

Multiscale modelling of carbonation in concrete made with RCA

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ABSTRACT: The objective of this work is to develop a carbonation model for concrete incorporating recycled concrete aggregates (RCA), with the aim of predicting and assessing the progression of carbonation. The broader goal is to evaluate the relative influence of key parameters on carbonation and, more importantly, to determine the overall impact of replacing natural aggregates with recycled ones. Understanding carbonation is essential, as it is a critical precursor to reinforcement corrosion—one of the primary degradation mechanisms in concrete structures. The numerical model has been developed based on various approaches from the literature. It was first implemented at a macroscopic scale, then extended to a multiscale framework to account for the intrinsic heterogeneity of concrete. This heterogeneity is represented through a representative volume element (RVE), which includes the mortar paste, aggregates, and the adherent mortar surrounding them. The model considers several coupled processes, as well as the chemical reactions resulting from the carbonation process within the concrete matrix. The implementation was carried out using the nonlinear finite element software LAGAMINE, developed at the University of Liège.

1 INTRODUCTION

Concrete is currently the most widely produced material in the construction sector, with an estimated global production of $14 \times 10^9 \text{ m}^3$ in 2020 (Global Cement and Concrete Association 2025), including approximately $1 \times 10^9 \text{ t}$ within the European Union (EU) (Eurostat 2014).

Consequently, the production of such vast quantities of concrete leads to the consumption of significant amounts of raw materials. Amongst these, aggregates are particularly critical resources due to their high demand and limited availability, with a consumption of approximately $2.6 \times 10^9 \text{ t}$ in 2023 in the EU, taking into account applications beyond concrete production (Aggregates Europe 2025). Meeting this demand requires extensive extraction activities, which are associated with several environmental impacts, including noise pollution, dust emissions, habitat destruction, and the depletion of natural reserves (Gavrilitea 2017, Rentier and Cammeraat 2022, Rangel-Buitrago et al. 2023).

Concrete waste also represents a major challenge. Production processes are not fully efficient, meaning that concrete waste is generated during manufacturing. In addition, concrete-like most materials—has a limited service life, generally estimated to range between 50 and 100 years. Eventually, all concrete structures reach the end of their service life and become waste (Xiao

2018). This leads to the generation of over $374 \times 10^6 \text{ t}$ of construction and demolition waste (CDW) per year in the EU (European Environment Agency 2020).

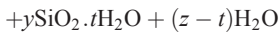
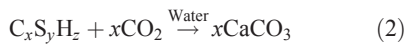
One way to address both issues - the depletion of natural resources and the accumulation of waste - is to shift from a linear to a circular economy model, enabling waste materials to be reused as secondary raw materials (Ige 2023). A promising approach is the production of recycled concrete aggregates (RCA) from concrete waste, to be used as a substitute for natural aggregates (NA) (Xiao 2018).

However, the introduction of these new materials also brings uncertainties, particularly regarding durability (McGinnis et al. 2017). RCA consists of natural aggregates surrounded by adhered mortar paste. This paste is more porous and contains microcracks, resulting in aggregates with higher water absorption than NA (Hussain et al. 2000). Consequently, RCA generally exhibits inferior properties compared with NA. To address these challenges, it is essential to deepen the understanding of the behaviour of these new materials.

Amongst the various degradation mechanisms affecting reinforced concrete, reinforcement corrosion is one of the most critical, costing up to $22.6 \times 10^9 \text{ USD}$ in infrastructure corrosion losses in the United States between 1999 and 2001 (not limited to reinforced concrete structures) (Koch et al. 2002). It can be triggered by several factors, including chloride

ingress, stray currents, and carbonation (Fanara 2024). The present work focuses on the latter process.

Carbonation is the reaction between gaseous CO_2 from the atmosphere and the carbonatable compounds present in concrete. The main carbonatable materials-listed in decreasing order of reactivity-are portlandite, calcium silicate hydrate (C-S-H) (De Schutter 2017), and, to a lesser extent, other phases such as ettringite (Von Greve-Dierfeld et al. 2020) or unhydrated clinker (Papadakis et al. 1991). The overall reactions for the two principal carbonation mechanisms are presented in Equations (1) and (2) (Papadakis et al. 1989, Thiery 2005). These global equations summarise a series of intermediate reactions that occur successively.



The impact of concrete produced with recycled concrete aggregates (C-RCA), compared with concrete made using natural aggregates (C-NA), on carbonation has already been investigated experimentally. Results generally show an increase in carbonation depth, indicating that the use of RCA reduces the carbonation resistance of concrete (Silva et al. 2015). Numerical models of this process provide deeper insight into the underlying mechanisms and offer predictive capabilities for the behaviour of concrete (Thiery 2005, Ibrahim 2024). Most existing models, however, focus on concrete made with NA and are limited to macroscale analyses.

The use of RCA increases the heterogeneity of concrete due to the presence of three distinct phases: natural aggregates, adhered mortar paste, and new mortar paste (Mi and Pan 2022). Furthermore, replacing NA-which has negligible porosity and is non-carbonatable-with RCA, which is both porous (Hussain et al. 2000) and carbonatable (Tiruta-Barna and Barna 2013, Sousanabadi Farahani et al. 2025), significantly influences the carbonation process (Buyle-Bodin and Hadjieva-Zaharieva 2002). A suitable approach to capture this complexity is the use of a multiscale modelling framework. Such models enable the heterogeneity of concrete to be represented while maintaining computational efficiency for large-scale simulations at the macroscale, where structural dimensions are typically on the order of metres in the construction sector (Fanara et al. 2024). This type of model has already demonstrated its capability to simulate chloride penetration in C-RCA (Fanara 2024) and, more generally, diffusion processes within concrete (Nilenius et al. 2015).

The two scales considered in this work are the macroscale and the mesoscale. The computation at the macroscale assumes a homogeneous medium and

applies mixture theory to model the different phases present, using uniform constitutive laws throughout the model. Conversely, the computation at the mesoscale accounts for the heterogeneity of the different phases-namely, the natural aggregate (NA), the adhered mortar paste, and the new cement paste-each of which is assigned its own material properties and constitutive equations. This level of computation provides information and properties that can only be obtained at the mesoscale, without the need for an excessively fine mesh over the entire element (Zupan and Korelc 2018, Fanara et al. 2024).

There are several possible approaches to performing multiscale computations, and the most appropriate method should be selected according to the specific problem to be addressed (Geers et al. 2010). In this study, the FE2 approach was adopted, as it is well suited to problems involving two well-separated scales, with limited coupling terms linking the different scales (Zupan and Korelc 2018).

The link between the different scales is established through a homogenisation technique, which may be either numerical (Smit et al. 1998) or analytical (Bensoussan et al. 1978). In this approach, the finite elements at the macroscale receive information at each integration point from finite elements at the lower scale (positioned at those points). The computations are first carried out at the smaller scale, and the resulting homogenised properties are then transferred to the macroscale analysis (Zupan and Korelc 2018).

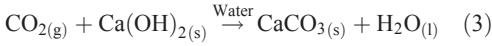
2 NUMERICAL MODEL

The model used in this study is a simplified representation of the real carbonation process. This model is based on the work of Saetta (Saetta and Vitaliani 2004). It considers several chemical species as reactants and products of the carbonation reaction: gaseous carbon dioxide, solid portlandite (calcium hydroxide), liquid water, and solid calcium carbonate. These species are denoted respectively as $\text{CO}_{2(g)}$, $\text{Ca}(\text{OH})_{2(s)}$, $\text{H}_2\text{O}_{(l)}$, and $\text{CaCO}_{3(s)}$. The subscripts indicate the physical state of each chemical species: solid (s), liquid (l), and gaseous (g). For the sake of simplicity, this article does not account for the movement or production of water, nor for the movement of air.

2.1 Chemical process

The modelling of the carbonation process was carried out following the work of Saetta et al. (Saetta et al. 1995, Saetta and Vitaliani 2004). This simplified approach, compared with other models (Thiery 2005, Ibrahim 2024), enables easier interpretation of the results due to the reduced number of variables and the lower amount of required input data. However, this simplification inevitably involves a loss of detailed information.

The carbonation process is assumed to consist of the reaction between solid calcium hydroxide present in the concrete and gaseous carbon dioxide, producing liquid water and solid calcium carbonate, as represented in Equation (3).



The kinetic of the process is described by the expression given in Equation (4). This formulation accounts for several factors through the inclusion of dimensionless coefficients: the relative humidity (since the reaction requires water to proceed), the concentrations of the reactants (the higher their availability, the faster the reaction rate), and the temperature, which is incorporated via the Arrhenius law (Saetta and Vitaliani 2004, Zha et al. 2015).

$$\frac{\partial \xi_c}{\partial t} = \alpha_1 f_1(RH) f_2(C_{\text{CO}_2}) f_3(C_{\text{Ca}(\text{OH})_2}) f_4(T) \quad (4)$$

$$f_1(RH) = \begin{cases} 0 & 0 \leq RH \leq 0,5 \\ \frac{5}{2}(RH - 0,5) & 0,5 \leq RH \leq 0,9 \\ 1 & 0,9 \leq RH \leq 1 \end{cases} \quad (5)$$

$$f_2(C_{\text{CO}_2}) = \frac{C_{\text{CO}_2}}{C_{\text{CO}_2,\text{max}}} \quad (6)$$

$$f_3(C_{\text{Ca}(\text{OH})_2}) = 1 - \left(1 - \frac{C_{\text{Ca}(\text{OH})_2}}{C_{\text{Ca}(\text{OH})_2,\text{max}}}\right)^m \quad (7)$$

$$f_4(T) = \exp\left(\frac{E_0}{R} \left(\frac{1}{T_0} - \frac{1}{T}\right)\right) \quad (8)$$

where t (s) is the time, ξ_c (–) is the carbonation degree, T (K) is the absolute temperature, RH (–) is the relative humidity in the concrete porosity, α_1 (s^{-1}) is a material parameter that must be calibrated experimentally, and a value of $2.8 \times 10^{-7} \text{ s}^{-1}$ was adopted based on the literature (Zha et al. 2015), $C_{\text{Ca}(\text{OH})_2}$ (kg m^{-3}) is the concentration of $\text{Ca}(\text{OH})_2$, $C_{\text{Ca}(\text{OH})_2,\text{max}}$ (kg m^{-3}) is the initial concentration of $\text{Ca}(\text{OH})_2$, m (–) is a dimensionless parameter, typically equal to 1, C_{CO_2} (kg m^{-3}) is the concentration of CO_2 , $C_{\text{CO}_2,\text{max}}$ (kg m^{-3}) is the CO_2 concentration at the concrete surface, E_0 ($\text{JK}^{-1} \text{ mol}^{-1}$) is the activation energy of the carbonation process, with a value of $48096 \text{ JK}^{-1} \text{ mol}^{-1}$ at a reference temperature T_0 (K), which was set to 296 K (Zha et al. 2015), and R ($\text{J mol}^{-1} \text{ K}^{-1}$) is the universal gas constant, equal to $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$.

The function f_4 in Equation (8) was redefined based on a dimensional analysis (Zha et al. 2015).

The sink term of CO_2 due to the carbonation reaction is determined from the carbonation degree, as expressed in Equation (9). The sink and source terms for the other chemical species are obtained by multiplying this reference term by their respective molar

mass ratios, since the stoichiometric coefficients are identical.

$$Q_{r,c} = \frac{M_{\text{CO}_2}}{M_{\text{Ca}(\text{OH})_2}} C_{\text{Ca}(\text{OH})_2,\text{max}} \frac{\partial \xi_c}{\partial t} \quad (9)$$

where $Q_{r,c}$ ($\text{kg m}^{-3} \text{ s}^{-1}$) is the sink term of CO_2 due to the carbonation reaction, M_{CO_2} (g mol^{-1}) is the molar mass of CO_2 , equal to $44.009 \text{ g mol}^{-1}$, and $M_{\text{Ca}(\text{OH})_2}$ (g mol^{-1}) is the molar mass of $\text{Ca}(\text{OH})_2$, equal to $74.093 \text{ g mol}^{-1}$.

The carbonation process affects other variables such as porosity, the water retention curve, and the diffusion coefficient (Ibrahim 2024). In this study, these variables are assumed to remain constant throughout the domain and to be unaffected by carbonation.

2.2 Carbon dioxide

The model assumes that CO_2 is transported only in the gaseous phase. Two transport mechanisms are considered: the first is *advection*, caused by the movement of dry air through the concrete porosity due to air pressure gradients; the second is *diffusion*, which occurs in response to concentration gradients. Since air pressure gradients are generally very small under typical carbonation conditions at atmospheric pressure, advective transport is negligible compared with diffusive transport (Zha et al. 2015).

The conservation equation for CO_2 within the concrete is expressed as:

$$\frac{\partial}{\partial t}(C_{\text{CO}_2}) + \nabla(D_{\text{CO}_2,\text{eff}} \nabla C_{\text{CO}_2}) + Q_{r,c} = 0 \quad (10)$$

where C_{CO_2} (kg m^{-3}) is the mass concentration of gaseous CO_2 and $D_{\text{CO}_2,\text{eff}}$ ($\text{m}^2 \text{ s}^{-1}$) is the effective diffusion coefficient of CO_2 .

The diffusion coefficient of CO_2 in the gaseous phase, denoted $D_{\text{CO}_2,\text{eff}}$ ($\text{m}^2 \text{ s}^{-1}$), represents an effective diffusion coefficient that accounts for the presence of the porous concrete medium and its degree of saturation. Several formulations are available in the literature, such as those proposed by (Papadakis et al. 1991, Thiery et al. 2007). Both models provide diffusion coefficients of the same order of magnitude and are primarily based on two key parameters: porosity and the water content within the pores. The main difference is that the latter model additionally accounts for other factors, such as temperature effects, through the bulk diffusion coefficient, which can vary with temperature - a feature not included in the Papadakis model. In this study, the Papadakis formulation was selected for its simplicity and ease of implementation. The adopted expression is presented in Equation (11).

$$D_{\text{CO}_2,\text{eff}} = 1.64 \times 10^{-6} \phi_p^{1.8} (1 - RH)^{2.2} \quad (11)$$

where ϕ_p (–) is the porosity of the cement paste (Papadakis et al. 1991).

Carbon dioxide can also dissolve in the pore water and subsequently dissociate; the resulting ionic species can then diffuse through the liquid phase. Since the diffusion coefficient in water is lower by approximately four orders of magnitude compared to that in air (Haynes 2014), the contribution of this mechanism to overall CO₂ transport is limited (De Schutter 2017). Nevertheless, it may be included to improve model accuracy (Thiery 2005, Ibrahim 2024).

2.3 Calcium hydroxide and calcium carbonate

Calcium hydroxide and calcium carbonate are assumed to remain in the solid phase while still participating in the reaction; that is, they are not transported within the concrete. Although some advanced models include dissolution–precipitation mechanisms of the solid phases and the transport of the corresponding ions in solution, these effects remain secondary compared with the flux of CO₂ considered in this study (Saetta et al. 1993). Their mass balance equation are seen in Equations (12) and (13).

$$\frac{\partial}{\partial t}(C_{\text{Ca(OH)}_2}) + \frac{M_{\text{Ca(OH)}_2}}{M_{\text{CO}_2}} Q_{r,c} = 0 \quad (12)$$

$$\frac{\partial}{\partial t}(C_{\text{CaCO}_3}) - \frac{M_{\text{CaCO}_3}}{M_{\text{CO}_2}} Q_{r,c} = 0 \quad (13)$$

where $C_{\text{Ca(OH)}_2}$ (kg m⁻³) is the mass concentration of Ca(OH)₂ per unit volume of concrete, C_{CaCO_3} (kg m⁻³) is the mass concentration of CaCO₃ per unit volume of concrete, M_{CO_2} (g mol⁻¹) is the molar mass of CO₂ (44.009 g mol⁻¹), $M_{\text{Ca(OH)}_2}$ (g mol⁻¹) is the molar mass of Ca(OH)₂ (74.093 g mol⁻¹), and M_{CaCO_3} (g mol⁻¹) is the molar mass of CaCO₃ (100.087 g mol⁻¹).

2.4 Multiscale: Homogenisation process

The multiscale approach used in this work follows the methodology described in (Fanara et al. 2024). For each Gauss point at the macroscale, the boundary conditions are determined and expressed as gradients of averaged quantities. These gradients are then applied as boundary conditions to the mesoscale problem. With these boundary conditions, the mesoscale problem is solved using the finite element method (FEM). The resulting fluxes at the mesoscale integration points are then homogenised using first-order homogenisation techniques to obtain a single equivalent value for each macroscale Gauss point. The macroscale problem can then be solved using FEM. Finally, the different steps are repeated until convergence is reached at both the macro- and meso-scales (Fanara et al. 2024).

The properties computed in the multiscale framework are the transport of CO₂ and water. By contrast, the carbonation reaction is evaluated at the macroscale, meaning that any variation in carbonatable material

content - such as differences arising from the presence of RCA - is not explicitly taken into account.

The models are implemented in LAGAMINE, a nonlinear finite element software developed at the University of Liège (col).

3 RESULT

3.1 Validation of reaction kinetic

The validation of the reaction kinetic is carried out to assess whether the model can correctly represent the carbonation process. In this case study, a homogeneous medium is considered, with initial concentrations of the reactants defined as $C_{\text{CO}_2,0}$ and $C_{\text{Ca(OH)}_2,0}$, while the concentrations of the reaction products (CaCO₃) are initially taken as zero. Transport fluxes are neglected, allowing the reaction to occur freely over time. The model developed in Section 2 thus reduces to the simplified system given in Equation (14). The time evolution of the concentrations of the different species is then obtained. The simplicity of the kinetic model described in Equation (4) enables an analytical solution to be derived, which can be compared with the numerical results for verification.

$$\frac{\partial}{\partial t}(C_{\text{CO}_2}) + Q_{r,c} = 0 \quad (14a)$$

$$\frac{\partial}{\partial t}(C_{\text{Ca(OH)}_2}) + \frac{M_{\text{Ca(OH)}_2}}{M_{\text{CO}_2}} Q_{r,c} = 0 \quad (14b)$$

$$\frac{\partial}{\partial t}(C_{\text{CaCO}_3}) - \frac{M_{\text{CaCO}_3}}{M_{\text{CO}_2}} Q_{r,c} = 0 \quad (14c)$$

The surface concentration of CO₂ was computed using the CO₂ content in air, expressed in %, based on the data reported by (Saetta and Vitaliani 2004). These values were adjusted using the ideal gas law to obtain mass (or molar) concentrations, and subsequently multiplied by the porosity and the degree of saturation in order to account for the pore volume actually accessible to CO₂. This procedure yields a surface concentration of CO₂ equal to 104.5×10^{-6} kg m⁻³.

The quantity of carbonatable material was determined following (Bunte and Rostasy 1994), as expressed in Equation (15). Alternative formulations have been proposed by (CEB 1997, Ta et al. 2016), and (Hyvert et al. 2010), which consider additional parameters; however, this additional complexity is not necessary for the present work.

$$C_{r,\text{CO}_2} = 0.0052 c_{\text{cement}} (\omega_{\text{cement,CaO}} - 3.2) \quad (15)$$

where C_{r,CO_2} (kg m⁻³) is the amount of CO₂ that can react with one cubic metre of concrete, c_{cement} (kg m⁻³) is the cement content of the concrete, and $\omega_{\text{cement,CaO}}$ (%) is the proportion of calcium oxide (CaO) in the cement.

Table 1. Parameters used for the kinetic verification.

Property	Value	Property	Value
c_{cement} (kg m^{-3})	432.5	$\omega_{\text{cement,CaO}}$ (%)	65.4
$C_{\text{CO}_2,0}$ (kg m^{-3})	104.5×10^{-6}	$C_{\text{Ca(OH)}_2,0}$ (kg m^{-3})	235.51
RH (%)	70	T (K)	293.15
φ (-)	0.127		

The Equation (15) provides the amount of CO_2 that can be fixed per unit volume of concrete, but not the initial amount of portlandite present. Subsequently, it is assumed that all available CO_2 reacts with Ca(OH)_2 (Steffens et al. 2002). This assumption enables the estimation of an equivalent amount of Ca(OH)_2 required to bind the predicted quantity of CO_2 , although it leads to a slight overestimation since a portion of the CO_2 would otherwise react with other carbonatable compounds.

Assuming a complete reaction of CO_2 with Ca(OH)_2 , the initial concentration of Ca(OH)_2 can be estimated using Equation (16):

$$C_{\text{Ca(OH)}_2,0} = \frac{M_{\text{Ca(OH)}_2}}{M_{\text{CO}_2}} C_{\text{r,CO}_2} \quad (16)$$

A comparison between analytical and numerical solutions is shown in Figure 1. The parameters used are summarised in Table 1.

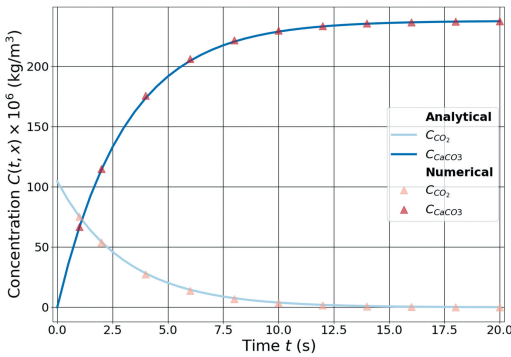


Figure 1. Comparison between the analytical and numerical solutions for the kinetic verification case.

The results show a decrease in the concentration of CO_2 , which progressively approaches zero as the reaction rate diminishes due to the depletion of reactants. The concentration of Ca(OH)_2 is not shown, as its initial value is several orders of magnitude higher and thus remains nearly constant throughout the simulation. The production of CaCO_3 increases

steadily until reaching a plateau corresponding to the expected amount predicted by Equation (17).

$$\lim_{t \rightarrow \infty} C_{\text{CaCO}_3}(t) = C_{\text{CO}_2}(t=0) \frac{M_{\text{CaCO}_3}}{M_{\text{CO}_2}} \quad (17)$$

$$= 237.66 \times 10^{-6} \text{ kg m}^{-3} \quad (18)$$

3.2 Results of the multiscale model and comparison with a simplified model

Having established that the model can reproduce the carbonation reaction described in Section 2.1, the combined effects of reaction and transport processes are now investigated through a simplified test case. To ensure the reliability of the results, the outcomes of the multiscale model are compared with those obtained from a simplified model.

The case study considers a one-dimensional homogeneous concrete element of 25 cm in length. At the mesoscale, the material is simplified as homogeneous. The element is exposed to air on its left-hand side, where the CO_2 concentration is prescribed and assumed to remain constant over time, acting as a boundary condition. The surface concentration of CO_2 is taken from Table 1 and is equal to $104.5 \times 10^{-6} \text{ kg m}^{-3}$.

Inside the concrete, the initial concentrations of CO_2 and CaCO_3 are set to zero, since no carbonation has yet occurred. Conversely, the initial concentration of Ca(OH)_2 is set to 235.51 kg m^{-3} . The relative humidity of the air within the concrete porosity is assumed to be homogeneous, kept constant at 70 %. The total porosity of the concrete is 0.127, leading to an effective diffusion coefficient for CO_2 of $2.4 \times 10^{-8} \text{ m}^2 \text{ s}^{-1}$, calculated from Equation (11).

The results of the multiscale model are presented in Figure 2, illustrating the concentration profiles along the specimen depth at different times.

The simulations reveal a transition in the chemical composition of the concrete, from a carbonated zone near the exposed surface to an uncarbonated zone deeper within the material. As time progresses, this transition advances further into the concrete. The development of this transition zone requires a certain period to form.

The emergence of the carbonation front can be understood through the change in the concavity of the concentration profiles: initially, the solution is concave, but over time a distinct carbonation front appears. This front is characterised by a convex region on the left-hand side of the profile and a concave region on the right, corresponding to the formation of an inflection point within the transition zone.

The location of this transition defines the carbonation front, which separates the carbonated region - where carbonation can no longer proceed due to the depletion of reactive calcium hydroxide (Ca(OH)_2) - from the uncarbonated region that remains unaffected.

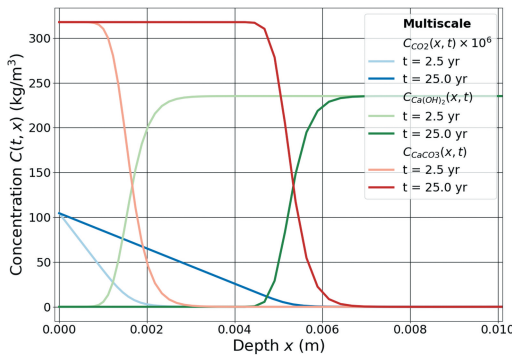


Figure 2. Spatial distribution of chemical species at $t = 20$ yr obtained from the multiscale models in the simplified case at different time.

The CO_2 concentration in the carbonated zone, extending from the surface to the reaction front, exhibits an approximately linear decrease to zero at the front. This behaviour indicates that diffusion is the rate limiting factor in the carbonation process under these conditions. The CO_2 does not penetrate deeply into the uncarbonated zone before reacting, resulting in a steep carbonation front. A higher diffusion coefficient leads to a smoother transition zone.

The first result shown in Figure 2 highlights the presence of a carbonation front whose depth evolves over time. In practice, carbonation depth tests aim to determine the position of this front in order to assess the extent of the carbonated zone and the remaining uncarbonated (pristine) concrete, thereby estimating the time before the carbonation front reaches the reinforcement bars and initiates corrosion (Ployaert 2008). This front - or rather, the transition zone - therefore plays a crucial role in carbonation depth assessments.

Experimentally, the carbonation front is most commonly identified using a pH indicator, typically phenolphthalein. The carbonation depth is determined from the variation of pH with depth, which reflects the chemical composition changes induced by carbonation (CEN 2006, Thiery 2005).

To reproduce this behaviour, several simplified models have been developed. These models generally assume the existence of a sharp transition between the carbonated and uncarbonated regions. They are referred to as *simplified* because they account for only a limited number of physical and chemical processes. Such models provide an estimate of the carbonation front depth as a function of time. Examples include those proposed by (Petre-Lazar 2001, Silva et al. 2014, Papadakis et al. 1989, CEB 1997, Hyvert 2009).

The results obtained from the multiscale model can be compared with those predicted by the simplified formulations. The main requirement for this comparison is the definition of a carbonation front that is physically relevant and can be effectively compared with the simplified models. The model presented in this study provides the local chemical composition

and thus offers an alternative way of defining the carbonation front, based on the variation of composition - or more precisely, on the degree of carbonation, denoted by ξ_c , as defined in Equation (19).

This approach, however, remains somewhat subjective, as the threshold value ($\xi_{c,th}$) depends on the chosen model. Selecting a different threshold would slightly modify the computed carbonation depth, but it would not significantly affect the overall trends observed. To overcome the ambiguity associated with defining the carbonation front solely from the degree of carbonation, some detailed models compute the pH directly from the chemical composition. Although the present model is capable of representing a distinct carbonation front, it remains too simplified to determine pH values explicitly (Thiery 2005).

$$\xi_c(t) = \frac{C_{\text{CaCO}_3}(t)}{\lim_{t \rightarrow \infty} C_{\text{CaCO}_3}(t)} \quad (19)$$

The carbonation depth at a given time is determined from the concentration profile of Ca(OH)_2 across the specimen depth. The reaction coefficient is then derived from this concentration. Since the finite element method provides results at discrete nodal points, interpolation is required to accurately locate the position of the carbonation front.

The simplified model chosen for comparison is that proposed by (Hyvert et al. 2009, Hyvert et al. 2010), presented below in Equation (20).

$$X_c = \sqrt{\frac{2k_e k_c k_t D_{\text{CO}_2, \text{eff}} \frac{P_{\text{CO}_2}}{RT} t}{\left(1 + \beta C_2 \left(\frac{P_{\text{CO}_2}}{P_{\text{atm}}}\right)^n\right) \left(\frac{C_2 \phi_p}{n+1} \left(\frac{P_{\text{CO}_2}}{P_{\text{atm}}}\right)^n + Q_1\right)}} \quad (20)$$

where X_c (m) is the carbonation depth, t (s) is the time, $D_{\text{CO}_2, \text{eff}}$ ($\text{m}^2 \text{s}^{-1}$) is the effective diffusion coefficient of CO_2 in concrete at atmospheric pressure, P_{CO_2} (Pa) is the partial pressure of CO_2 at the concrete surface, P_{atm} (Pa) is the atmospheric pressure, R ($\text{JK}^{-1} \text{mol}^{-1}$) is the universal gas constant, equal to $8.314 \text{ JK}^{-1} \text{mol}^{-1}$, and T (K) is the absolute temperature. The parameters n (—) and β ($\text{m}^3 \text{mol}^{-1}$) are independent of the concrete composition and cement type: n accounts for the chemical affinity of C-S-H with respect to CO_2 and has a value of 0.67, while β represents the reduction in porosity caused by carbonation of the C-S-H phase and has a value of $23.5 \times 10^{-3} \text{ m}^3 \text{mol}^{-1}$. Q_1 (mol m^{-3}) is the initial concentration of calcium contained in portlandite, calcium monosulfoaluminate, and calcium trisulfoaluminate phases within the concrete, and C_2 (mol m^{-3}) is the initial concentration of calcium bound within the C-S-H phase of the cement paste. ϕ_p (—) is the ratio between the volume of cement paste and the total concrete volume, k_e (—) is a parameter defined by climatic conditions -

Table 2. Parameters used in the simplified model.

Property	Value	Property	Value
k_e (—)	1.0	k_c (—)	1.0
k_t (—)	1.0	$D_{CO_2,eff}$ (m ² s ⁻¹)	2.4×10^{-8}
Q_1 (mol m ⁻³)	3.18	C_2 (mol m ⁻³)	0.0
T (K)	293.15		

primarily the degree of saturation of the concrete - k_c (—) accounts for the curing conditions, and k_t (—) represents the influence of any thermal treatment applied to the concrete.

The result comparing the carbonation depth between the prediction of the simplified model and the multiscale model are presented in Figure 3. The parameters used in the simplified model are summarised in Table 2.

The results obtained from the multiscale model highlight an interesting feature of the carbonation process: the *initiation period*. This period corresponds to the time interval between the moment when the concrete is first exposed to CO₂ and the formation of a distinct carbonation front, which subsequently advances towards the core of the concrete (Thiery 2005).

The results also clearly show similar trends and closely matching values, but with a constant offset between the numerical model and Hyvert's model. Even though Hyvert's model would have been delayed by the initiation period (108.8 d), it rapidly recovers the undelayed solution because of its time dependence, since $\lim_{t \rightarrow \infty} \sqrt{t + \varepsilon} \approx \sqrt{t}$ for sufficiently large t . Thus, the initiation period becomes negligible for long-term tests. The remaining difference between the two approaches arises because the carbonation front is not perfectly sharp.

To minimise the discrepancy between the multiscale results and Hyvert's model, the value of $\xi_{c,th}$ can be adjusted. The carbonation depth depends directly on the chosen threshold degree of carbonation: a higher $\xi_{c,th}$ yields a smaller estimated depth, while a lower value yields a larger one.

In Hyvert's formulation, the CO₂ concentration is assumed to vary linearly between the carbonation front, where it is equal to zero, and the imposed surface concentration. The reaction is considered instantaneous, the carbonation front is assumed to be steep, and the diffusion coefficient is treated as constant. These assumptions closely match the behaviour reproduced by the numerical model, which exhibits a linear distribution of CO₂ up to the carbonation front - exactly the distribution used to compute the CO₂ flux in Hyvert's formulation. In the results, the progression of the carbonation front is governed by the transport of CO₂, as the reaction is almost instantaneous compared with diffusion. This produces a relatively sharp carbonation front.

As a consequence, both models extract nearly the same quantity of CO₂ from the surface and therefore consume almost the same amount of carbonatable

material. Integrating the degree of carbonation over the depth yields comparable values. Hyvert's expression, which assumes an infinitely sharp carbonation front, therefore provides the mean position of the front. Under the assumption of an almost point-reflection symmetry in the spatial distribution of chemical species at the transition zone in the numerical model, the equivalent threshold is $\xi_{c,th} = 0.5$. If the carbonation front becomes asymmetric, this equivalence no longer holds, and the optimal threshold becomes the value of $\xi_{c,th}$ that corresponds to the mean depth, as determined from the degree of carbonation using Equation (2):

$$\int_0^1 X_{c,num}(\xi_c) d\xi_c = \int_0^1 X_{c,Hyvert}(\xi_c) d\xi_c \quad (21a)$$

$$= X_{c,Hyvert} = \bar{X}_c \quad (21b)$$

An increase in the diffusion coefficient or a reduction in the reaction kinetics would progressively cause the results to diverge, as the carbonation front would become smoother and the concentration distribution would no longer satisfy the assumptions of Hyvert's model.

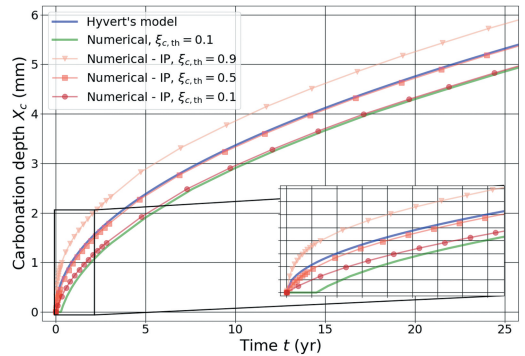


Figure 3. Comparison of carbonation depth predictions obtained from the simplified and multiscale models for different value of $\xi_{c,th}$, with and without the initiation period (IP).

This agreement is illustrated in Figure 3, where Hyvert's model is compared with the numerical results obtained using different values of $\xi_{c,th}$, with the initiation period removed so that all curves start from the origin. Under these conditions, the two solutions coincide almost exactly for $\xi_{c,th} = 0.5$, as expected.

Table 3. Parameters used to define the property of the different phase: Natural aggregates (NA), Adherent Mortar Paste (AMP), New Mortar Paste (NMP), in the RVE.

Property	NA	Adherent MP	New MP
Diffusion Coefficient (m ² s ⁻¹)	0	2.4×10^{-9}	2.4×10^{-8}
Carbonatable material (kg m ⁻³)	235.51	235.51	235.51

The model is therefore comparable to simplified models while providing additional information regarding the spatial distribution of the chemical composition.

3.3 Academic application

Having demonstrated that the model provides reliable results in a simplified case, it is now applied to a more practical case study to investigate the influence of recycled concrete aggregates (RCA). The case setup is similar to the simplified example presented in Section 3.2, with the main difference being that, in this study, the multiscale model employs a RVE containing recycled concrete aggregates (RCA).

A key concept in multiscale modelling is the *representative volume element* (RVE). It is defined as the smallest volume capable of representing the processes or properties occurring at a given scale, and it is essential for accurately capturing the behaviour and properties at higher scales (Li and Sitnikova 2020). The more realistic the RVE, the more representative and reliable the computed values are.

The RVE generation method is based on the random sequential addition (RSA) algorithm proposed by (Nilenius 2014). In summary, the method takes as input a particle size distribution and surface fraction. Aggregates are first generated with an initial ellipsoidal shape, defined by an aspect ratio and a given size range. These are then modified to obtain octagonal aggregates with random surface irregularities. The aggregates are placed randomly within the RVE, ensuring that no interpenetration occurs with previously placed particles or with the domain boundaries. Finally, an adherent mortar paste layer is generated according to the specified surface fraction of adherent mortar paste. When the target surface fraction for a given size interval is reached, the

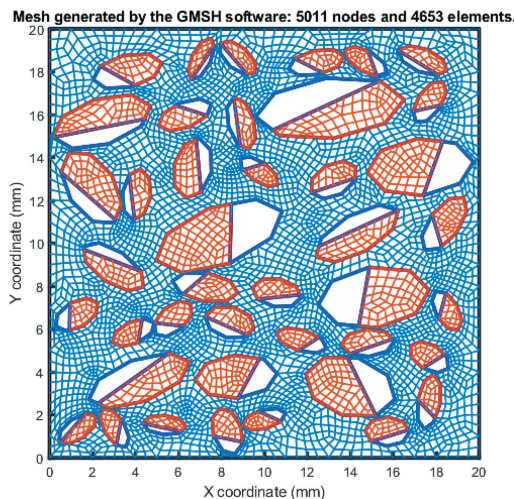


Figure 4. Representative Volume Element (RVE) of the concrete made with recycled concrete aggregates (C-RCA).

process proceeds to the next smaller size range until all intervals have been used (Fanara et al. 2024). Once generated, the RVE is meshed using the Gmsh software (Geuzaine and Remacle 2009).

Based on this method, the RVEs of concrete produced with recycled concrete aggregates (RCA) were generated. The resulting RVE obtained for the C-RCA case is shown in Figure 4, together with its corresponding mesh. The unmeshed regions represent the natural aggregates, while the red mesh corresponds to the adhered mortar paste. Consequently, the combination of the unmeshed regions and the red meshed zones constitutes the recycled concrete aggregate phase, whereas the blue mesh represents the new cement paste.

The results obtained from the multiscale simulations using the homogeneous and C-RCA RVEs are compared in Figure 5.

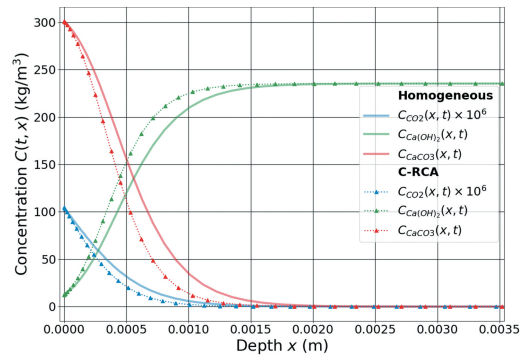


Figure 5. Comparison between multiscale results for the homogeneous and C-RCA concretes under the same environmental conditions at $t = 139$ d.

The results in Figure 5 clearly show that introducing aggregates leads to a marked decrease in the effective diffusion coefficient. This occurs because the adhered mortar paste (AMP) exhibits a lower diffusion coefficient than the new mortar paste (NMP), and because the NA phase is essentially impermeable. As a consequence, the global CO_2 concentration is lower than in the homogeneous case, which results in a lower carbonation depth.

The outcome would have been different if the diffusion coefficient of CO_2 in the AMP had been higher than that in the NMP, which could be justified by the presence of microcracks within the AMP. In that situation, the results would be influenced not only by the increased diffusivity but also by the reduced amount of carbonatable material due to possible pre-carbonation of the AMP, as well as by the presence of the inert NA phase, which contains no carbonatable compounds.

Based on Equation (21), it is possible to estimate the effective diffusion coefficient by using the mean depth corresponding to the degree of carbonation

and the elapsed time. This value can then be related to Hyvert's formula Equation (20), allowing the effective diffusion coefficient to be determined for the different cases.

4 CONCLUSION

The model is capable of representing the carbonation process within concrete, either by assuming a homogeneous medium or by considering the heterogeneity of the material through the presence of aggregates.

Despite its simplicity, the model can predict the evolution of carbonation depth with the correct order of magnitude while accounting for the heterogeneity of concrete at relatively low computational cost, particularly for large structural elements. This makes it suitable for comparing reference concrete with concrete produced using recycled concrete aggregates and represents a first step towards a more faithful simulation of the carbonation process.

In addition, the simplified model provides a practical means of estimating carbonation depth over time, enabling validation or comparison of numerical models in specific cases. It can also be used to obtain an approximate value of the effective diffusion coefficient of CO_2 .

Future work will focus on refining the model by explicitly accounting for the production and transport of water, as well as its influence on the relevant transport properties. In parallel, experimental data will be collected to enable direct comparison with real measurements and further validation of the model.

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