Modelling study of CO_2 sequestration by mineral waste carbonation

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1. Introduction

Waste generation by economic activities and households, 2020

(% share of total waste)

	Mining and quarrying	Manufacturing	Energy	Construction and demolition	Other economic activities	Households
EU	23.4	10.9	2.3	37.1	16.8	9.5
Belgium	0.0	20.9	1.5	30.5	39.3	7.8
Bulgaria	81.6	4.2	5.2	1.6	5.4	2.0
Czechia	0.3	12.1	1.1	42.9	27.7	15.9
Denmark	0.1	5.4	3.9	54.8	17.8	18.0
Germany	1.3	13.7	2.0	56.3	17.1	9.6
Estonia	15.2	24.6	35.0	9.8	12.0	3.4
Ireland (¹)	14.2	24.7	1.1	13.6	35.1	11.4
Greece	36.6	17.8	6.1	1.1	20.4	18.0
Spain	2.3	12.5	0.7	30.7	31.8	22.0
France	0.1	7.1	0.4	67.6	14.2	10.7
Croatia	11.6	7.5	1.1	23.8	35.8	20.2
Italy	0.8	15.2	0.9	37.8	28.8	16.6
Cyprus	6.9	9.5	0.1	50.2	16.2	17.0
Latvia	0.0	17.0	4.1	9.7	46.6	22.6
Lithuania	1.0	32.7	2.3	8.3	34.8	20.9
Luxembourg	1.1	6.5	0.3	82.1	7.7	2.2
Hungary	0.8	15.8	11.2	27.1	15.9	29.1
Malta	1.3	1.0	0.0	82.7	8.5	6.5
Netherlands	0.1	10.6	0.4	65.4	16.2	7.4
Austria	0.1	7.5	0.6	76.5	8.7	6.7
Poland	36.6	16.1	6.6	13.0	20.0	7.8
Portugal	0.1	17.8	1.3	10.7	38.3	31.8
Romania	84.3	4.6	3.1	0.9	4.1	3.0
Slovenia	0.1	17.9	12.1	6.3	55.2	8.4
Slovakia	1.6	24.0	5.5	9.0	41.4	18.5
Finland	75.1	8.2	0.8	11.8	1.9	2.1
Sweden	76.5	3.1	1.2	9.3	6.8	3.1
Iceland (¹)	0.0	24.4	0.0	3.9	31.5	40.2
Liechtenstein (¹)	1.6	1.5	0.0	88.6	1.6	6.7
Norway	1.3	13.6	1.6	44.2	20.9	18.4
Montenegro	25.3	2.5	29.0	13.8	10.8	18.5
North Macedonia	35.1	35.0	0.5	3.8	25.6	0.0
Serbia	77.9	1.9	13.5	1.2	2.0	3.5
Turkey	25.6	19.2	22.6	0.0	6.1	26.5
Bosnia and Herzegovina	11.3	27.3	46.3	1.3	0.4	13.4
Kosovo (²)	19.9	9.4	52.5	0.2	17.8	0.2

(¹) 2018

(²) This designation is without prejudice to positions on status, and is in line with UNSCR 1244/1999 and the ICJ Opinion on the Kosovo Declaration of Independence.

Source: Eurostat (online data code: env_wasgen)

eurostat

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[1] 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

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2. CO_2 capture by mineral carbonation by using construction waste

Mineral Loop Project

CO_2 capture by mineral carbonation by using construction waste → Design → Develop → Install → Operate → Industrial pilot

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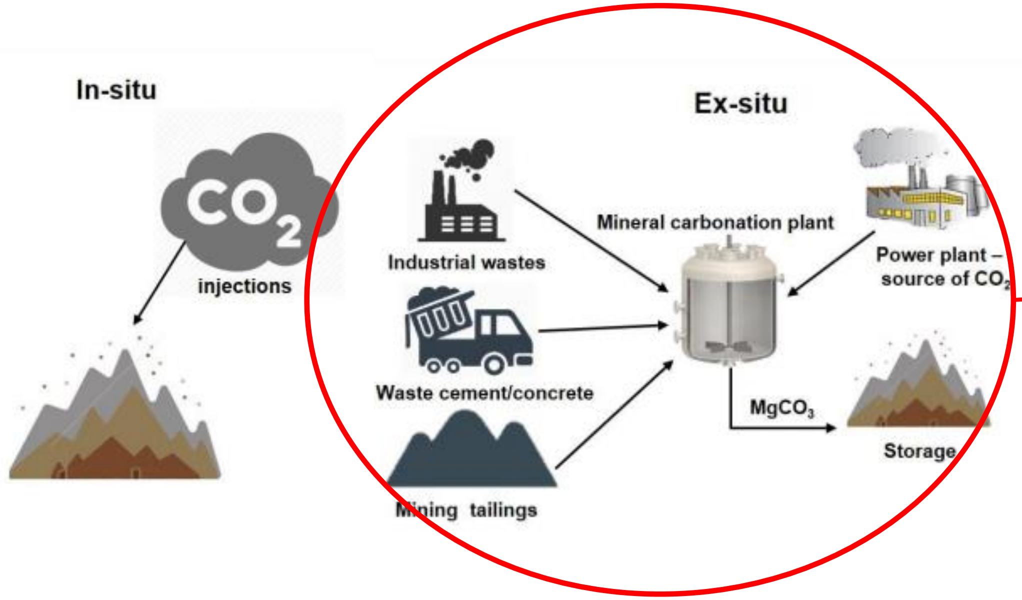
2. CO_2 capture by mineral carbonation by using construction waste

Mineral carbonation process



Direct carbonation

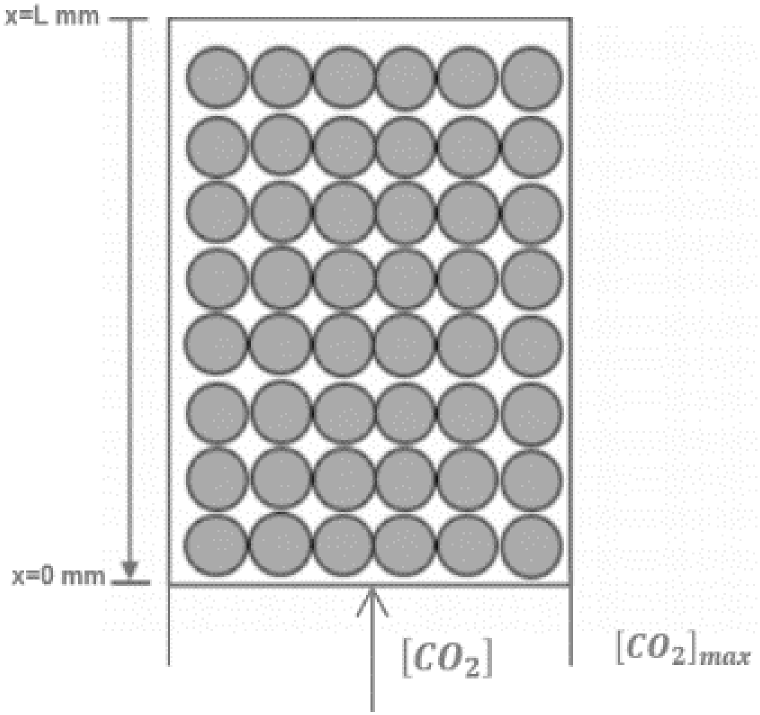
-Gas-solid carbonation of hydrated lime

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

3. Coupling between chemical reactions and transfer phenomena

Dual-scale modelling-COMSOL multiphysics

- **Physical interactions:** CO_2 diffusion between the particles and inside the particles *f(porosity, liquid water saturation)*
- **Chemical reactions:** $Ca(OH)_2$ carbonation *f(liquid water saturation)*

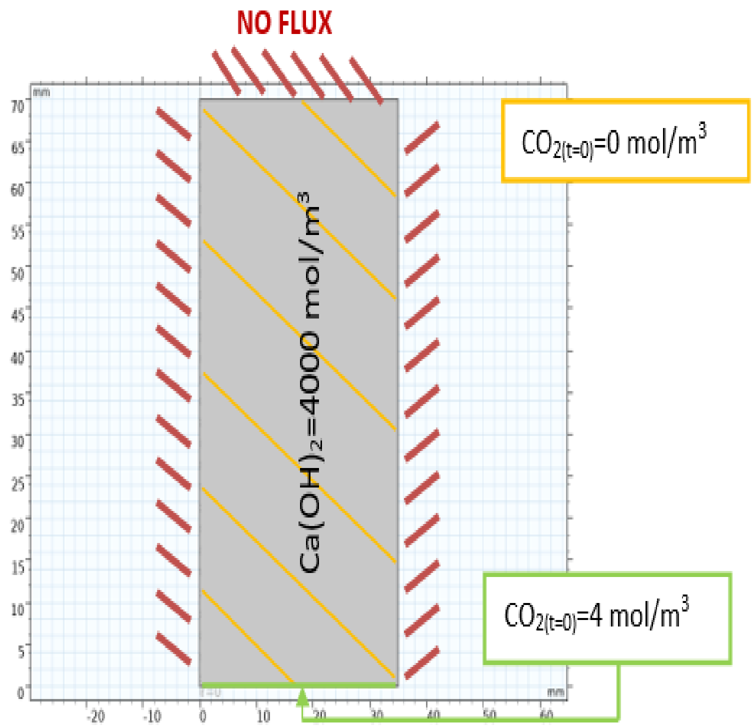


[2] P.Belin G.Habert N.Rousse M.Thiery, P.Dangla. 'Carbonation kinetics of a bed of recycled concrete aggregates: a laboratory study on model materials.' Available online: https://doi.org/10.1016/j.cemconres.2013.01.005

3. Coupling between chemical reactions and transfer phenomena

Model proposed-Basic case [2]

- Cylindrical reactor→Axisymmetric 2D model with spherical particles
  - Diameter: 70 mm
  - Radius: 35 mm
  - Length: 75 mm
- $Ca(OH)_2 + CO_2 \Rightarrow CaCO_3 + H_2O$
  - Rate constant(kc): 0,00025m^3/mol s
- P: 1 atm, T: 23 °C

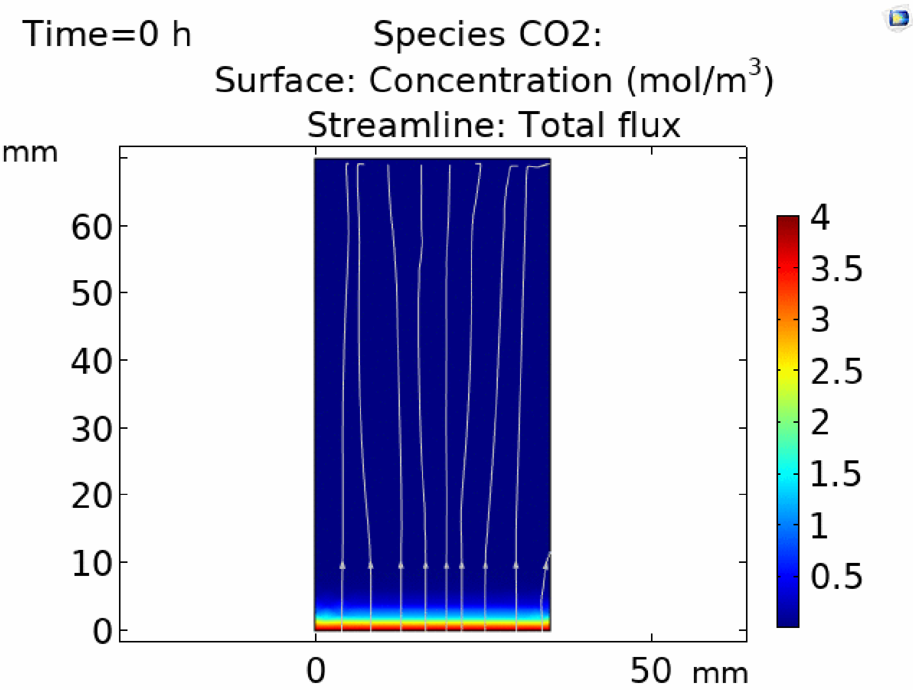


[2] P.Belin G.Habert N.Rousse M.Thiery, P.Dangla. 'Carbonation kinetics of a bed of recycled concrete aggregates: a laboratory study on model materials.' Available online: https://doi.org/10.1016/j.cemconres.2013.01.005

4. COMSOL results

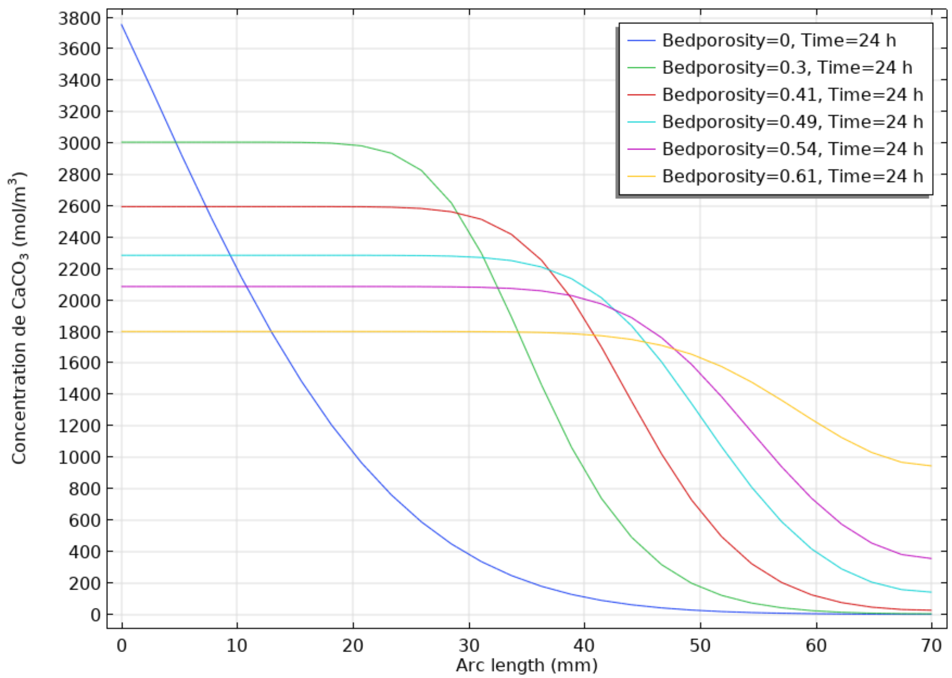
- Sensitivity analysis of various parameters in the model, considering the following parameters as constants when not modified:

  - Liquid water saturation in the bed(SL) = 0
  - Liquid water saturation in the pellet(sl) = 0.28
  - Porosity of the granular bed = 0.4 (%volume fraction of voids to the total volume of the matrix)
  - Porosity of the particle = 0.49 (%volume fraction of voids to the total volume of the matrix)
  - Particle radius = 1mm



4. COMSOL results

- Sensitivity Analysis Results: Influence of bed porosity on $CaCO_3$ concentration

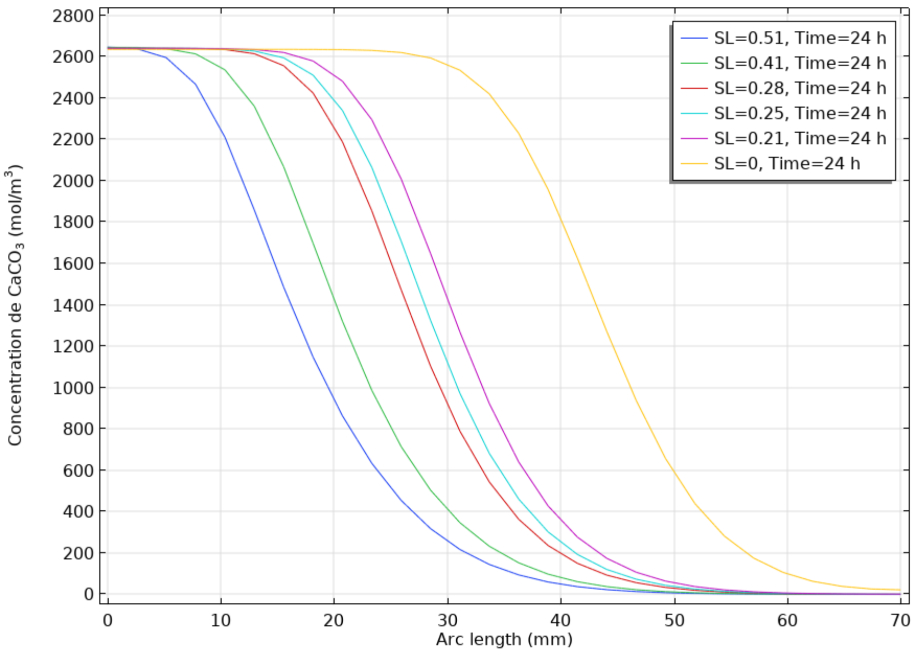


↑ Bed porosity ↑ Evolution of the $CaCO_3$ « front »

↑ Bed porosity ↓ Maximum local concentration of $CaCO_3$

4. COMSOL results

- Sensitivity Analysis Results: Influence of the liquid water saturation in the bed on $CaCO_3$ concentration

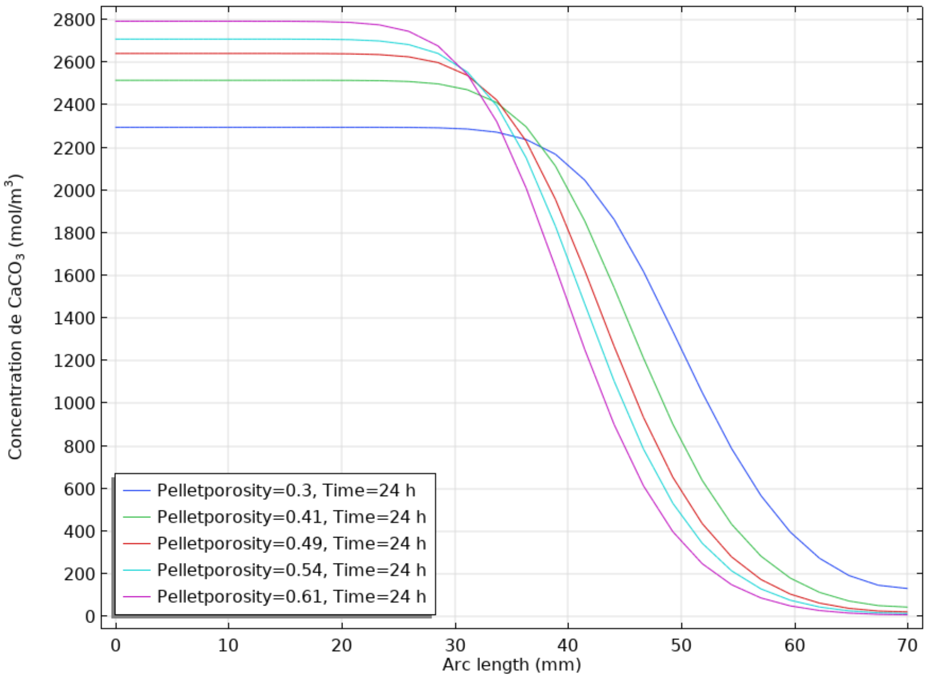


⬇ Liquid water saturation in the bed ⬆ Evolution of the $CaCO_3$ « front »

No noticeable influence on the maximum local concentration of $CaCO_3$

4. COMSOL results

- Sensitivity Analysis Results: Influence of the pellet porosity on $CaCO_3$ concentration



↑ Pellet porosity ↓ Evolution of the $CaCO_3$ « front »

↑ Pellet porosity ↑ Maximum local concentration of $CaCO_3$

4. COMSOL results

- Literature validation[2]

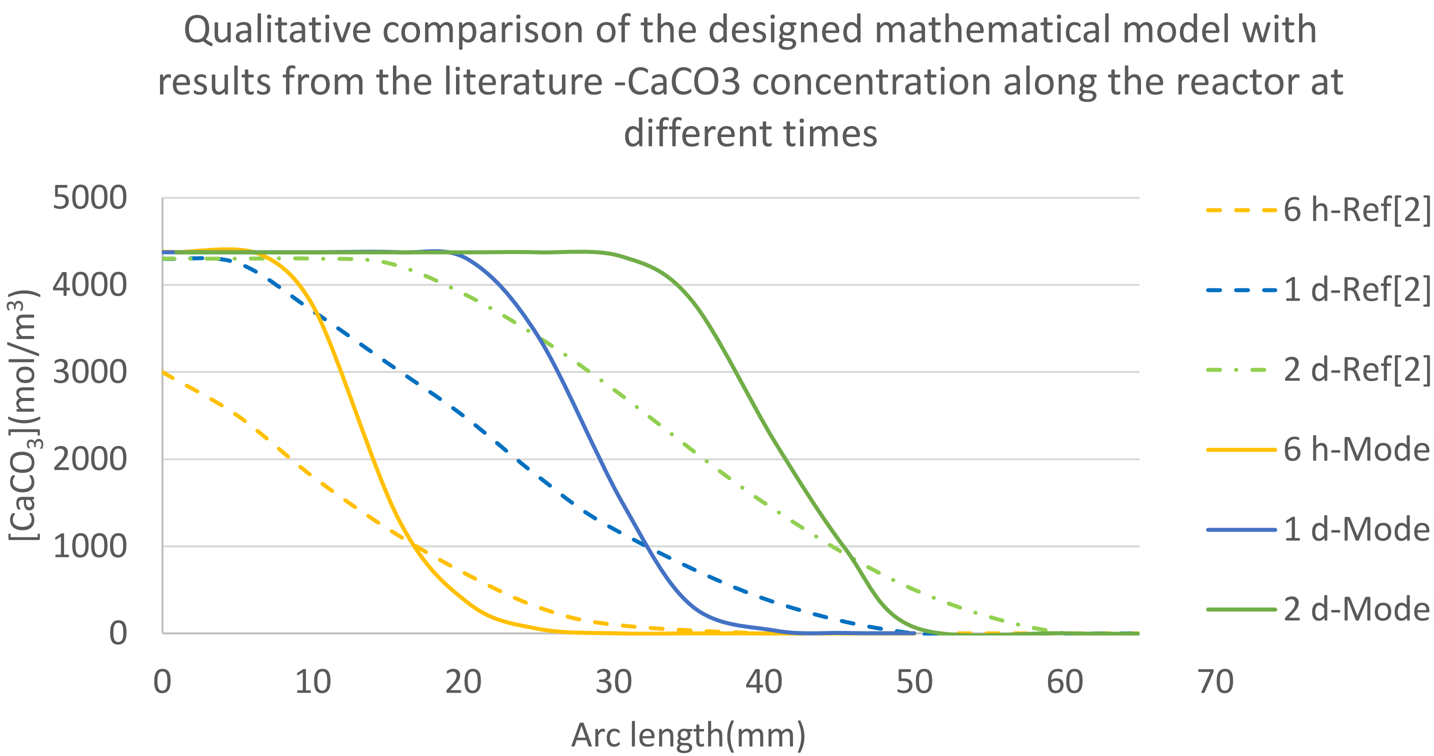
<u>Characteristics of two samples</u>

Samples	w/c	Carbonatable material (mol/m^3)	sl	Pellet posority	SL	Bed porosity
C80	0.8	5700	0.21	0.61	0	0.4
C55	0.55	6800	0.28	0.49	0	0.4

[2] P.Belin G.Habert N.Rousse M.Thiery, P.Dangla. 'Carbonation kinetics of a bed of recycled concrete aggregates: a laboratory study on model materials.' Available online: https://doi.org/10.1016/j.cemconres.2013.01.005

4. COMSOL results

- Validation with results from the literature- C80



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[2] P.Belin G.Habert N.Rousse M.Thiery, P.Dangla. 'Carbonation kinetics of a bed of recycled concrete aggregates: a laboratory study on model materials.' Available online: https://doi.org/10.1016/j.cemconres.2013.01.005

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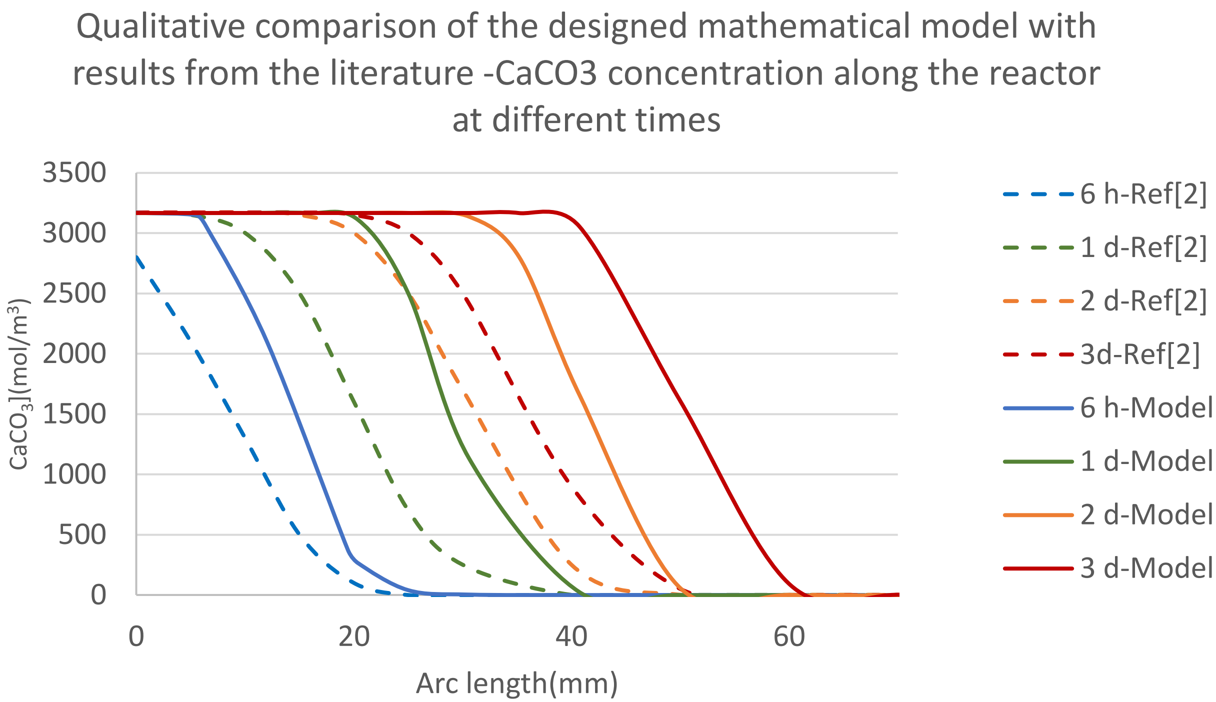
4. COMSOL results

- Validation with results from the literature -C55



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5. Conclusions

- An increase in bed porosity promotes the progression of the $CaCO_3$ front but does not enhance its maximum local concentration
- The lower the liquid water saturation of the bed, the better the progression of the $CaCO_3$ front.
- Higher pellet porosity leads to a higher maximum local concentration of $CaCO_3$.
- Qualitative agreement with the results from the literature is achieved.
- Model improvements implemented include the introduction of pellet porosity and the variation of liquid water saturation through the carbonation process

Thank you for your attention!

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