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Development of *OptiCon*: A Mathematical Model with a Graphical User Interface for Designing Sustainable Portland Cement Concrete Mixes with Budget Constraint

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Abstract: The production of Portland Cement Concrete (PCC) generates significant environmental impacts that increase climate change and decrease people's quality of life. Recent studies highlight the potential to reduce these environmental burdens by partially replacing Portland cement with Supplementary Cementitious Materials (SCMs) and coarse aggregates with Recycled Concrete Aggregate (RCA). However, designing PCCs with simultaneous contents of SCMs and RCA is not easily manageable because current design procedures fail to adjust all of the variables involved. In order to overcome these limitations, this research introduces a novel mathematical model designed to develop operationally efficient PCC mixes that are both environmentally sustainable and cost-effective. The proposed model, denominated *OptiCon*, employs the Life-Cycle Assessment and Life-Cycle Costs Analysis methodologies to evaluate the incorporation of three different SCMs (i.e., fly ash, silica fume, and steel slag) and RCA into PCC mixes. *OptiCon* is also integrated within a graphical user interface in order to make its implementation straightforward for potential users. Thus, *OptiCon* is operationalized through an algorithm, offering a replicable approach that can be adapted to various contexts, providing both a theoretical framework and a practical tool for state agencies, engineers, suppliers, and other stakeholders to adopt more environmentally friendly practices in concrete production. Furthermore, a case study from northern Colombia analyzed thirty mix design scenarios with varying supplier conditions (foreign, local, or mixed), calculating costs and CO_2 emissions for a fixed concrete volume of 1 m^3. The findings demonstrated that utilizing *OptiCon* can achieve substantial reductions in both CO_2 emissions and production costs, underscoring the model's efficiency and practical impact.

Keywords: life cycle assessment; life cycle costs analysis; Portland Cement concrete; recycled concrete aggregate; supplementary cementing material

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1. Introduction

Portland Cement Concrete (PCC) is the composite material most widely used worldwide for construction purposes [1,2]. Although there is a wide range of different PCCs, the standard one is made from the mixing of coarse aggregates (i.e., gravel), fine aggregates (i.e., sand), Portland Cement (PC), and water [3,4]. In order to satisfy the global demand for PCC, it is necessary to consume immense quantities of natural resources, which generates a high depletion of non-renewable resources and, consequently, accelerates global warming potential and climate change [1,3]. In addition to the high environmental impact associated with PCCs, their production implies elevated monetary costs [5,6]. The preceding has led various researchers to explore ways to increase the sustainability of this industry [7,8]. Thus, two alternatives stand out, i.e., partially replace the coarse aggregates and PC with Recycled Concrete Aggregate (RCA) and Supplementary Cementing Materials (SCMs), respectively [9,10]. These alternatives are described below.

Overall, the PC is produced industrially in a four-stage process [11,12]: (i) initially, limestone and clay (or sometimes shale) are mixed and ground; (ii) then, the mixture is heated up to approximately 1500 °C; (iii) next, the mixture is ground to obtain the clinker; and (iv) finally, a small quantity of gypsum is added to the clinker (around 5% by weight) to obtain the PC. Remarkably, the main problem of this industrial process is the heightened environmental impact generated (especially during the exploitation of quarries and heating) [13,14]. Therefore, producing PCC with the least amount of PC is crucial to achieving sustainable development. In this way, partially replacing PC with SCMs is an ideal strategy [15,16]. Moreover, it has been demonstrated that using SCMs provides economic benefits and improves the mechanical performance of PCCs [15,17]. Although there is no consensus on the definition of SCMs, a standard connotation is that this term includes materials (even wastes, residues, co-products, and by-products) that have cementing-type chemical reactions (in some cases also pozzolanic-type reactions) [18,19]. Notably, within the wide variety of SCMs, fly ash, silica fume, and steel slag are some of the most used [19,20]. On the one hand, fly ash is the residue formed by fine particles of burned fuel, which are expelled from boilers, incinerators, and furnaces after the industrial combustion of flue gases [21,22]. On the other hand, silica fume is an ultrafine powder by-product obtained from silicon and ferrosilicon alloy fabrication, which maintains the shape of amorphous solid spherical particles [23,24]. Meanwhile, steel slags are the by-products of processing steel (and other iron-based alloys) in smelting ores, which are condensed and pulverized to obtain a fine powder material [25,26].

The production of PCCs consumes a massive quantity of natural aggregates (i.e., sand and gravel). In order to extract these aggregates, it is necessary to exploit quarries on a large scale. Consequently, the preceding industrial process causes significant resource consumption (i.e., energy and water), emissions to the atmosphere (e.g., carbon dioxide, nitrogen oxide, particle size less than 10 µm, sulfur dioxide, and carbon monoxide), and generation of a non-negligible amount of leachate material (e.g., mercury, lead, hazardous waste, aldehydes, and benzo[a]pyrene) [27,28]. Thus, a remarkable strategy to mitigate the depletion of natural aggregates (and thus reduce the associated environmental burdens) in the fabrication of PCCs, is to partially replace coarse aggregates with coarse RCA. Likewise, various studies found that PCC with coarse RCA contents also developed significant economic and mechanical-behaviour advantages over traditional PCC [9,10]. Typically, RCAs are obtained by recycling (i.e., crushing and sieving) the PCC at the end of its useful life [29,30]. Accordingly, RCAs can mainly be reached by demolishing old rigid pavements and buildings [31,32]. Notably, fine aggregates are generally not substituted with fine RCA because they can have counterproductive effects on the mechanical performance of the mixtures [32,33].

Although numerous research efforts have been reported in the literature on designing PCCs with SCMs or RCA contents, few studies have addressed the simultaneous incorporation of these materials; some of these remarkable case studies can be consulted in [9,10,34]. However, these investigations present a limited scope; i.e., the design procedure is based on trial-and-error experimental tests that fail to maximize the sustainability components of these technologies. The preceding reveals a gap in the literature. Accordingly, to improve the current state-of-the-art, this study presents a novel mathematical model for designing sustainable PCC mixes, incorporating budget constraints.

The model presented in this work arises from the need to create PCC mixes that are operationally efficient, environmentally friendly, and budget-friendly. Utilizing Life Cycle Assessment (LCA) and Life Cycle Costs Analysis (LCCA) methodologies, this study evaluates three different SCMs: fly ash, silica fume, and steel slag. A case study in the northern region of Colombia demonstrated significant reductions in CO_2 emissions and production costs. This model not only provides a practical tool but also offers a replicable approach that can be adapted to various contexts, benefiting state agencies, engineers, suppliers, and other stakeholders in adopting more sustainable practices in concrete production.

The following sections of this manuscript are explained below. Section 2 presents a brief overview of the LCA and LCCA methodologies. Then, in Section 3, the linear programming model proposed to design PCCs is developed. In Section 4, the simulation results obtained through a computational tool (i.e., the so-called *OptiCon*) are shown and described. Afterward, Section 5 discusses the optimization proposal and its outcomes. Meanwhile, Section 6 exhibits the main conclusions of this investigation and recommends some future research lines.

2. Background

The search for sustainable development in the civil infrastructure sector has led many researchers to explore ways to modify traditional materials [35,36]. In this way, it is necessary to estimate the sustainable performance of these novel materials. For these purposes, two methodologies stand out, i.e., the LCA and LCCA [28,30]. Notably, both methodologies can analyze a material (and even products, projects, services, processes, or activities) under an entire life cycle or for selected stages [37,38]. Specifically, the LCA assesses the environmental impacts, whilst the LCCA evaluates the monetary costs [39].

LCA and LCCA are versatile decision-making tools that have been used successfully as a theoretical basis for developing design optimization software/frameworks, e.g., ref. [40] publicly released "*WMA-RCA PEIC*" to estimate the environmental impact of warm mix asphalts. Meanwhile, refs. [41–43] created "*OPTIPAV*" to compute the profitability of economic investments for pavement management. Remarkably, refs. [44,45] conceived "*CONCRETop*" to optimize the inclusion of RCA and fly ash in PCCs under a comprehensive standpoint (i.e., considering mechanical, environmental, and economic criteria). Another interesting approach was that proposed by [46], an investigation in which the authors used genetic algorithms to achieve an LCA–LCCA integration to establish the optimal dosages of raw materials in the fabrication of eco-friendly asphalt mixtures.

Following this research path, this investigation uses an LCA–LCCA integration as the foundation of the sustainability criteria within the linear programming approach. Hence, it is necessary to describe these methodologies adequately. Thus, the basics of LCA and LCCA are explained below.

2.1. LCA Methodology

According to the International Organization for Standardization (ISO), the LCA is a standardized methodology that can be used for the following purposes [37,38]: (i) to estimate the potential environmental impacts of activities, materials, processes, products, projects, and services; (ii) to recognize possibilities of enhancing environmental performances; (iii) to inform decision-makers and other stakeholders on planning for a sustainable strategy; (iv) to establish an appropriate indicator regarding environmental behaviour; (v) to generate an environmental product declaration and other types of environmental claims; and even, (vi) to implement an ecolabelling scheme in marketing campaigns. Currently, the standards that regulate the implementation of LCAs worldwide are ISO-14040 and ISO-14044 [37,38]. On the one hand, the ISO-14040 standard specifies the principles and frameworks related to LCAs. On the other hand, the ISO-14044 standard establishes the minimum requirements and general guidelines for LCA execution. Notably, the most relevant aspect of these regulations is the specification that an LCA must be composed of the subsequent four phases [37,38]:

- Goal and scope definition phase: in this step, it is required to define the goal, system description, boundaries, functional unit, and data source. Hence, this phase specifies the assessment's depth and level of detail. All these aspects must be in accordance with the objectives of the study.
- Life Cycle Inventory (LCI) analysis phase: in this step, it is necessary to establish the LCI according to the previously defined system boundaries. In this way, the LCI must collect the input and output data associated with the raw materials, energy, distances, residues, by-products, pollutants, and other important information.
- Life Cycle Impact Assessment (LCIA) phase: in this step, selecting the categories used to classify the environmental burdens is essential. This number of classes can be from 1 (usually, the global warming potential, which is the CO_2 equivalent emitted into the atmosphere) to higher than 10.
- Interpretation phase: in the final step, the environmental impacts are calculated following the previously defined LCI and LCIA. Likewise, the results are examined under a suitable statistical approach. Notably, the only compulsory analysis is the characterization (i.e., the report of the resultant magnitude for each impact category). Meanwhile, normalization, grouping, weighting, and data quality analysis are optional.

The other valuable guideline for the LCA execution is the framework released by the Federal Highway Administration (a state agency of the U.S. federal government) [47]. The main contribution to the literature of this manual is the establishment of four approaches to defining the system boundaries (especially planned for the civil infrastructure sector): cradle-to-gate, cradle-to-site, cradle-to-laid, and cradle-to-grave. Figure 1 shows the description of these approaches. The preceding is essential because the proper choice of a system boundaries approach can affect the consistency of the results and their harmony with the appointed objectives [37,38].

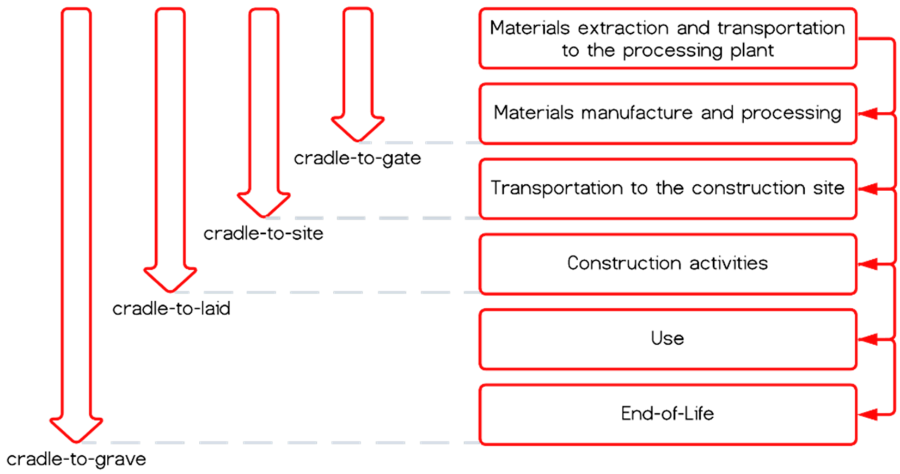

Figure 1. System boundaries suggested by the Federal Highway Administration. Adapted from: [28,48].

2.2. LCCA Methodology

The LCCA (also known as Life Cycle Costing, LCC) is an objective methodology to compute and manage the monetary costs of activities, materials, processes, products, projects, and services throughout its life cycle (whether in whole or in part) [49,50]. The LCCA is older than the LCA; however, it has had less time to be standardized. The ISO 15686-5 standard is the international regulation for the LCCA [39]. Thus, the LCCA can assess the cost-effectiveness of different alternatives considering all the cash flow (i.e., capital inflows and outflows) in a specific analysis period [51,52]. Consequently, the LCCA employs several financial indicators to integrate the user and agency costs at a precise accounting point (in time), i.e., generally the "year zero" [53,54]. Notably, the most typical financial indicators are the net present value, residual cost, benefit/cost ratio, internal rate of return, and equivalent uniform annual cost [55,56]. Overall, when an LCCA is developed parallel to an LCA, the same system boundaries and functional units are often adopted [28,30]. In other words, LCCAs are easily integrated with LCAs [57,58]. The preceding comprises the main advantage of the LCCA over other economic/financial techniques.

3. Linear Programming Model

This study develops a mixed-integer linear programming model to design eco-friendly PCCs under budgetary constraints. In this way, the objective of this model is to minimize the CO_2 emissions and the production costs associated with PCC fabrication. For these purposes, two technologies were simultaneously addressed: (i) partially replace the PC with three SCMs (fly ash, steel slag, and silica fume); and (ii) partially replace the coarse aggregates with coarse RCA. Notably, considering the goal of this study, the cradle-to-gate approach was followed. Tus, the estimation of environmental impacts and production costs only take into account three stages, i.e., raw materials extraction/production, materials transport to the concrete plant, and mixture production. Figure 2 shows the system boundaries handled. On the other hand, it is well known in the literature that transportation distances for raw materials are crucial to estimating sustainability performance [27,28]. Hence, typical distances between suppliers and the concrete plant are assumed in order to obtain accurate outcomes. Below, the proposed linear programming model is described in detail. Thus, the mathematical components that simulate the LCA, LCCA, and the dosage restrictions that guarantee the designed PCCs develop outstanding mechanical performance are explained. For all purposes, a functional unit defined as 1 m^3 of PCC (produced in a traditional concrete plant) is considered.

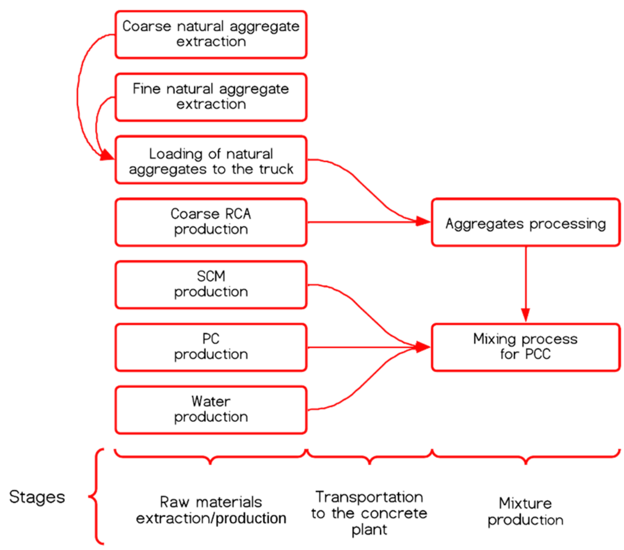

Figure 2. System boundaries addressed in this study.

3.1. LCA-Based Objective Function and Variables

The model proposed by this study considers three types of values: decision variables, parameters, and user-inserted values. On the one hand, the decision variables are those that correspond to the amount (in tons) of each material required to produce 1 m^3 of PCC. In this way, the following nomenclature is followed: tons of SCM i per m^3 of concrete (x_i), tons of PC per m^3 of concrete (P), tons of gravel per m^3 of concrete (G), tons of RCA per m^3 of concrete (R), tons of sand per m^3 of concrete (S), tons of water per m^3 of concrete (W), tons of admixture j per m^3 of concrete $\left(y_j\right)$. On the other hand, the parameters considered are CO_2 emissions (tons) per ton of SCM i (α_i), CO_2 emissions (tons) per ton of PC (e_P), CO_2 emissions (tons) per ton of gravel (e_G), CO_2 emissions (tons) per ton of RCA (e_G), CO_2 emissions (tons) per ton of sand (e_S), CO_2 emissions (tons) per ton of water (e_W), CO_2 emissions (tons) per ton of admixture j $\left(\delta_j\right)$ and tons of emitted CO_2 per ton*kilometer (i.e., tkm) of the mean of transportation k (E_k). Meanwhile, the user-inserted values are the amount of concrete in m^3 (a), the linear distance between the supplier of SCM i and the concrete plant in km (θ_i), the linear distance between the supplier of PC and concrete plant in km d_P, the linear distance between the supplier of Gravel and concrete plant in km d_G and the linear distance between the supplier of RCA and concrete plant in km d_R. Table 1 describes all the decision variables, parameters, and user-inserted values.

Table 1. Description of all variables of the model.

Symbol	Description	Unit
a	Amount of required concrete	m^3
x_i	tons of SCM i per m^3 of concrete	ton
P	tons of PC per m^3 of concrete	ton
G	tons of gravel per m^3 of concrete	ton
R	tons of RCA per m^3 of concrete	ton
S	tons of sand per m^3 of concrete	ton
W	tons of water per m^3 of concrete	ton
y_j	tons of admixture j per m^3 of concrete	ton
z_i	Usage of SCM i (1 if yes; 0 otherwise)	-
α_i	CO_2 emissions per ton of SCM i	-
e_p	CO_2 emissions per ton of PC	ton
e_G	CO_2 emissions per ton of gravel	ton
e_R	CO_2 emissions per ton of RCA	ton
e_S	CO_2 emissions per ton of sand	ton
e_S	CO_2 emissions per ton of water	ton
δ_j	CO_2 emissions per ton of water	ton
e_{mp}	CO_2 emissions per m^3 of concrete due to the mixing process	ton
Z_{min}	CO_2 emissions per m^3 of concrete	ton
E_k	emitted CO_2 per tkm of the mean of transportation k	ton
θ_i	linear distance between the supplier of SCM i and concrete plant	km
d_P	linear distance between the supplier of PC and concrete plan	km
d_G	linear distance between the supplier of Gravel and concrete plant	km
d_R	linear distance between the supplier of RCA and concrete plant	km
w/b_{min}	Minimum water–binder ratio	-
w/b_{max}	Maximum water–binder ratio	-
β_{01}	The intercept of the Linear Regression Model (LRM) for coarse aggregate	-

Table 1. *Cont.*

Symbol	Description	Unit
β_{11}	The slope of the LRM for coarse aggregate	-
β_{02}	The intercept of the LRM for sand	-
β_{12}	The slope of the LRM for sand	-
τ_i	density of SCM i	tons/m^3
ρ_P	density of PC	tons/m^3
ρ_G	density of gravel	tons/m^3
ρ_R	density of RCA	tons/m^3
ρ_S	density of sand	tons/m^3
ε_j	Minimum dosage (decimal) of admixture j	-
φ_j	Maximum dosage (decimal) of admixture j	-
γ_i	Maximum replacement fraction of SCM i	-
μ	Maximum replacement fraction of RCA	-
ϑ_i	estimated cost per ton of SCM i	US dollars
C_P	estimated cost per ton of PC	US dollars
C_G	estimated cost per ton of gravel	US dollars
C_R	estimated cost per ton of RCA	US dollars
C_S	estimated cost per ton of sand	US dollars
C_W	estimated cost per ton of water	US dollars
σ_j	estimated cost per ton of admixture j	US dollars
ω_k	estimated cost per tkm in means of transportation k	US dollars
q	Other transport-related costs	US dollars
b	Budget for concrete	US dollars

Equation (1) presents the mathematical model that defines the proposed objective function, i.e., minimizing CO_2 emissions (under budget restrictions). The terms of this equation are explained below. First, the sum of emissions due to production includes the sum of the emissions of the n supplementary cementing materials ($\sum_{i=1}^{n}(\alpha_i x_i)$), the individual contributions of PC ($e_P P$), gravel ($e_G G$), RCA ($e_R R$), sand ($e_S S$) and water ($e_W W$), and, lastly, the sum of the emissions due to the production of the m admixtures (($\sum_{j=1}^{m}(\delta_j y_j)$).

Meanwhile, the second part of Equation (1) refers to emissions related to transportation. It should be noted that the unit of the mean for transport is expressed in tkm, so to obtain the full impact it must be multiplied by the length and weight. $\theta_i x_i$ is the multiplication of the weight and distance to travel of each SCM; likewise, $d_P P$, $d_G G$ and $d_R R$ are the multiplication of the weight and the distance to travel of PC, gravel, and RCA, respectively. All of this is then multiplied by the emissions of the o means of transportation ($\sum_{k=1}^{o} E_k$). In the second part of the equation, a component should only be multiplied by the correspondent mean(s) of transportation. Notably, the transportation of non-replaceable materials is not considered for this study since their election is fixed and does not depend on the distance between the supplier and the concrete plant, as occurs with their counterpart. It should be noted that this objective function is based on the LCA methodology, in which all individual environmental contributions are summarized to obtain the total environmental impact [37,38].

Finally, the e_{mp} constant represents the CO_2 emissions generated by the mixing process stage. In previous investigations [27,28], it was determined that (i) the mixing process of 1 m^3 of PCC generates an energy consumption of 1287 MJ (differences in the mix design have a negligible effect on this value); (ii) for every 1 MJ of energy consumed, 95.3 g of CO_2 emissions are generated; and (iii) therefore, the e_{mp} constant takes a value of 0.123 ton-CO_2 per m^3 of PCC. Thus, e_{mp} is a constant equally applicable to all possible PCC designs; then, the stage of the mixing process will be excluded from further analysis. Hence, the rest of the manuscript focuses on evaluating the other two stages, i.e., raw materials extraction/production and transportation to the concrete plant.

$$Z_{min} = a\left(\sum_{i=1}^{n}(\alpha_i x_i) + (e_P P) + (e_G G) + (e_R R) + (e_S S) + (e_W W) + \sum_{j=1}^{m}(\delta_j y_j) + \sum_{k=1}^{o} E_k\left(\sum_{i=1}^{n}(\theta_i x_i) + (d_P P) + (d_G G) + (d_R R)\right) + e_{mp}\right) \quad (1)$$

3.2. Mechanical Performance Constraint

One of the main concerns of the model is that it should be able to ensure the compressive strength of the generated mixture as the first indicator of functionality, which is represented in the model by Equation (2). This equation is based on Abram's Law (Equation (2)), which states that the compressive strength of PCC has an inverse relation to the water–binder ratio (*w/b* ratio, i.e., the amount of water divided by the sum of all cementing materials) [59–61]. Thus, the smaller the *w/b* ratio, the greater the compressive strength [62,63]. It is essential to highlight that, although the *w/b* ratio is not the only variable that influences the strengths of PCC, it is one of the most important factors to consider [4,64]. Therefore, this parameter is used as the central axis of the mechanical performance constraint. No additional or derived variables have been included to avoid introducing unnecessary complexity to the model. Regardless, it is worth mentioning the other factors that significantly affect the strengths of PCC beyond mix proportions, such as binder types and compositions, aggregate properties, chemical compatibility of raw materials, degree of compaction, curing conditions, and even environmental exposures [65–68].

$$\frac{w}{b}_{min}\left(\sum_{i=1}^{n}(x_i) + P\right) \le W \le \frac{w}{b}_{max}\left(\sum_{i=1}^{n}(x_i) + P\right) \quad (2)$$

$$strength = \frac{K_1}{K_2^{\frac{W}{b}}}, \ where\ K_1\ and\ K_2\ are\ constants \quad (3)$$

Due to the fact that constants K_1 and K_2 are related to the time elapsed before testing, it can be inferred that any mixture with the same *w/b* ratio will have the same strength if tested after the same time-lapse. Equation (3) also defines a range of *w/b* ratios to restrain the solution to a specific compressive strength value, according to the values given by the water–binder ratio curve. The preceding means that the amount of water divided by all cementing materials should be contained between a lower and upper limit. The equation is cleared since all constraints must be linear to fit the mixed integer linear programming model. The amount of cementing material now multiplies both the lower and upper bound of the *w/b* ratio.

3.3. Material Proportion Constraints

The model can bring water and cementing materials into the mix by restraining the water and binder ratio. Nevertheless, it must also add coarse and fine aggregates and admixtures in suitable proportions. Fixed proportions for conventional PCC exist but, by analyzing several concrete mixtures designed by [9,10], in which SCMs and RCA are included simultaneously, it was noted that these proportions could not be followed. Therefore, several statistical analyses were made to find a dependent variable(s) that can predict the contents of coarse and fine aggregates in such mixes. It was then found that the total volume of cementing materials could most accurately predict the volume of coarse and fine aggregates through Linear Regression Models (LRMs), which are compatible with the mixed integer linear programming model that this study proposes. Respectively, Equations (4) and (5) are the LRM proposed structure for coarse and fine aggregates. Thus, the model should be trained first with a set of previously designed mixes that integrate the same materials as the mixes to be generated.

β_{01} and β_{11} are the intercept and slope, respectively, of the LRM that predicts the required amount of coarse aggregate. Likewise, β_{02} and β_{12} have the same meaning for the LRM that predicts the required amount of sand. Other parameters that are introduced are the density of SCM i in tons/m^3 (τ_i), the density of PC in tons/m^3 (ρ_P), the density of gravel in tons/m^3 (ρ_G), the density of RCA in tons/m^3 (ρ_R) and the density of sand in tons/m^3 (ρ_S).

$$\beta_{01} + \beta_{11}\left(\sum_{i=1}^{n}\left(\frac{x_i}{\tau_i}\right) + \left(\frac{P}{\rho_P}\right)\right) = \left(\frac{G}{\rho_G}\right) + \left(\frac{R}{\rho_R}\right) \quad (4)$$

$$\beta_{02} + \beta_{12}\left(\sum_{i=1}^{n}\left(\frac{x_i}{\tau_i}\right) + \left(\frac{P}{\rho_P}\right)\right) = \frac{S}{\rho_S} \quad (5)$$

On the other hand, admixtures are chemical solutions added to the mixture immediately before or during mixing to modify the properties of concrete (fresh or hardened) [69,70]. The manufacturers determine the optimal dosage of these substances as proportions based on the contents of cementing materials. Usually, it is not a fixed amount but presented with a lower and upper bound [71,72]. Considering these conditions, Equation (6) is proposed as the optimal dosage range for admixtures, where ε_j is the minimum dosage (decimal) of admixture j and φ_j is the maximum. Regarding the constraints, it should be noted that admixtures are not limited because their volume is insignificant for the concrete mix. Once again, the equation must be linear, and the density is raised to the power of minus one; the density of water is dismissed, since it is 1 ton/m^3. Equation (7) represents this constraint.

$$\varepsilon_j\left(\sum_{i=1}^{n}(x_i) + P\right) \leq\ y_j \leq \varphi_j\left(\sum_{i=1}^{n}(x_i) + P\right),\ for\ j = 1, 2, \ldots, m \quad (6)$$

$$\sum_{i=1}^{n}\left(x_i \tau_i{}^{-1}\right) + \rho_P{}^{-1}P + \rho_G{}^{-1}G + \rho_R{}^{-1}R + \rho_S{}^{-1}S + W = 1\ \left(m^3\right) \quad (7)$$

3.4. Replacement Percentage Constraints

Respectively, neither SCMs nor coarse RCA can be used as a 100% replacement for PC or gravel; thus, the model should restrain the amounts added to the mix. Previous studies have determined the optimal replacement ratios for both cases, SCMs and RCA [73,74]. These investigations state that these materials should not be used beyond a fixed percentage. For instance, for one given SCM, the amount added divided by the sum of all cementing materials should be less than or equal to a constant, as expressed in Equation (8), where γ_i is the maximum replacement fraction of the SCM i. Meanwhile, for RCA, the equation is modified as in Equation (9) with the corresponding variables; in this case μ is the maximum replacement fraction of RCA.

$$(1 - \gamma_i)x_i \leq \gamma_i P\ ,\ for\ i = 1, 2, \ldots, n \quad (8)$$

$$(1 - \mu)\mathrm{R} \leq \mu G \quad (9)$$

3.5. Binary Constraints

Additional constraints must be included in the model to guarantee that only one SCM is used at a time. This is because using several SCMs simultaneously can generate adverse effects on the compressive strength [75–78]. In operations research, this type of constraint is known as an "either-or constraint", and the intention is to pick one option or another. In this case, the continuous variable must take either a positive value or zero for each SCM. Furthermore, if one of the SCM variables x_i takes a positive value, then all others should be zero. For this purpose, binary variables must be introduced. Considering that Equation (7) restrained the total volume of all materials to one cubic meter, it is inevitable that the amount of any given SCM will be less than one ton. Hence, Equation (10) is proposed to introduce binary variables. These binary variables z_i can take only two values: 1 if the associated continuous variable takes a positive value, i.e., the corresponding SCM is chosen, and 0 otherwise. At this point, it is still possible for more than one binary variable z_i to take a positive value, meaning that another constraint must be included to indicate that, among all binary variables, only one can take the value of 1. Finally, Equation (11) summarizes all these variables and equals their result to a lesser or equal one, meaning that either or any SCM can be chosen.

$$x_i \leq z_i \text{ , } for\ i = 1, 2, \ldots, n \tag{10}$$

$$\sum_{i=1}^{n} z_i \leq 1 \tag{11}$$

3.6. Budgetary Constraint Through LCCA

In order to estimate total production costs, the LCCA technique is implemented. For these purposes, the required total monetary investment is selected as the financial indicator. The costs considered by the proposed model are the purchase and transportation costs of all materials. a in Equation (12) is the amount of required concrete inserted by the user; the following seven terms refer to the cost of purchase of materials, where ϑ_i is the estimated cost per ton of SCM i, C_P is the estimated cost per ton of PC, C_G is the estimated cost per ton of gravel C_R is the estimated cost per ton of RCA, C_S is the estimated cost per ton of sand, W is the estimated cost per ton of water, and finally, σ_j is the estimated cost per ton of admixture j. As in the minimization target equation, the second part corresponds to the transportation costs of replaceable materials. Likewise, the transportation costs are expressed in tkm. Hence, this should be multiplied by the distance and the weight of each material to obtain the total cost. Finally, q are the other transport-related costs (i.e., transportation costs of non-replaceable materials). Non-transport-related costs can also be included in this value. The summation of all considered costs must be less or equal to the user's budget b, so it can be guaranteed that the generated mix is the best option environmentally while still being financially feasible.

$$\begin{aligned} a\Bigg(&\sum_{i=1}^{n} (\vartheta_i x_i) + (C_P P) + (C_G G) + (C_R R) + (C_S S) + (C_W W) + \sum_{j=1}^{m} (\sigma_j y_j) \\ &+ \sum_{k=1}^{o} \omega_k \left(\sum_{i=1}^{n} (\theta_i x_i) + (d_P P) + (d_G G) + (d_R R) \right) \Bigg) + q \leq b \end{aligned} \tag{12}$$

3.7. Nonnegativity Constraints

Finally, the quadrant in which the feasibility region must be found must be stated. The preceding means that the continuous variables, i.e., the amount of every material, must be greater than zero (Equations (13)–(19)), and binary variables can only take values of either 1 or 0 (Equation (20)).

$$x_i \geq 0\ \forall\ i\ \in\ n \tag{13}$$

$$P \geq 0 \tag{14}$$

$$G \geq 0 \tag{15}$$

$$R \geq 0 \tag{16}$$

$$S \geq 0 \quad (17)$$

$$W \geq 0 \quad (18)$$

$$y_j \geq 0 \, \forall \, j \, \in \, m \quad (19)$$

$$z_i \, \epsilon \, \{0, 1\} \, \forall \, i \, \in \, n \quad (20)$$

3.8. Model Training

In order to evaluate whether the model proposed reduces CO_2 emissions compared to a regular concrete mix, it is necessary to assess its performance in different case scenarios. Therefore, the first step is to choose the sample size of cases to be evaluated and, to do so, the Law of Large Numbers and the Central Limit Theorem are considered; thus, the sample is set to n = 30. The preceding means that 30 hypothetical cases will be evaluated. Then, a regular mix and an algorithmic-generated mix are designed for each case.

The model must be trained with a set of previously designed mixes that integrate the same materials as the mixes to yield. For this purpose, the 30 designs generated by [9,10] were adopted. In this regard, the SCMs used are fly ash, steel slag, and silica fume. Furthermore, RCA and admixtures (i.e., retarding plasticizer and superplasticizer) are also considered. The compressive design strength of all 30 mixes is 28 MPa. On the other hand, all transport is assumed to take place in a medium-heavy truck, i.e., a typical concrete trucks. It is important to note that the distances must be reported as one-way type (i.e., linear) for practical purposes. The bulk densities of these materials are shown in Table 2. These values were derived from prior research and field observations [9,10,28]. These values reflect the material's behaviour in bulk form, rather than its intrinsic density (i.e., specific gravity). Regardless, considering the high flexibility and adaptability of the proposed model, each user can assign representative density values for their contexts.

Table 2. Bulk densities of considered materials. Adapted from: [9,10,28].

Materials	Bulk Density (ton/m^3)
Fly Ash	1.31
Steel slag	1.21
Silica Fume	0.28
PC	1.44
Gravel NMS 3/4″	1.77
RCA 3/4″	2.39
Sand	1.60
Water	1.00
Superplasticizer	1.20
Retarding Plasticizer	1.15

Table 3 shows all the CO_2 emissions to be considered in this study, except for the retarding plasticizer, since its associated environmental impacts are negligible (at least at the typical amounts used) [28]. On the other hand, the superplasticizer admixture slightly surpasses the environmental burdens of PC. Nonetheless, this additive is employed minimally, at around 0.6–1% of the total mass of cementing materials, as suggested by [73,74]. Therefore, its global impact is also minimal compared to PC. By replacing the parameters of Equation (1) with the values in Table 3, a generic equation for CO_2 emissions of PCC, including the transportation of raw materials, is obtained (Equation (21)). The preceding expression is taken as the minimization target of the binary linear programming problem.

$$Z_{min} = a\Big(1.01\times10^{-5}x_{fly\ ash} + 6.68\times10^{-5}x_{slag} + 3.92\times10^{-5}x_{silica\ fume} + (0.93P) + (7.3\times10^{-2}G) + (1.69\times10^{-3}R) + (3.1\times10^{-3}S) + (5.7\times10^{-4}W) + \big(1.84y_{superplasticizer}\big) + (2.35\times10^{-4})\big(\theta_{fly\ ash}x_{fly\ ash} + \theta_{slag}x_{slag} + \theta_{silica\ fume}x_{silica\ fume} + (d_P P) + (d_G G) + (d_R R)\big)\Big) \quad (21)$$

Table 3. CO_2 emissions associated with PCC production. Adapted from: [79–81].

Materials	CO_2 Emissions (Emitted Ton/Ton Produced)
Fly Ash	1.01×10^{-5}
Steel slag	6.68×10^{-5}
Silica Fume	3.92×10^{-3}
PC	0.93
Gravel NMS 3/4″	7.30×10^{-2}
RCA 3/4″	1.69×10^{-3}
Sand	3.10×10^{-3}
Water	5.7×10^{-4}
Superplasticizer	1.84
Medium-heavy truck	2.35×10^{-4} (ton/tkm)

As stated earlier, the compressive strength is restrained to 28 MPa, which means that the *w/b* ratios can range from 0.4295 to 0.4975. Therefore, by replacing these parameters and the summation for the SCMs considered in Equation (3), the compressive strength constraint for this case study was obtained as Equation (22). Consequently, by analyzing the concrete mixes adopted from [9,10], two regression models were developed: one for fine aggregates (i.e., natural sand) and another for coarse aggregates (i.e., natural gravel and RCA). Figure 3 shows these models. In both cases, significant adjustments were obtained.

$$0.43\left(x_{fly\ ash} + x_{slag} + x_{silica\ fume} + P\right) \le W \le 0.50\left(x_{fly\ ash} + x_{slag} + x_{silica\ fume} + P\right) \quad (22)$$

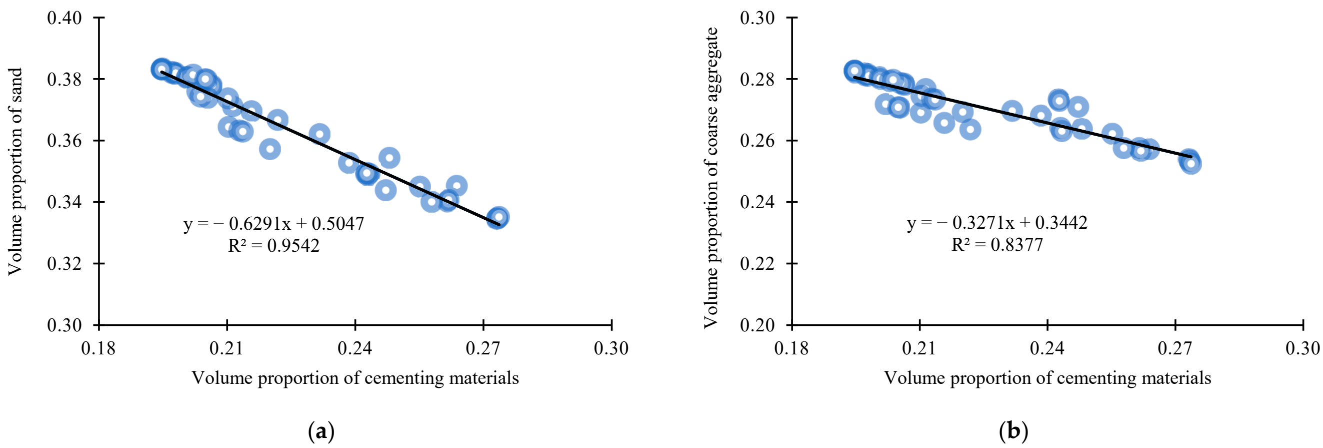

Figure 3. Adjusted models for aggregates based on the volume of cementing materials. (**a**) Regression model for fine aggregates. (**b**) Regression model for coarse aggregates.

After validating the assumptions of both linear regression models, the parameters obtained were replaced in Equations (4) and (5) for coarse aggregates (Equation (23)) and fine aggregates (Equation (24)), respectively.

$$0.50 - 0.63\left(\frac{x_{fly\ ash}}{\tau_{fly\ ash}} + \frac{x_{slag}}{\tau_{slag}} + \frac{x_{silica\ fume}}{\tau_{silica\ fume}} + \frac{P}{\rho_P}\right) = \left(\frac{G}{\rho_G}\right) + \left(\frac{R}{\rho_R}\right) \quad (23)$$

$$0.34 - 0.33\left(\frac{x_{fly\ ash}}{\tau_{fly\ ash}} + \frac{x_{slag}}{\tau_{slag}} + \frac{x_{silica\ fume}}{\tau_{silica\ fume}} + \frac{P}{\rho_P}\right) = \frac{S}{\rho_S} \quad (24)$$

In this study, the superplasticizer and retarding plasticizer were used to improve workability and retard the setting of the mix. According to [82,83], the effective dosage of superplasticizer varies from 0.6% to 1.0%, and a dose of 75–400 mL per every 100 kg of cementitious is suggested. Furthermore, a range from 0.086% to 0.460% was considered by converting this into mass. By replacing these parameters in Equation (6), the two restraint equations for admixtures are obtained: Equation (25) for superplasticizer and Equation (26) for retarding plasticizer.

$$6\times10^{-3}\left(\frac{x_{fly\ ash}}{\tau_{fly\ ash}} + \frac{x_{slag}}{\tau_{slag}} + \frac{x_{silica\ fume}}{\tau_{silica\ fume}} + \frac{P}{\rho_P}\right) \le y_{superplasticizer} \le 1\times10^{-2}\left(\frac{x_{fly\ ash}}{\tau_{fly\ ash}} + \frac{x_{slag}}{\tau_{slag}} + \frac{x_{silica\ fume}}{\tau_{silica\ fume}} + \frac{P}{\rho_P}\right) \quad (25)$$

$$8.6\times10^{-4}\left(\frac{x_{fly\ ash}}{\tau_{fly\ ash}} + \frac{x_{slag}}{\tau_{slag}} + \frac{x_{silica\ fume}}{\tau_{silica\ fume}} + \frac{P}{\rho_P}\right) \le y_{ret.\ plast} \le 4.6\times10^{-3}\left(\frac{x_{fly\ ash}}{\tau_{fly\ ash}} + \frac{x_{slag}}{\tau_{slag}} + \frac{x_{silica\ fume}}{\tau_{silica\ fume}} + \frac{P}{\rho_P}\right) \quad (26)$$

Lastly, by modifying Equation (7) to add the materials considered, the amount of concrete produced is restrained, as is reported in Equation (27).

$$x_{fly\ ash}{\tau_{fly\ ash}}^{-1} + x_{slag}{\tau_{slag}}^{-1} + x_{silica\ fume}{\tau_{silica\ fume}}^{-1} + {\rho_P}^{-1}P + {\rho_G}^{-1}G + {\rho_R}^{-1}R + {\rho_S}^{-1}S + W = 1\ \left(\mathrm{m}^3\right) \quad (27)$$

Additionally, it is necessary to develop constraints for fly ash, steel slag, silica fume, and coarse RCA. The first three are obtained by modifying Equation (8). In contrast, the constraint for RCA is obtained by replacing Equation (9). As proposed by [74], fly ash can replace up to 40% of PC (Equation (28)), steel slag can replace up to 70% of PC (Equation (29)), and silica fume can replace up to 15% of PC (Equation (30)). On the other hand, ref. [73] recommends a maximum replacement of RCA of 45% (Equation (31)).

$$\left(1 - 0.4\right)x_{fly\ ash} \le 0.4P \quad (28)$$

$$\left(1 - 0.7\right)x_{slag} \le 0.7P \quad (29)$$

$$\left(1 - 0.15\right)x_{silica\ fume} \le 0.15P \quad (30)$$

$$(1 - 0.45)\mathrm{R} \le 0.45G \quad (31)$$

For the binary constraints, Equation (16) must be modified for each SCM considered in this case study, i.e., fly ash (Equation (32)), steel slag (Equation (33)), and silica fume (Equation (34)). Likewise, Equation (17) should be adjusted as the summation of the binary variables of every SCM, as in Equation (35).

$$x_{fly\ ash} \le y_{fly\ ash} \quad (32)$$

$$x_{slag} \le y_{slag} \quad (33)$$

$$x_{silica\ fume} \leq y_{silica\ fume} \tag{34}$$

$$y_{fly\ ash} + y_{slag} + y_{silica\ fume} \leq 1 \tag{35}$$

Regarding the budgetary constraint, each case is different depending on the suppliers. Thus, several suppliers for all replacement materials were surveyed (national and international); then, prices per ton and linear distance from the supplier to the concrete plant (taking as reference the northern region of Colombia) were documented. Suppliers were intentionally selected so that different scenarios could be evaluated to determine whether the selection of SCMs or RCA is distance sensitive. In addition, prices for sand, water, superplasticizer, and retardant were also quoted, but the supplier was consistently fixed in all 30 cases as these are not relevant materials for this study.

The first 10 cases were built upon assuming that all materials suppliers were foreigners. Another 10 cases were simulated as if suppliers of replacement materials were foreigners and conventional materials were local. All suppliers were local in the last 10 cases. For practical purposes, a case will be understood as the unique combination of supplier conditions for every material considered in this study, i.e., case number one is built under the assumption that all suppliers are foreigners. Therefore, the costs and distances of all materials (i.e., replaceable and non-replaceable) correspond to foreign suppliers, which differs from case number two. Other transportation costs were not included, and the amount of concrete needed was fixed to 1 m^3.

To determine the value of the budgetary constraint, in each case a regular concrete mix was built, and the costs (as well as the emissions) were calculated and later used as budge (b). Besides the 30 algorithmic-generated cases, 30 cases of regular concrete mixes in equal conditions were also built to make comparisons. In order to calculate the average cost of transportation, FCL and LCL shipping costs with different weights and volumes, also from different origins and destinations, were quoted. Then, the total price was divided by distance and weight, obtaining the price per tkm. Finally, an average of all these values was calculated to get a cost of USD 0.0739 per tkm. The preceding will be taken as the value of the c_t parameter. Thus, the final constraint is defined as Equation (36).

$$\begin{aligned}\Big(\vartheta_{fly\ ash}x_{fly\ ash} &+ \vartheta_{slag}x_{slag} + \vartheta_{silica\ fume}x_{silica\ fume} + (C_P P) + (C_G G) + (C_R R) + (C_S S) + (C_W W) \\ &+ \sigma_{superplasticizer}y_{superplasticizer} + \sigma_{ret.plast}y_{ret.plast} \\ &+ \$0.0739\Big(\theta_{fly\ ash}x_{fly\ ash} + \theta_{slag}x_{slag} + \theta_{silica\ fume}x_{silica\ fume} + (d_P P) + (d_G G) + (d_R R)\Big)\Big) \leq b\end{aligned} \tag{36}$$

3.9. Software Release

Using the Python 3.9 programming language, all the equations, mathematical expressions, constraints, and model training results were integrated into a single graphical user interface, thus developing the so-called *OptiCon* software. The model was programmed and solved using the PuLP library, which employs CBC (COIN-OR Branch and Cut) solver by default for linear programming problems. Branch and Cut is a method of combinatorial optimization used to solve integer linear programming problems through the Branch and Bound algorithm and the cutting planes method to satisfy all constraints [84–86]. It is worth highlighting that Tkinter was utilized as the primary library for designing/assembling the associated graphical user interface. Figure 4 shows a screenshot of *OptiCon*. The authors are willing to share this software upon request in order to contribute to the evolution of the state-of-the-art.

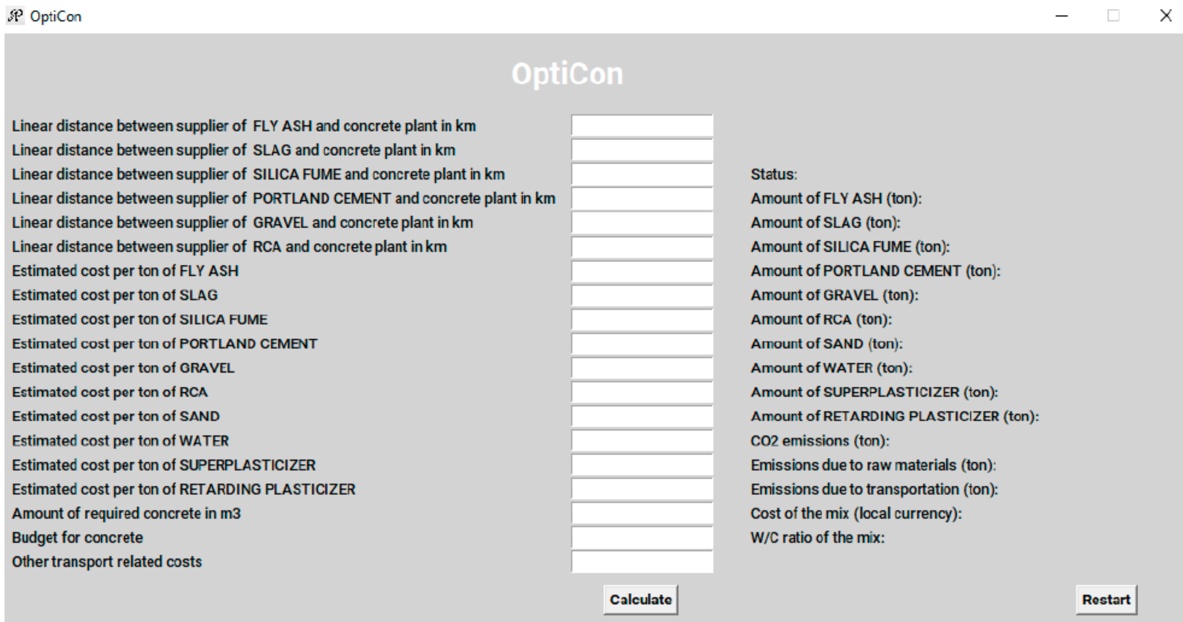

Figure 4. *OptiCon*'s graphical user interface.

4. Simulation Results

In order to evaluate the capabilities of the proposed mathematical-based model, 30 cases were analyzed. In these cases, the price and distance conditions of the raw materials varied as follows:

- Cases type I: In 10 cases, foreign suppliers were considered for all materials.
- Cases type II: In 10 cases, foreign suppliers were considered for SCMs, and local suppliers were considered for the relevant conventional materials (PC and gravel).
- Cases type III: In 10 cases, local suppliers were considered for all materials.

It must be noted that RCA was always quoted from local suppliers. Furthermore, in 14 of the 30 cases that were simulated, silica fume was the chosen SCM, and in the remaining cases this was steel slag. The preceding means that fly ash was never the most appropriate alternative. The data associated with the environmental impacts and production costs were collected during this step. Subsequently, a statistical analysis of the environmental and financial performance of algorithmic-generated mixes was conducted. For these purposes, a Mann–Whitney–Wilcoxon test was performed with $\alpha = 0.05$. Regarding the CO_2 emissions, the hypotheses to be evaluated are shown in Equation (37).

$$\begin{aligned} H_o &: \mu_{emissions\ conventional} = \mu_{emissions\ opticon} \\ H_1 &: \mu_{emissions\ conventional} > \mu_{emissions\ opticon} \end{aligned} \tag{37}$$

The Mann–Whitney–Wilcoxon test delivered a Z value of 3.08; hence p-value $= 1.03 \times 10^{-3}$. With this result, it can be affirmed that the average CO_2 emissions of conventional PCCs are statistically more significant than those of the mixtures obtained with the model proposed by this study, thus validating that it achieves its target. Figure 5 exhibits the comparison between the emissions of both types of PCCs. In all scenarios analyzed, emissions from standard concrete mixes consistently exceeded those of algorithm-generated mixes, with the disparity being most pronounced when all suppliers were foreigners.

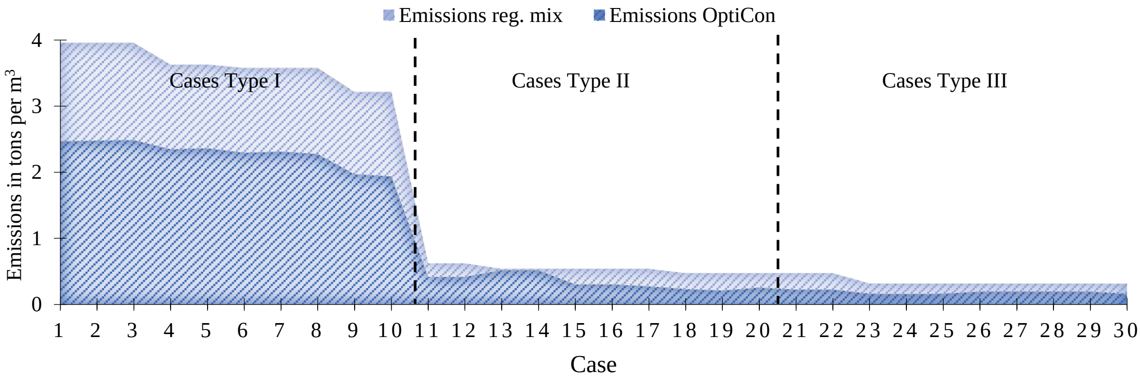

Figure 5. Comparison of CO_2 emissions between the proposed scenarios.

Regarding the sources of the emissions of the algorithmic-generated mixes, transportation represents a significant percentage of the total emissions, especially in type I cases, but also in type II and some of type III. For instance, in the 30 cases that were simulated, transportation alone provided (on average) 47% of the total emissions and up to 89% in type I. The preceding information is plotted in Figure 6.

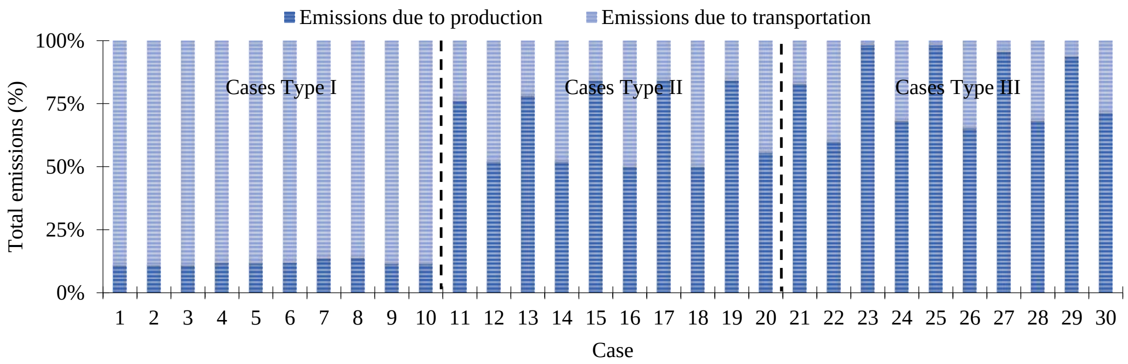

Figure 6. Comparison of sources of emissions between the proposed scenarios.

Regarding the emissions due to the production process, the algorithmic-generated mixes reduced an average of 66% and up to 76% of emissions compared to the conventional PCCs, as seen in Figure 7.

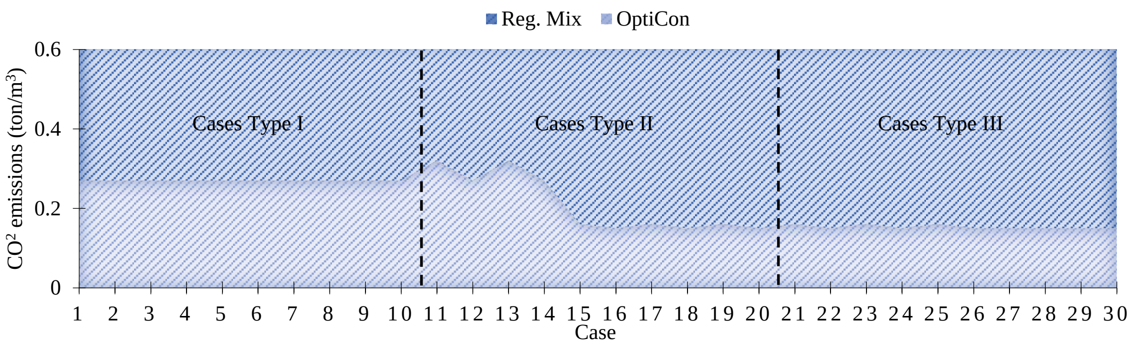

Figure 7. Comparison of emissions due to production.

Besides the environmental analysis, a financial analysis was carried out. The cost of conventional PCCs calculated as a budgetary constraint was now used to prove if there was an economic benefit of using *OptiCon* as a design tool. The cost of the conventional and algorithmic-generated mixes was compared by performing a Mann–Whitney–Wilcoxon test. Equation (38) presents the hypothesis for testing; once again, a value of $\alpha = 0.05$

was used. Consequently, the Mann–Whitney–Wilcoxon test delivered a Z value of 3.10; hence p-value $= 9.77 \times 10^{-4}$. With this result, it can be stated that the average cost of conventional concrete mixes is statistically more significant than that of the mixes obtained with the proposed mathematical/computational model. Figure 8 exhibits the financial difference between traditional and algorithmic-generated mixes; once again, the gap gets smaller when suppliers are local. Although reducing costs is not the solution's target, a financial benefit is obtained, since SCMs and RCA are residues and, therefore, cheaper than newly extracted/produced raw materials.

$$\begin{aligned} H_o &: \mu_{cost\ conventional} = \mu_{cost\ opticon} \\ H_1 &: \mu_{cost\ conventional} > \mu_{cost\ opticon} \end{aligned} \quad (38)$$

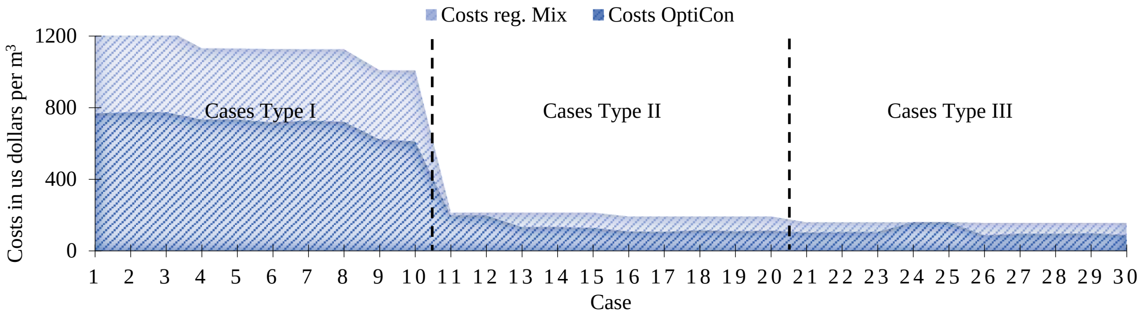

Figure 8. Comparison of costs per m^3 between the proposed scenarios.

5. Discussion

The 30 cases observed an average reduction of 39.74% in CO_2 emissions and 33.87% in production costs. An SCM was chosen in all cases, with steel slag being the most suitable alternative. To further explore this, the last ten cases were simulated again, omitting the possibility of using steel slag, and in all these cases, silica fume was selected. Thus, the amount needed of the other SCMs is reduced by a smaller density, reducing the environmental impacts associated with PCC fabrication.

A significant result is that replacing a PC with an SCM was preferable in all cases, even when the SCM suppliers' distances were greater than those of PC suppliers. Furthermore, the selection of the SCM is heavily influenced by how far the supplier is located from the concrete plant. Figures 5–8 show that the material transportation stage significantly impacts both environmental and financial performance. For instance, silica fume was chosen in type I cases since distances were smaller than other SCMs, and the amount used was considerably smaller, thus reducing emissions and costs. Conversely, in type II cases, both the emissions and costs dropped massively, showing that most of the environmental burdens and costs in type I cases are due to transportation and not to the materials extraction/production stage. Notably, in this category, there are also two cases (i.e., cases 13 and 14) with similar results for CO_2 emissions.

Meanwhile, type III cases achieve more satisfactory sustainability within 30 cases. Remarkably, when choosing local suppliers, the emissions due to transportation are reduced. However, it is also possible to reduce PC usage even more, as it is possible to use more of the chosen SCM, obtaining eco-friendly PCC designs. Because of this, it is recommended that local suppliers are preferred when the quality of materials is not compromised.

Regarding transportation means, all transport was assumed to be made by medium-heavy trucks regardless of the length or actual means of transportation that should be used (e.g., a ship for intercontinental travel and a truck for local travel). Since emissions for medium-sized ships or heavy trucks are less than those of medium-heavy trucks, actual emissions could be slightly lower than those calculated with this assumption. On the other hand, comparing the magnitudes of CO_2 emissions generated throughout the PCC production process, it is clear that the mixing process stage generates an insignificant environmental impact (i.e., only 0.123 ton-CO_2 per m3 of PCC) compared to the two other stages (i.e., raw materials extraction/production and transportation to the concrete plant).

It is essential to recognize that this mathematical model is only a decision-making support tool; thus, the user must perform experimental validation. This is because the quality of the raw materials governs the mechanical behaviour of the PCCs. Other aspects that should be addressed experimentally are the mixing, placing, compaction, and curing processes. Otherwise, it cannot be guaranteed that the PCC design obtained with the model can meet the minimum technical requirements established by state agencies.

In light of the above, the study's findings underscore the critical role of integrating sustainability considerations into the design of PCC mixes. The novel mathematical model developed in this research provides a robust framework for optimizing both the environmental and economic aspects of PCC production. Several key strengths of the mathematical model are highlighted below:

- The model effectively demonstrates how the partial replacement of PC with SCMs, such as steel slag and silica fume, can significantly reduce CO_2 emissions. This finding is crucial as it addresses the high environmental burden associated with PC, which is the most detrimental component of emissions.
- Incorporating budget constraints into the model ensures that the proposed sustainable mixes are environmentally friendly and economically feasible. The cost analysis showed that using SCMs and RCA can lead to substantial cost savings, making the adoption of these materials more attractive to stakeholders.
- The model's flexibility in adapting to various contexts and scenarios is one of its major strengths. It can accommodate different combinations of SCMs and RCA and adjust for varying transportation distances and material costs. This adaptability makes it applicable in diverse geographical and economic settings.
- The mathematical model enables precise optimization of material proportions, ensuring that the mixes meet specific performance criteria while minimizing environmental and economic costs. This approach goes beyond the traditional trial-and-error methods, providing a more systematic and efficient way to design sustainable PCC mixes.
- Integrating LCA and LCCA methodologies within the model ensures a comprehensive evaluation of both environmental and economic impacts. This dual approach allows for a more balanced and informed decision-making process.
- The model's structured approach and reliance on well-established LCA and LCCA methodologies mean that other researchers and practitioners can replicate and adapt it. This potential for replication enhances its value as a tool for advancing sustainable practices in the construction industry.
- The analysis highlights the significant impact of transportation distances on both costs and emissions. The model's ability to factor in these distances provides critical insights into how to strategically source materials to optimize sustainability outcomes.

Thus, the mathematical model presented in this study offers a powerful tool for designing sustainable PCC mixes. Its strengths lie in its ability to reduce environmental impacts, ensure economic feasibility, adapt to various contexts, optimize material use, and provide a comprehensive and replicable framework for sustainable concrete production. By addressing the limitations of traditional design methods, this model represents a significant advancement in the field of sustainable construction materials.

6. Conclusions

This research presents a novel mathematical model for designing sustainable PCC mixes, incorporating budget constraints and using an algorithm to operationalize the method. The main conclusions that this study determined are presented below:

- Under a cradle-to-gate approach, the mixing process is the stage that generates the smallest environmental burden in PCC production. Meanwhile, the raw materials extraction/production stage carries most of the contaminating potential. Thus, the transportation stage is located in the intermediate position.
- Hauling distances of raw materials are critical to computing the economic profitability and environmental impacts of PCC production. Thus, examining strategies to reduce transport distances is essential to increasing the industry's sustainability.
- PC is the raw material that generates the most elevated environmental detriments. Hence, partially replacing PC with SCMs is crucial to optimization of sustainability criteria. Furthermore, even the use of SCMs acquired at a considerably greater haulage distance than PCs has been shown to continue generating economic–environmental benefits.
- Among the three SCMs evaluated, the steel slag yielded the most satisfactory performance (in terms of cost-effectiveness and environmental burden), followed by silica fume. Otherwise, fly ash was the most suitable alternative in none of the scenarios evaluated.
- Although replacing coarse aggregates (gravel) with coarse RCA does lead to improvements in sustainability benchmarks, these advantages are minuscule compared to the other technique (reducing PC consumption).
- The proposed mathematical model is a high-capacity tool that enables a wide range of eco-friendly PCC designs. The versatility of this model allows for the simultaneous consideration, analysis, and definition of numerous potential scenarios, offering a replicable approach adaptable to various contexts.
- This model provides both a practical tool and a theoretical framework that can benefit state agencies, engineers, suppliers, and other stakeholders in adopting more sustainable practices in concrete production.
- Finally, it is worth highlighting that *OptiCon* offers significant flexibility, allowing users to easily incorporate additional SCMs based on regional availability, project requirements, or specific preferences. While fly ash, silica fume, and steel slag were chosen for their typical and readily available nature in Colombia, the software's adaptable framework ensures compatibility with other SCMs, such as mineral powder, red mud, and even nanomaterials.

Future Research Lines

In order to improve this investigation, the following recommendations are proposed to be addressed in future research lines: (i) develop a new objective function to allow the simultaneous minimization of additional environmental impact categories (e.g., acidification, carcinogenic, ecotoxicity, eutrophication, fossil fuel depletion, non-carcinogenic, ozone depletion, respiratory effects, and smog); (ii) consider other aspects related to chemo-mechanical behaviour, e.g., alkali–silica reaction, slump, and tensile strength; (iii) provide the possibility for users to choose between several financial indicators (e.g., benefit/cost ratio, equivalent uniform annual cost, internal rate of return, net present value, and residual cost) to conduct the optimization process; (iv) assess the feasibility of using other construction residues (e.g., asphalt shingles, crumb rubber, masonry bricks, reclaimed asphalt pavement, and waste glass) as a partial replacement for natural aggregates; (v) incorporate different means of transportation to model the hauling of raw materials; (vi) include a graphical sensitivity analysis within the outputs received by users; and (vii) utilize a genetic algorithm approach (or another artificial intelligence branch) to enhance the software execution.

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Data Availability Statement: Some or all of the data, models, or code supporting this study are available from the corresponding author upon reasonable request.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CBC	COIN-OR Branch and Cut
CO_2	Carbon dioxide
ISO	International organization for standardization
LCA	Life cycle assessment
LCC	Life cycle costing
LCCA	Life cycle costs analysis
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LRMs	Linear regression models
PC	Portland cement
PCC	Portland cement concrete
RCA	Recycled concrete aggregate
SCMs	Supplementary cementitious materials

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