

Mesoscale modelling of carbonation in concrete made with RCA

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Why use a mesoscale model for C-RCA?

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Recycled concrete aggregate

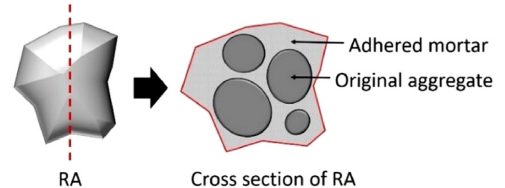


Figure 1: Schematic representation of a RCA [[Ng and Engelsen, 2018](#)]

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- ▶ is a natural aggregate surrounded by mortar [[Zhang and Bao, 2023](#)]

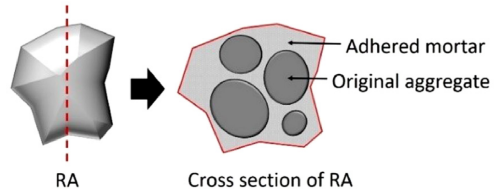


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- ▶ is a natural aggregate surrounded by mortar [[Zhang and Bao, 2023](#)]
- ▶ is a porous aggregate due to the presence of the adhered mortar [[Hussain et al., 2000](#)]

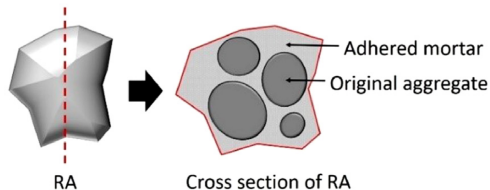


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- ▶ is a natural aggregate surrounded by mortar [Zhang and Bao, 2023]
- ▶ is a porous aggregate due to the presence of the adhered mortar [Hussain et al., 2000]
- ▶ contains unreacted cement and carbonatable materials within the mortar [Zhihai, 2023]

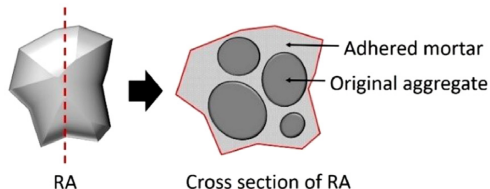


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Concrete made with RCA (C-RCA)

- ▶ Strong material heterogeneity

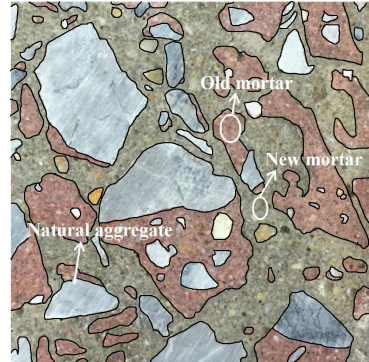


Figure 2: Concrete with pigmented RCA, adapted from [Mi et al., 2019])

Carbonation mechanisms in C-RCA

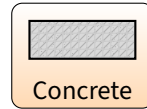


Figure 3: Schematic representation of the carbonation mechanisms in C-RCA, from parent concrete to final concrete.

Carbonation mechanisms in C-RCA

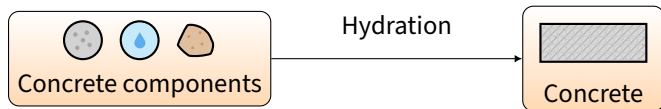


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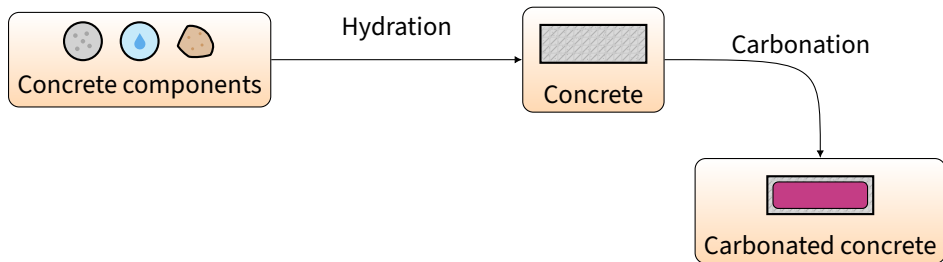


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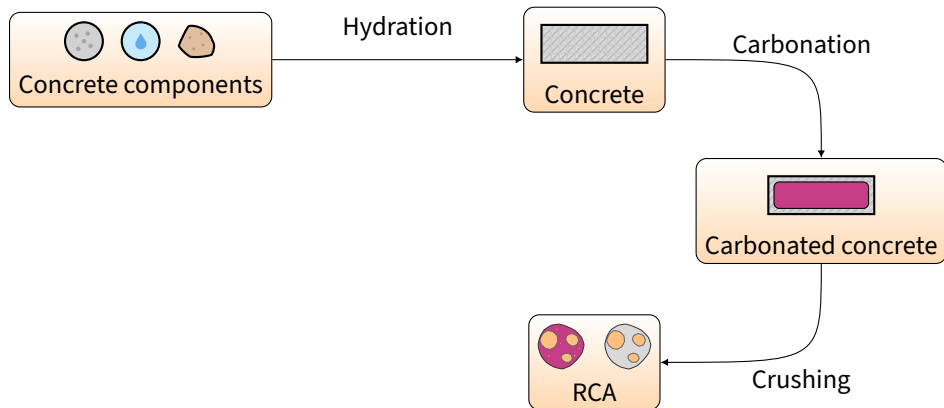


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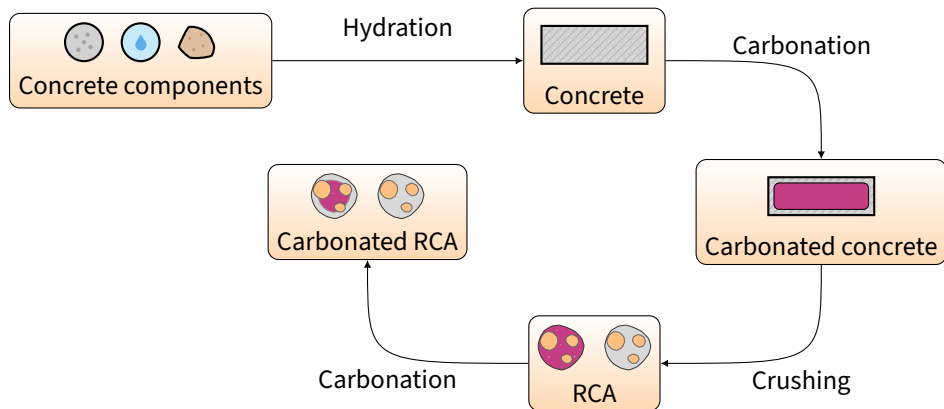


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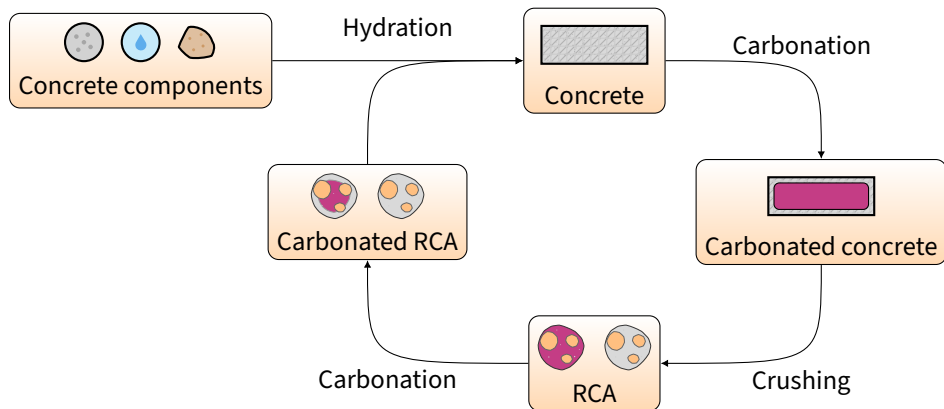


Figure 3: Schematic representation of the carbonation mechanisms in C-RCA, from parent concrete to final concrete.

Proposed approach

Combines

- ▶ Mesoscale modelling (RVE)
- ▶ Simplified carbonation model ($X_c = \alpha\sqrt{t}$)

Provides

- ▶ Effective diffusion coefficient
- ▶ Carbonatable material content

Enables efficient parametric analysis

Model framework

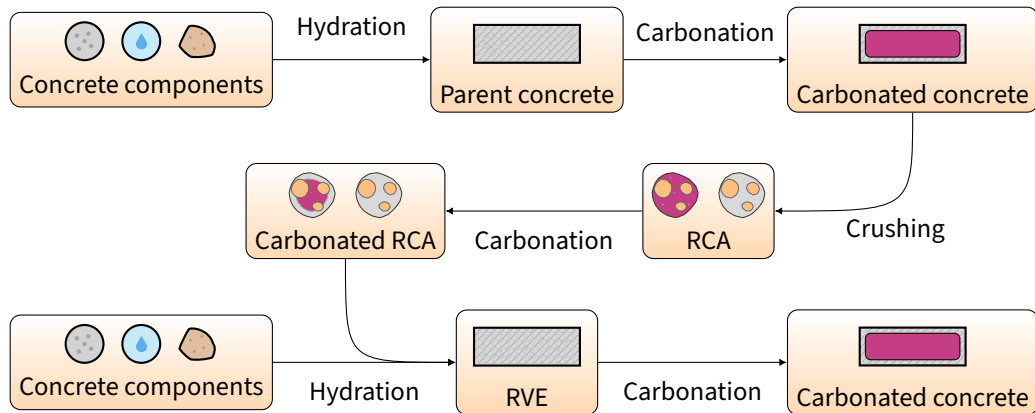


Figure 4: Computational workflow for C-RCA carbonation.

Sensitivity analysis

Input parameters

- ▶ Reference value: i_{ref}
- ▶ Range of variation: $i_{\text{min}} = i_{\text{ref}} - \Delta_i$ and $i_{\text{max}} = i_{\text{ref}} + \Delta_i$

Model outputs

- ▶ Reference carbonation depth: $X_{c,50,\text{ref}}$
- ▶ Perturbed carbonation depths: $X_{c,50,i_{\text{min}}}$ and $X_{c,50,i_{\text{max}}}$

Sensitivity metrics

- ▶ Parameter variability: $V_i = \frac{\Delta_i}{i_{\text{ref}}}$
- ▶ Relative impact: $I_i = \max \left(\frac{|X_{c,50,i_{\text{max}}} - X_{c,50,\text{ref}}|}{X_{c,50,\text{ref}}}, \frac{|X_{c,50,\text{ref}} - X_{c,50,i_{\text{min}}}|}{X_{c,50,\text{ref}}} \right)$

Sensitivity analysis

	C_{Cement}	$D_{\text{CO}_2, \text{eff}}$	C_{CO_2}	t_{Carbo}	Others
Hydration PC	$C_{\text{Cement, AMP}}$	$D_{\text{CO}_2, \text{eff, AMP}}$			
Carbonation PC			$C_{\text{Pre, CO}_2}$	t_{Pre}	thk_{Slab}
Carbonation RCA			$C_{\text{Post, CO}_2}$	t_{Post}	
Hydration C-RCA	$C_{\text{Cement, NMP}}$	$D_{\text{CO}_2, \text{eff, NMP}}$			α_{RCA}
Carbonation C-RCA			$C_{\text{RVE, CO}_2}$		

Table 1: Parameters varied during hydration and carbonation, from parent concrete to C-RCA.

Sensitivity analysis

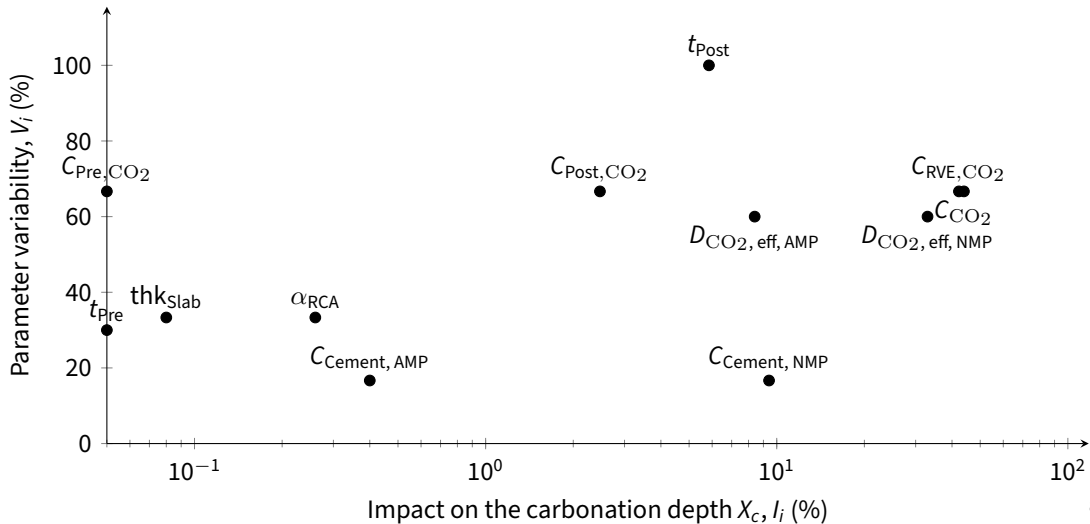
Phase-dependent material properties

Property	NA	Adherent MP	New MP
$D_{\text{CO}_2, \text{eff}} (\text{m}^2 \text{s}^{-1})$	0.0	2.5×10^{-8}	2.5×10^{-8}
$C_{\text{Cement}} (\text{kg m}^{-3})$	0.0	600	600

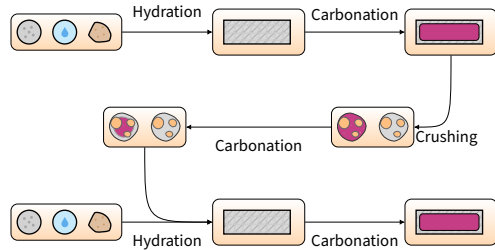
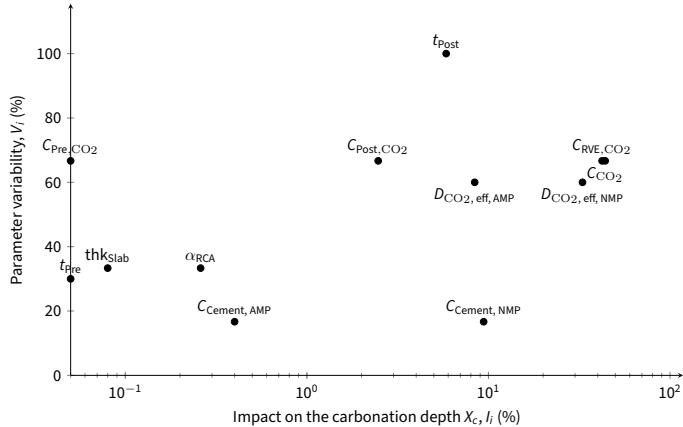
Global parameters

	Property	Reference	Unit	Property	Reference	Unit
PC	$C_{\text{Pre}, \text{CO}_2}$	0.045	%	t_{Pre}	50.0	yr
	thk_{Slab}	300	mm			
RCA	$C_{\text{Post}, \text{CO}_2}$	0.045	%	t_{Post}	0.5	yr
C-RCA	$C_{\text{RVE}, \text{CO}_2}$	0.045	%	C_{CO_2}	0.045	%
	α_{RCA}	75.0	%			

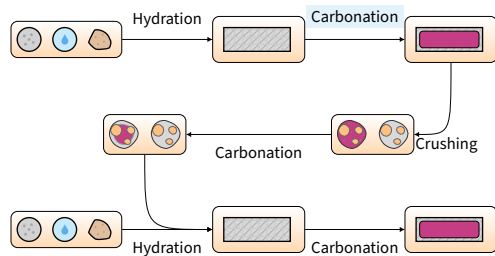
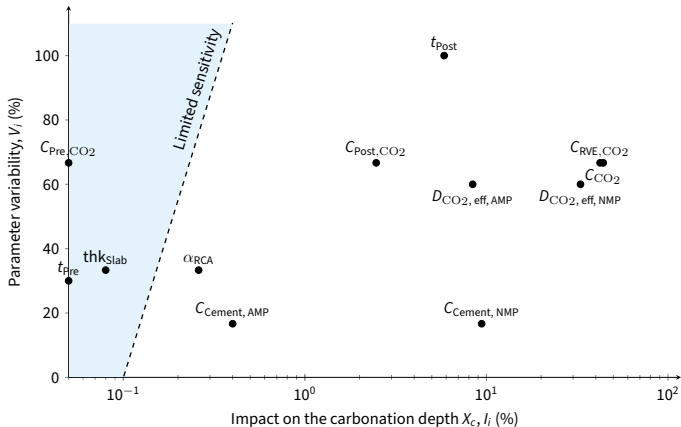
Results



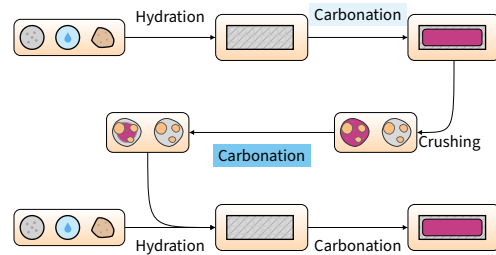
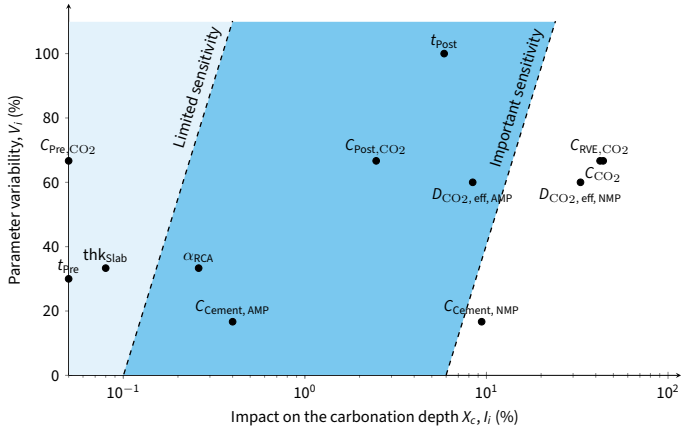
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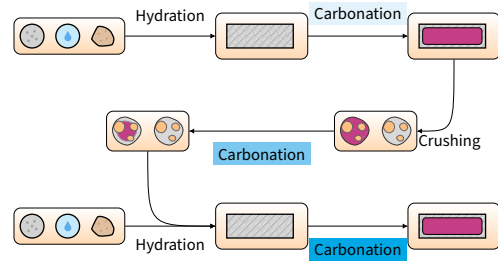
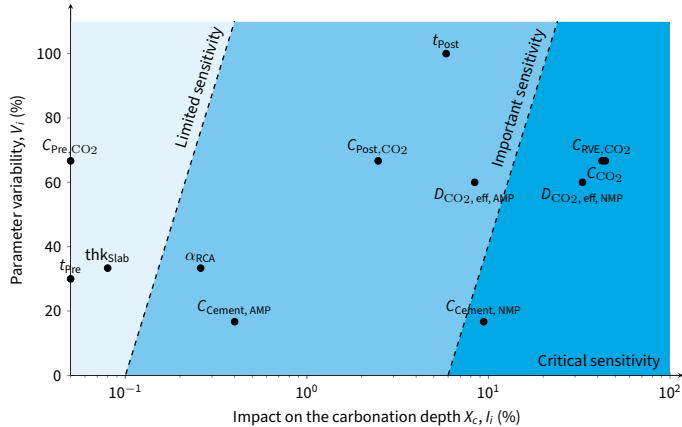
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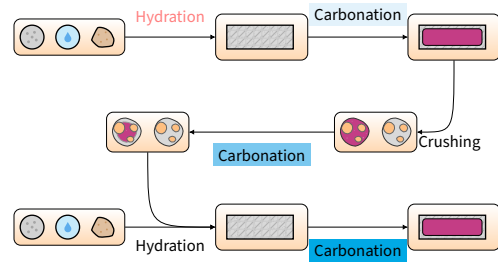
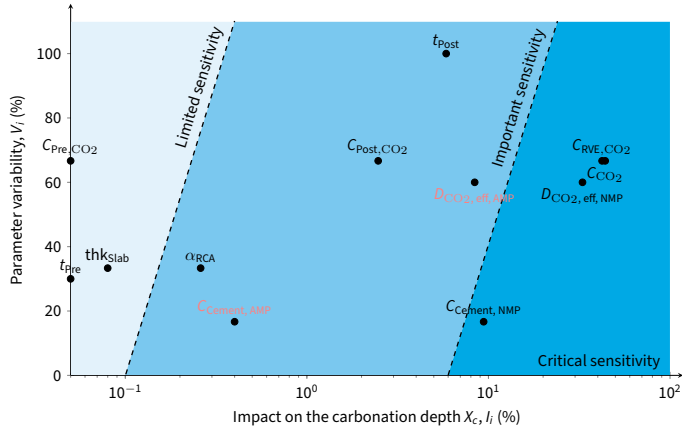
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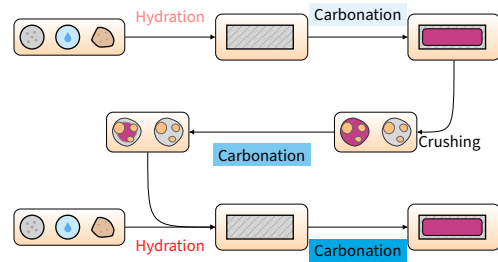
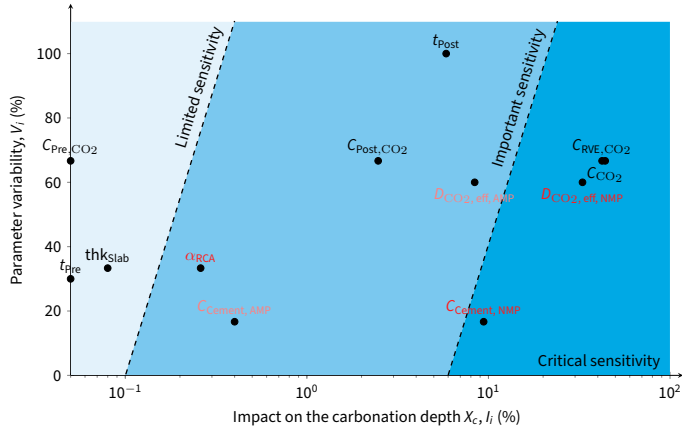
Results



Results



Results



Conclusion

Main contributions

- ▶ Hybrid approach combining RVE-based properties and a simplified carbonation model
- ▶ Efficient comparison of RCA-related parameters

Practical Relevance

- ▶ Identification of key controlling parameters
- ▶ Dominant influence of NMP properties

Future work

- ▶ Extend the range of parameters investigated
- ▶ Improve modelling
- ▶ Experimental validation



Acknowledgements:

This work is funded by the Wallonia-Brussels Federation — Concerted Research Actions EsPOIR



Sensitivity Analysis

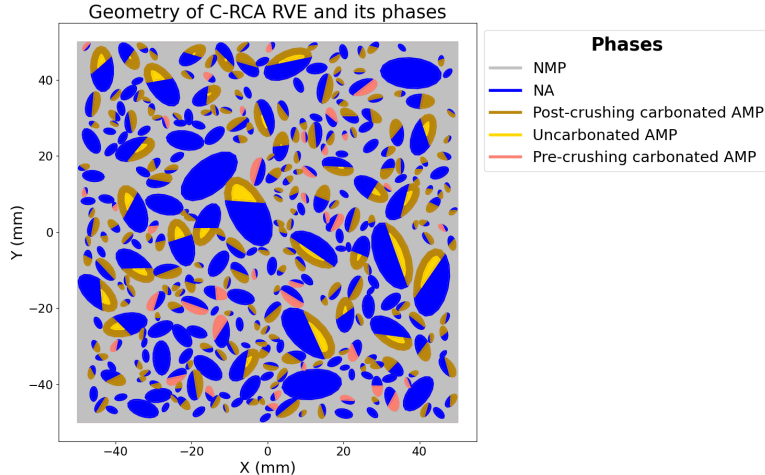


Figure 5: Example of a generated RVE based on the reference parameter set.

Model framework

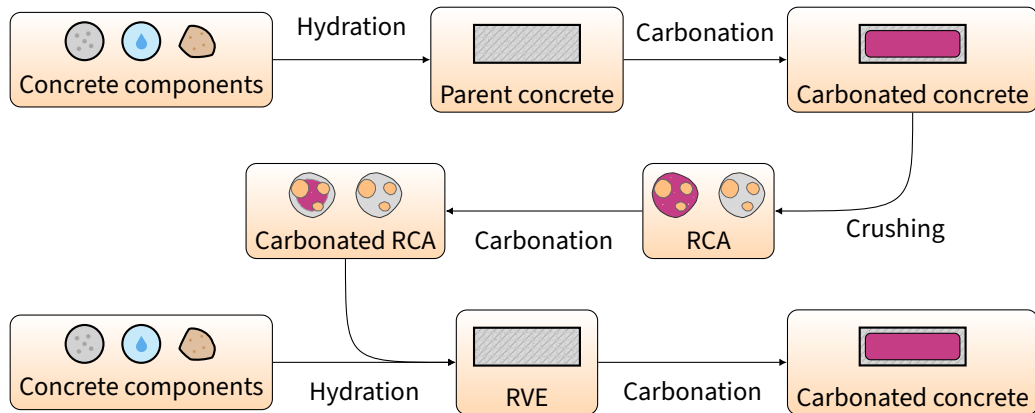
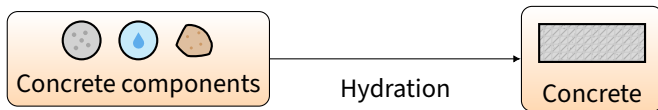


Figure 6: Computational workflow for C-RCA carbonation.

hydration process in C-RCA

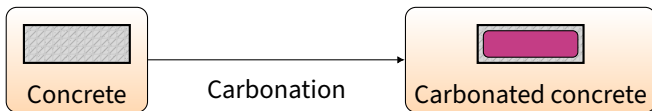


Hydration model [CEB, 1997, Hyvert et al., 2010]:

$$C_{\text{Ca(OH)}_2} = 0.75 \cdot C_{\text{Cement}} \cdot \omega_{\text{CaO,Cement}} \cdot \alpha_h \cdot \frac{M_{\text{Ca(OH)}_2}}{M_{\text{CaO}}} \quad (1)$$

$$\alpha_h = 1 - \exp\left(-3.3 \cdot \frac{W}{C}\right) \quad (2)$$

Carbonation mechanisms in C-RCA



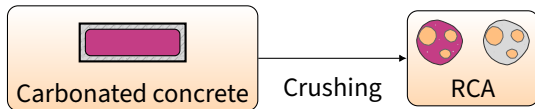
Carbonation model [[Hyvert, 2009](#)]:

$$X_c = k\sqrt{t} = \sqrt{\frac{2D_{\text{CO}_2, \text{eff}} \frac{P_{\text{CO}_2}}{RT}}{\left(1 + \beta C_2 \left(\frac{P_{\text{CO}_2}}{P_{\text{atm}}}\right)^n\right) \left(\frac{C_2}{n+1} \left(\frac{P_{\text{CO}_2}}{P_{\text{atm}}}\right)^n + Q_1\right)}} \sqrt{t} \quad (3)$$

$$Q_1 = \left(\frac{C_{\text{Ca(OH)}_2}}{M_{\text{Ca(OH)}_2}} + 4 \frac{C_{\text{AF}_m}}{M_{\text{AF}_m}} + 6 \frac{C_{\text{AF}_t}}{M_{\text{AF}_t}} \right) \cdot 10^3 \quad (4)$$

$$C_2 = n_{\text{CSH}} \frac{C_{\text{CSH}}}{M_{\text{CSH}}} \cdot 10^3 \quad (5)$$

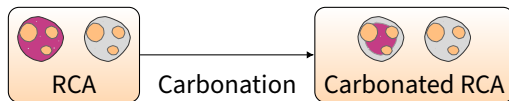
Pre-crushing carbonation of RCA



Pre-crushing carbonation of RCA

$$P_{\text{Pre-carbonated,RCA}} = \frac{V_{\text{Carb,Elem}}}{V_{\text{tot,Elem}}} \approx \frac{A_{\text{Carb,Elem}}}{A_{\text{tot,Elem}}} \approx \frac{2 \cdot X_c}{thk_{\text{Elem}}} \quad (6)$$

Carbonation mechanisms of RCA



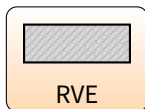
Carbonation of RCA [Hyvert, 2009]:

$$X_c = k\sqrt{t} = \sqrt{\frac{2D_{\text{CO}_2, \text{eff}} \frac{P_{\text{CO}_2}}{RT}}{\left(1 + \beta C_2 \left(\frac{P_{\text{CO}_2}}{P_{\text{atm}}}\right)^n\right) \left(\frac{C_2}{n+1} \left(\frac{P_{\text{CO}_2}}{P_{\text{atm}}}\right)^n + Q_1\right)}} \sqrt{t} \quad (7)$$

$$Q_1 = \left(\frac{C_{\text{Ca(OH)}_2}}{M_{\text{Ca(OH)}_2}} + 4 \frac{C_{\text{AF}_m}}{M_{\text{AF}_m}} + 6 \frac{C_{\text{AF}_t}}{M_{\text{AF}_t}} \right) \cdot 10^3 \quad (8)$$

$$C_2 = n_{\text{CSH}} \frac{C_{\text{CSH}}}{M_{\text{CSH}}} \cdot 10^3 \quad (9)$$

Carbonation mechanisms in C-RCA



Effective RVE properties

$$\bar{Q}_1 = \frac{1}{|\Omega|} \int_{\Omega} Q_1(x, y) d\Omega \quad (10)$$

$$\bar{C}_2 = \frac{1}{|\Omega|} \int_{\Omega} C_2(x, y) d\Omega \quad (11)$$

$$\bar{J} = \frac{1}{|\Omega|} \int_{\Omega} J(x, y) d\Omega = -D_{\text{CO}_2, \text{eff}} \nabla C_{\text{CO}_2} = -D_{\text{CO}_2, \text{eff}} \frac{C_{\text{CO}_2}(x=0) - C_{\text{CO}_2}(x=L)}{L} \quad (12)$$

Model Framework

1. RVE generation with different phases:
 - ▶ Natural aggregates (NA)
 - ▶ Adherent mortar paste (AMP)
 - ▶ New mortar paste (NMP)
2. Assignment of phase properties
3. Computation of effective properties
4. Input into simplified carbonation model

Main assumptions

Hydration

- ▶ Only portlandite ($\text{Ca}(\text{OH})_2$) is considered

Carbonation

- ▶ Sharp carbonation front
- ▶ Uniform carbonated layer
- ▶ Diffusion governed by carbonated zone

Crushing

- ▶ Negligible effect on diffusion properties [[Bouarroudj et al., 2023](#)]

Sensitivity analysis

	C_{Cement}	$D_{\text{CO}_2, \text{eff}}$	C_{CO_2}	t_{Carbo}	Others
Hydration PC	$C_{\text{Cement, AMP}}$	$D_{\text{CO}_2, \text{eff, AMP}}$			
Carbonation PC			$C_{\text{Pre, CO}_2}$	t_{Pre}	thk_{Slab}
Carbonation RCA			$C_{\text{Post, CO}_2}$	t_{Post}	
Hydration C-RCA	$C_{\text{Cement, NMP}}$	$D_{\text{CO}_2, \text{eff, NMP}}$			α_{RCA}
Carbonation C-RCA			$C_{\text{RVE, CO}_2}$		

Table 2: Parameters varied during hydration and carbonation, from parent concrete to C-RCA.

Sensitivity analysis

Property	T	P_{atm}	RH	$\frac{W}{C}$	$\omega_{\text{CaO,Cement}}$
Value	283.15	101325	0.6 to 0.7	0.5	0.65
Unit	K	Pa	—	—	—

Table 3: Fixed parameters used in the simulations.

Sensitivity analysis

Property	NA	Adherent MP	New MP
$D_{\text{CO}_2, \text{eff}} (\text{m}^2 \text{s}^{-1})$	0.0	2.5×10^{-8}	2.5×10^{-8}
$C_{\text{Cement}} (\text{kg m}^{-3})$	0.0	600	600

Table 4: Reference values and variations of phase-dependent material properties for natural aggregates (NA), adherent mortar paste (AMP), and new mortar paste (NMP).

Sensitivity analysis

Property	NA		Adherent MP		New MP	
	Reference	Δ	Reference	Δ	Reference	Δ
$D_{\text{CO}_2, \text{eff}}$ ($\text{m}^2 \text{s}^{-1}$)	0.0	0.0	2.5×10^{-8}	1.5×10^{-8}	2.5×10^{-8}	1.5×10^{-8}
C_{Cement} (kg m^{-3})	0.0	0.0	600	100	600	100

Table 5: Reference values and variations of phase-dependent material properties for natural aggregates (NA), adherent mortar paste (AMP), and new mortar paste (NMP).

Sensitivity analysis

	Property	Reference	Δ	Unit	Property	Reference	Δ	Unit
PC	C_{Pre,CO_2}	0.045	0.030	%	t_{Pre}	50.0	15.0	yr
	thk_{Slab}	300	100	mm				
RCA	C_{Post,CO_2}	0.045	0.030	%	t_{Post}	0.5	0.5	yr
C-RCA	C_{RVE,CO_2}	0.045	0.030	%	C_{CO_2}	0.045	0.030	%
	α_{RCA}	75.0	25.0	%				

Table 6: Reference values and ranges of variation of the parameters for parent concrete (PC), recycled concrete aggregates (RCA), and concrete incorporating RCA (C-RCA).

Sensitivity analysis

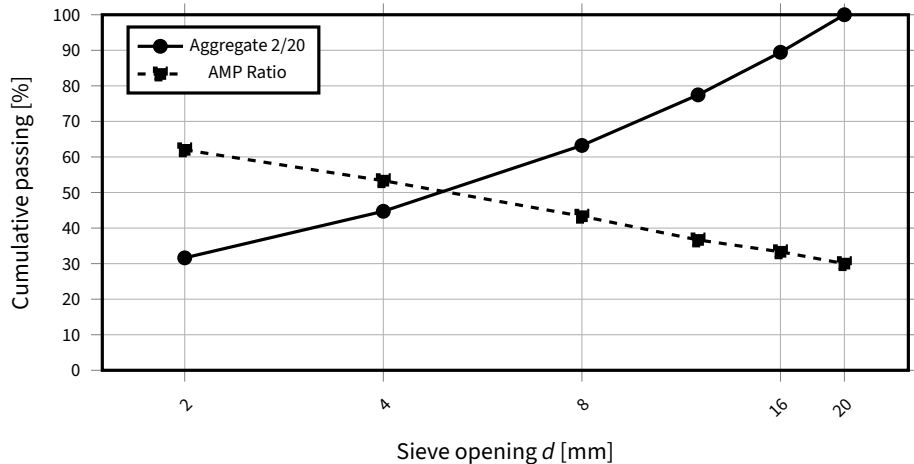


Figure 7: Granulometric curves of aggregates used in the sensitivity analysis

Sensitivity analysis

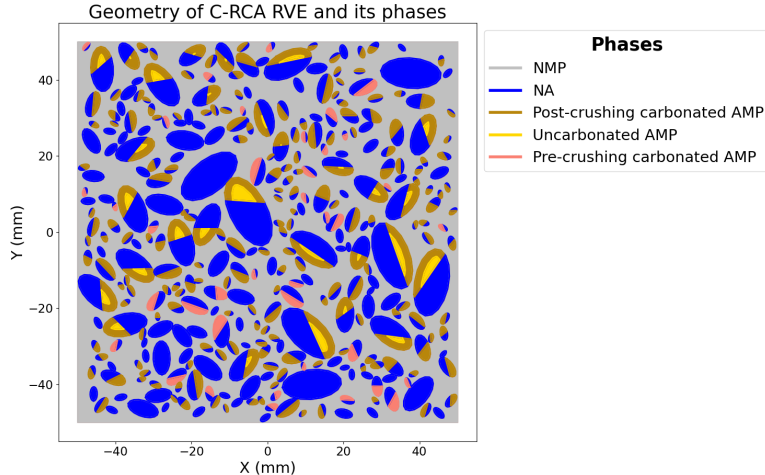


Figure 8: Example of a generated RVE based on the reference parameter set.

Results

Main observations

- ▶ Limited influence of pre-carbonation for thick parent elements
- ▶ Moderate influence of post-crushing carbonation
- ▶ Dominant role of NMP properties on carbonation behaviour
- ▶ Possible parameter interactions: effects may be amplified or compensated

Results valid in the vicinity of the reference case

Interpretation

Key takeaways

- ▶ Crushing increases exposed surface → enhanced carbonation of RCA
- ▶ Carbonation is irreversible → cumulative and memory effects
- ▶ NMP properties govern the final carbonation behaviour

Helps explain variability observed in experiments

Expected geometry-dependent trends $\left(\frac{\chi_c \cdot S_{PC,Air}}{V_{PC}} \right)$

- ▶ Low ratio : Pre-carbonation $\ll$ post-carbonation $\ll$ C-RCA carbonation
- ▶ Intermediate ratio : Post-carbonation $\ll$ pre-carbonation $\ll$ C-RCA carbonation
- ▶ High ratio : Post-carbonation $<$ pre-carbonation $\lll$ C-RCA carbonation

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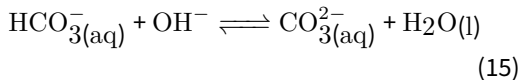
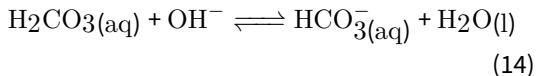
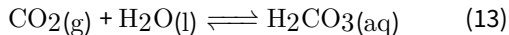
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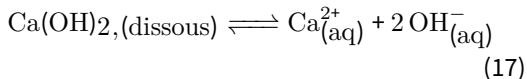
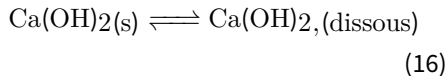
Helps explain variability observed in experiments

Carbonation Reaction

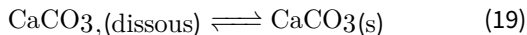
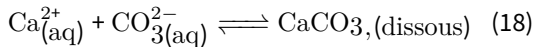
Dissolution and acid-base equilibrium:



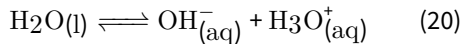
Dissolution and dissociation:



Reaction and precipitation:



Autoprotolysis:



Nomenclature du milieu cimentier

	Formule complète	Formule abrégée	Dénomination courante	
Eau	H ₂ O	H	Eau	
Composants de base	CaO	C	Chaux	
	SiO ₂	S	Oxyde de silicium	
	Al ₂ O ₃	A	Oxyde d'aluminium	
	Fe ₂ O ₃	F	Oxyde de fer	
	Na ₂ O-K ₂ O	N-K	Oxydes alcalins	
	MgO	M	Oxyde de magnésium	
Composants hydrauliques	CaSO ₄	<u>S</u>	Anhydrite	Sulfate de calcium
	CaSO ₄ .H ₂ O	<u>S</u>	Gypse	
	3CaO.Al ₂ O ₃	C ₃ A	Aluminate tricalcique	Aluminates de calcium
	4CaO.Al ₂ O ₃ .Fe ₂ O ₃	C ₄ AF	Alumino-ferrite tétracalcique	
	3CaO.SiO ₂	C ₃ S	Silicate tricalcique	Silicate de calcium
	2CaO.SiO ₂	C ₂ S	Silicate dicalcique	

Table 7: [Druart and Xhonneux, 2018]

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