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CARBON DIOXIDE BINDING ABILITY IN CONCRETES: METHODOLOGY AND MODELING

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Abstract.

Carbonation of concretes is a natural physico-chemical process that can be described as a reaction between the carbon dioxide contained in the air and the cement matrix. Carbonation concerns all concretes types in contact with the ambient air but also concretes in ground, from production stage to use and end-of-life stages. The amount of carbon dioxide bound varies according to the type of binder, the compacity of concrete and the environmental conditions during the use and the end-of-life stages. To consider the re-carbonation of concrete, works have been carried out within the framework of the European standardization group CEN/TC229/WG5 and in CEN/TC104. A methodology to consider the re-carbonation of concrete structures has been proposed in the NF EN 16757 standard on environmental product declarations for concrete and concrete elements. In addition, FD CEN/TR 17310 provides detailed recommendations regarding carbonation and absorption of carbon dioxide in concrete and give some precisions for application of NF EN 16757. This is an important topic towards a sustainable development in the current context of circular economy and CO_2 uptake related to the French energy labelling (E+C-). In this paper, numerical and analytical carbonation models are used to estimate the CO_2 binding ability of concrete structures. The obtained results are compared to the methodology proposed in Appendix BB of NF EN 16757 standard. They confirm that the methodology described in the NF EN 16757 standard leads to estimated degree of carbonation of the same order of magnitude. The advantage of using more advanced models lies in a better consideration of environmental parameters, the possibility to simulate the behaviour of crushed concrete, its reuse in new concrete as recycled aggregate and the possibility to simulate the carbonation of concretes in ground. This is an immediate perspective in the ongoing work in the French national project FastCarb on accelerated carbonation of recycled concrete aggregates.

Keywords: Concrete products, concrete structures, modeling, re-carbonation, standardization.

1. Introduction

Concrete is the most widely used building material in the world because the raw materials are generally considered lowly exhaustible and ubiquitous on the globe. In addition, its manufacturing process is well controlled and its cost price low. However, due to the use of cement and its success in construction works, concrete production can generate considerable CO_2 emissions. Today the cement sector is among the main emitters with between 5 and 7% of global emissions [1].

How can this situation be reconciled with, on the one hand, the need for countries to continue to offer an efficient, robust and affordable solution and, on the other hand, the need to fight effectively against global warming?

The building sector is actively working on solutions to reduce its CO_2 emissions. Current research considers many aspects:

- To reduce the carbon intensity of cement production operations;
- To control the environmental impact of concrete products on their entire life cycle;
- To optimize the processes of concrete production and construction;
- To better recycle concrete into concrete;
- To work in partnership with the construction industry to jointly contribute to green building systems.

This study is part of a national research project: The FastCarb Project. The aim of the FastCarb project is firstly to store CO_2 in the Recycled Con-

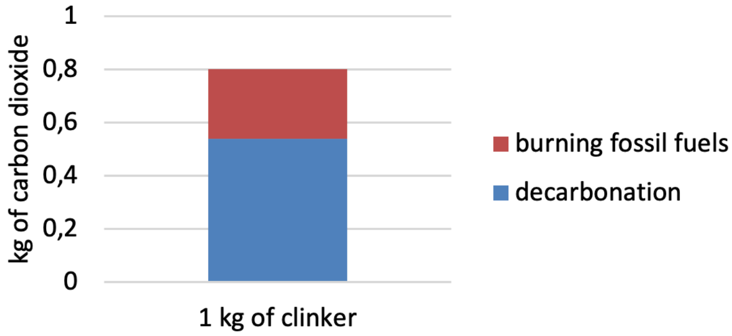

Figure 1. Carbon footprint of 1kg of clinker.

Type of cement	Carbon footprint*
CEM I	765 kg of CO_2/ton
CEM II/A-S - CEM II/A-L	671 - 676 kg of CO_2/ton
CEM II/B-L or LL - CEM/B-M	579 - 585 kg of CO_2/ton
CEM III/A	400 kg of CO_2/ton
CEM III/B	274 kg of CO_2/ton
CEM V/A	468 kg of CO_2/ton

* not including carbon dioxide emissions from the combustion of secondary fuels

Table 1. Carbon footprint of the different types of cement in France (in average) [2].

crete Aggregates (RCA), in order to reduce the environmental impact of concrete in the structures and secondly to improve the quality of these aggregates by reducing their porosity.

Today one of the main issues for the concrete profession is to better evaluate the carbon footprint of concrete and concrete structures. To solve this question, the quantity of carbon dioxide that could be stored by a building during its life time has to be correctly calculated. The objective of this study is to quantify the CO_2 stored by a building during its life time using different methods and models.

2. Context and objectives of the study

Cement is a widely used building material whose main hydraulic constituent is clinker. To manufacture the clinker, the active "raw material" of the cement, the calcination of the limestone and the clay in the kilns at very high temperature (1,450 °)C generates carbon dioxide due to decarbonation of limestone and to combustion reactions during pyroprocessing. This decarbonation step represents about 60% of CO_2 emissions of the production process [1, 3, 4]. The Figure 1 presents the carbon footprint of the production of clinker and the Table 1 gives the footprint of the different types of cement.

The carbon dioxide emitted during the manufacturing of cement can for a part be stored again by the natural phenomena of carbonation during the concrete life time. During the life of the structure, the concrete could store carbon dioxide at a level of 10 to 15% of the CO_2 emitted during the decarbonation of the limestone necessary for the manufacture of cement [1]. It is important to note that this percentage is average on the scale of the building. Some parts carbonate more than others (exposed/not exposed parts, porous masonry compared to civil engineering parts. . .).

These numbers take into account decarbonation and combustion of primary fuels but do not consider CO_2 emissions due to the combustion of "wastes" like tyres or waste oils for example. This is this value which is used for the LCA.

The standard NF EN 16757 presents a methodology and a model to evaluate the quantity of carbon dioxide that can be stored during concrete lifetime in function of the environment and the materials as concrete strength classes.

In this study, the numerical model SDReaM-crete is used to estimate the capacity of CO_2 storage of concrete. The results are compared to those obtained with the NF EN 16757 model. Then the CO_2 storage capacity of a R+5 building is estimated and compared to the amount of carbon dioxide emitted during its construction.

3. Presentation of the models

3.1. Model of the standard NF EN 16757 [5]

The NF EN 16757 standards model is an analytic model which considers environment as well as material parameters. The equation 1 gives the carbonation depth. The equation 2 presents the model to

	Material	Environment
x_c: carbonation depth (mm) (Equation 1)	X	X
k: carbonation rate (mm/year0.5)	X	X
K_k: correction to k−factor	X	–
t: time (year)	–	–
U_{tcc}: maximum theoretical uptake in CO_2/kg of cement (0.49 for CEM I)	X	–
C: cement content (kg/m^3)	X	–
D_c: degree of carbonation (−)	–	X

Table 2. Parameter of the NF EN 16757 model.

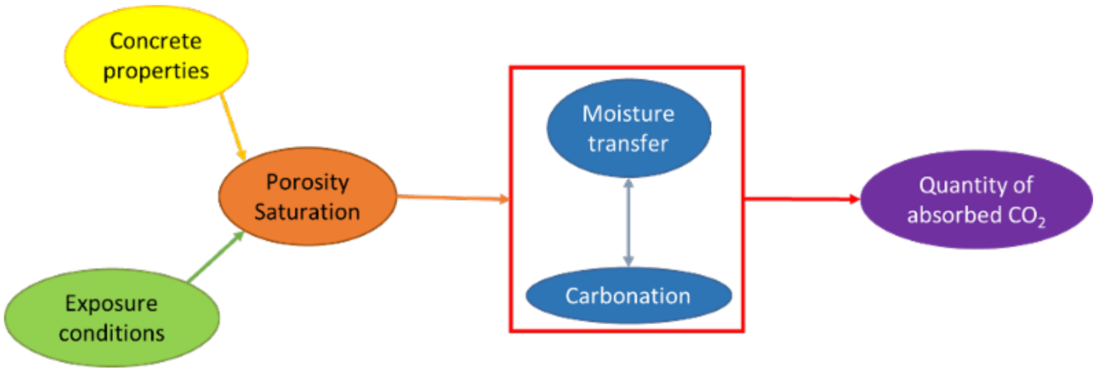

Figure 2. Schematic presentation of the SDReaM-crete model (only carbonation and hydric parts).

Properties	Value considered
Resistance class	C25/30
CEM I 52.5 N [kg/m^3]	280
Aggregates [kg/m^3]	1 922
Efficient water [l/m^3]	168
W_{eff}/C	0.60
Relative humidity [%]	80 ± 10
CO_2 concentration [%]	0.04

Table 3. Properties of studied concrete and environment.

estimate the CO_2 stored and the table 2 presents the parameters.

$$x_c = k \cdot \sqrt{t} \tag{1}$$

$$CO_{2\,\mathrm{uptake}} = k \cdot K_k \left(\frac{\sqrt{t}}{1000}\right) U_{tcc} \cdot C \cdot D_c \tag{2}$$

Each of these factors is detailed in Appendix BB of the standard. The Appendix BB also gives values for the parameters that depend on the material and the environment.

3.2. Model SDReaM-crete

The SDReaM-crete durability model was developed at Cerib with LMDC [5, 6]. It is a numerical model based on mass conservation equations. This model can simulate the chloride ingress, the carbonation, the moisture transfers as well as the development of the corrosion of the rebars in concretes exposed to wetting-drying cycles. It can be used in a deterministic context or in a probabilistic context to achieve reliability calculations for concrete products or concrete works. In this study, it is used to calculate the carbonation depth and then the amount of CO_2 absorbed by the concrete during its service phase. The quantity of stored CO_2 is calculated with the carbonation depth and the trapezoidal rules. The figure 2 presents a schematic representation of the SDReaM-crete durability model.

4. Results

4.1. Comparison between analytical method and numerical method

The first phase of this study consisted of estimating the amount of CO_2 that can be absorbed per square meter of exposed concrete with both models presented in the precedent section.

The properties of the considered concrete and environment are presented in the Table 3.

Properties	Value considered
k: carbonation rate (mm/year0.5)	1.6
K_k: correction to k-factor	1 (CEM I)
U_{tcc}: maximum theoretical uptake in CO_2/kg of cement	0.49 (CEM I)
D_c: degree of carbonation (-)	0.85 (outdoor exposed to the rain)

Table 4. Details of the considered value for the calculation with the NF EN 16757 model.

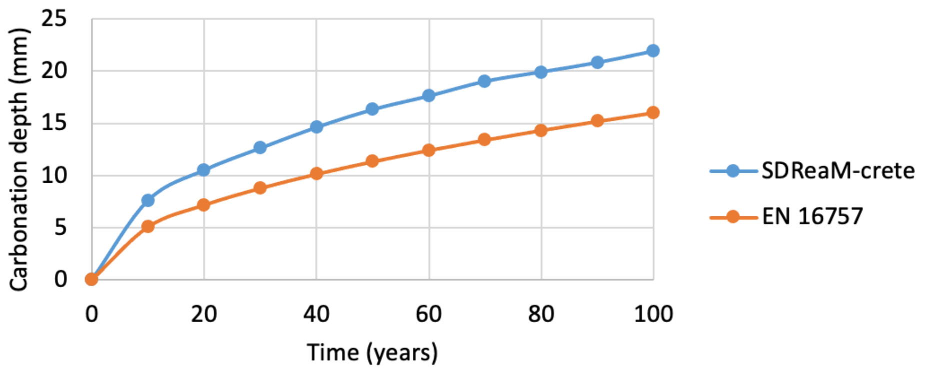

Figure 3. Carbonation depth of the studied concrete calculated with SDReaM-crete model and NF EN 16757 model.

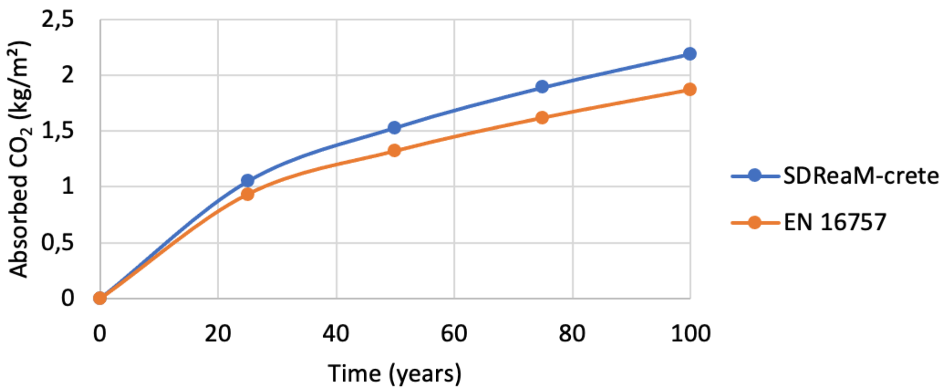

Figure 4. Absorbed carbon dioxide calculated with two models and two methods.

The figure 3 presents the carbonation depth calculated with SDReaM-crete model and with the Equation 1 (EN 16757 on the figure). The two models (SDReaM-crete et Eq. 1) provide results slightly different. That can be explained by the different parameters taken into account by the two models. The standard model is based on the law at the root of time while the numerical model considers more precisely the formulation and the environment of the concrete. That will be discussed later.

Considering that the carbonation reaction can be summarized as (Eq. 3):

$$Ca(OH)_2 + CO_2 \leftrightarrow CaCO_3 + H_2O \qquad (3)$$

The Equation 3 means that the consumption of one mol of CO_2 leads to the production of one mol of calcite. With SDReaM-crete model, the amount of calcite in the concrete can be calculated and, by extension, the amount of carbon dioxide consumed according to the Equation 3.

The Figure 4 presents the quantity of stored CO_2 for one square meter of the considered concrete. The orange curve was obtained using the Equation 2. The blue curve was obtained using the depth of carbonation calculated by SDReaM-crete and then using the mathematical method of the trapezoids.

These results show that two different models and methods, that consider very different parameters, are leading to very close results in this specific scenario. Both method and model have advantages and disadvantages: the analytical model has the advantage of being quick and easy to use. In fact, the standard NF EN 16757 details each of the parameters and proposes values to be considered depending on the resistance of the concrete and its environment. The numerical model seems more complete than the standard model because of the phenomena it considers (water cycle, detailed composition of concrete...). However,

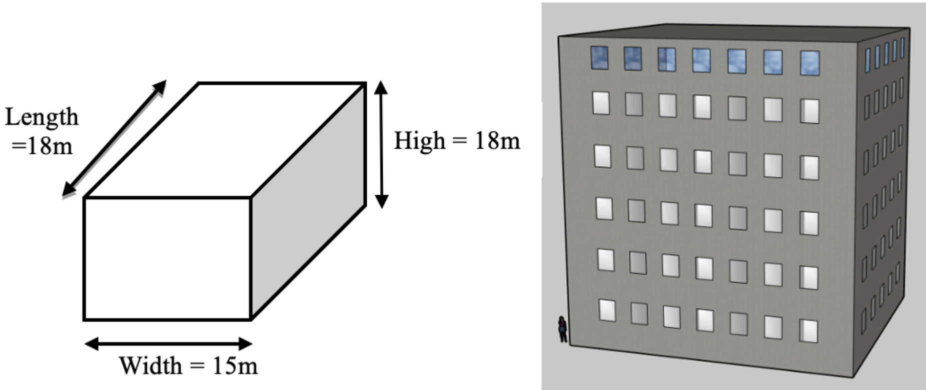

Figure 5. Illustration of the building modelized for the study.

	Outdoor	Indoor
k: carbonation rate (mm/year0.5)	1.6 (exposed to rain)	4.6 (with cover)
K_k: correction to k-factor	1.05	1.05
t: time (year)	50	50
U_{tcc}: maximum theoretical uptake in CO_2/kg of cement	0.41	0.41
C: cement content (kg/m3)	300	300
D_c: degree of carbonation $(-)$	0.85 (exposed to rain)	0.4 (dry climate)
Quantity of stored CO_2 (according to Eq. 2, kg/m^2)	1.24	1.68

Table 5. Values considered for the study.

the calculation times can be longer and obtaining the input data can sometimes be complicated in an operational context. In this study, the standard model will be used (Eq. 2).

4.2. Application to a Five-Storey Building [7]

In this paragraph, the NF EN 16757 model is applied to a R+5 building made with CEM II/A (case of an exposed architectural concrete, we only take into account the facade, external and internal) and the result is compared to the amount of CO_2 emitted during the decarbonation of the clinker needed for the building construction.

The Figure 5 presents an illustration the Five-Storey building studied.

The first step of the study is to determine the quantity of carbon dioxide emitted during the building construction (only considering decarbonation of cement).

The cement used for the construction of this building is CEM II/A-L and contains 80% clinker. The amount of clinker required for this building is therefore 48 384kg. Then it is possible to calculate the quantity of carbon dioxide emitted during the decarbonation phase (0.54kg for 1kg of clinker): 26ă127kg of CO_2 emitted.

Then we can calculate the quantity of carbon dioxide stored by the building with the model of the NF EN 16757 standard (Eq. 2). The Table 5 presents the values of the parameters used for the simulation. All these values were determined using annex BB of standard NF EN 16757.

After calculating the amount of carbon dioxide that can be absorbed per square meter of concrete, we can calculate the amount of CO_2 that can be stored by this building after 50 years of life (Eq. 4).

$$\begin{aligned}\text{Total } CO_{2\,\text{uptake}} = \\ \left(\text{outdoor } CO_{2\,\text{uptake}} + \text{indoor } CO_{2\,\text{uptake}}\right) \\ \cdot \text{surface of exposed concrete}\end{aligned} \tag{4}$$

So, the quantity of carbon dioxide that can be stored by the building is 2ă943.4 kg CO_2. If we compare this value to the quantity of CO_2 emitted during the construction (by the decarbonation phase, 26 127kg) we can highlight that the ratio is around 11.3%, which corresponds to the value of the literature [1] (Eq. 5).

$$\frac{\text{Total } CO_{2\,\text{uptake}}}{\text{Emitted } CO_{2\,\text{decarbonation}}} = \frac{2943.4}{26\,127} = 0.113 \tag{5}$$

This study was carried out on a fictitious and heavily simplified building at first. A single concrete for the whole building has been considered but in reality, we can observe significant divergences due to the possible variety of concretes encountered, e.g., porous masonry concrete or more efficient and dense concretes in some cases. The direct following will be to do the same work on an existing building for which we have all the material and environmental data. Both models can be used.

5. Conclusion

As an integral part of the national project FastCarb, this study made it possible to carry out a bibliographic study on the ability of concrete to capture CO_2 during its service phase. Several models of different levels (analytical, numerical ...) exist today. NF EN 16757 is the Product Category Rules for concrete and concrete elements. One model to take into account the carbonation phenomena in the context Environmental Product Declaration (EPD) for the calculation methodology is presented in the NF EN 16757 standard. This standard is the reference document when performing EPDs for concrete elements following EN 15804+A1 standard. Moreover FD CEN/TR 17310 [8] provides technical and scientific elements to support the carbonation treatment part of the NF EN 16757.

In the first part of this study, two different models and methods for calculating the quantity of stored CO_2 were compared. The results show that the model of standard NF EN 16757, although analytical and "simple", allows to obtain results close to those obtained with a numerical model taking into account many different parameters.

Then, the model proposed in the standard was used to assess the amount of carbon dioxide captured by a Five-Storey Building during its service phase (only the facade). The calculations highlight the ability of the concrete to capture part of the CO_2 emitted during the decarbonation of the clinker. With approximately 11.3% of the emitted CO_2 which can be reabsorbed, the results confirm the literature. It is important to note that this value could be increased significantly if carbonation continued after the demolition of the structure.

This last point is the direct perspective of the work reported in this article. Recent results show that it is possible to recapture up to 50 to 60% of the CO_2 emitted during the decarbonation of limestone for traditional concrete [1]. This value including the percentage of carbonation during the service life of the building, this means that the recycling phase alone stores around 40% to 45% of the CO_2 emitted during the decarbonation of limestone. Investigations and calculations are currently underway to precise the CO_2 storage capacity of a Recycled Concrete Aggregate (RCA) and the best condition to optimize the carbonation of RCA.

Acknowledgements

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