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Data-driven optimization tool for the functional, economic, and environmental properties of blended cement concrete using supplementary cementitious materials

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A R T I C L E I N F O

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A B S T R A C T

The need to produce more sustainable concrete is proving imminent given the rising environmental concerns facing the industry. Blended cement concrete, based on any of the prominent supplementary cementitious materials (SCMs) such as fly ash, ground granulated blast-furnace slag, silica fume, calcined clay and limestone powder, have proven to be the best candidates for sustainable concrete mixes. However, a reliable sustainability measure includes not only the environmental impact, but also the economic and functional ones. Within these five SCMs, their environmental, economic and functional properties are found to be conflicting at times, making a clear judgement on what would be the optimum mix not a straightforward path. A recent framework and tool for concrete sustainability assessment ECO_2, sets a reliable methodology for including the functional performance of a concrete mix depending on project-based specifications. Therefore, in this study, a recently published regression model, *Pre-bcc* was used to predict the functional properties of a wide grid search of potentially suitable blended cement concrete mixes. Hence, an open access novel genetic algorithm tool "*Opt-bcc*" was developed and used to optimize the sustainability score of these mixes based on a set selection of user-defined project-specific functional criteria. The optimized mixes using the *Opt-bcc* model for each strength class were compared against the mix design proposed by other optimization models from the literature and were found to be at least 70% cheaper and of 30% less environmental impact.

1. Introduction

Recent reports by the World Bank show that the highest rate of growth in population is happening among low-income countries, which currently constitute around 40% of the global population [1]. This increase in population size is associated with a 65% increase in the urbanization within these countries, a social trend that is encouraged by the urban policies within most of these countries [2].

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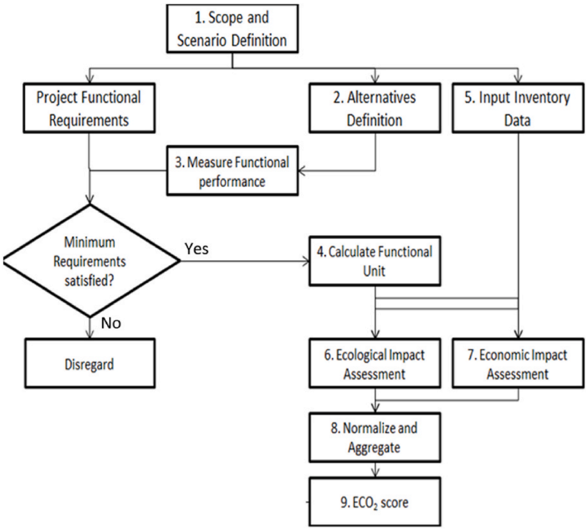

Fig. 1. A basic flowchart for the ECO_2 algorithm.

Hence, consolidating its position as the most used building material worldwide; concrete use in low-income communities is expected to rise from a current yearly rate of 15 billion tonne to at least the double by 2050 [3]. Therefore, there is a real necessity for concrete to be more affordable and accessible (Muller et al., 2014). However, sustainability is not only based on cost, but a combination of it with social and environmental performance [4]. Concrete is already relatively affordable material that is easy to manufacture almost anywhere in the world [5]. It has, on the other side, been under severe criticism lately by environmental researchers and policy makers for being a major contributor to the rising global warming concerns [6]. Concrete is, mainly due to the production of ordinary Portland cement (OPC), responsible for around 6% of the global CO_2 [7] emissions as well as the yearly risk of depleting >50 billion tonnes of aggregates [8].

Driven by the incentive to limit the alarming global warming potential through creating more sustainable concrete, several strategies were proposed in recent publications, out of which there is almost a consensus that utilizing blended cement is the most effective [9]. Blended cement concrete (BCC) is a type of concrete where OPC is partially replaced with various additions called supplementary cementitious materials (SCMs). The most prominent SCMs, are fly ash (FA), which is a by-product of coal combustion, ground granulated blast-furnace slag (GGBS), which is a by-product of steel manufacturing, silica fume (SF), which is generated from glass manufacturing, finely ground limestone, i.e. limestone powder (LP) and calcined clay (CC) [10]. Replacing OPC partially with varying percentages of one or two of these SCMs is claimed to produce a lower environmental impact and hence would make for more sustainable concrete [11].

In a recent publication of the authors [12], a concrete sustainability assessment framework – ECO_2 – was developed, defining sustainability as the user-weighted average of the economic and environmental impact of concrete based on specific functional requirements. The framework shown in Fig. 1, which will be explained in later sections in details, builds on user-defined performance criteria such as minimum slump, strength and a target service life and performs a life cycle assessment to calculate the environmental and economic impact using parameters such as: global warming potential, ozone layer depletion and net present value of money.

The functional requirements related to minimum slump, strength and target service life were assessed for each mixture evaluated by a non-linear multi-layered machine learning (ML) regression model – Pre-bcc – published recently by the authors [13]. As can be seen in Table 1, even though other ML models have been developed for the prediction of these properties, the Pre-bcc is currently the only alternative that covers both a wide range of SCMs (5) and the functional properties required.

The objective of this paper is to investigate, through the ECO_2 sustainability assessment framework [12] and the Pre-bcc model [13], the optimum BCC mixes based on a combination of SCMs under study for several strength and durability requirements. Current optimization approaches to find the most sustainable blended cement concrete mixes that achieve a combination of the functional compliance while minimizing the cost and environmental impact are based on Evolutionary Algorithms (EA) [31,32]. These are a class of optimization algorithms inspired by the concepts of evolutionary theory (survival of the fittest and the processes of selection, mutation, etc.). An EA builds an initial population of individuals P_o, and until reaching either convergence or a maximum number of iterations, the algorithm evaluates the population using some mapping $F : P \rightarrow R$, and applies a set of operators $H = \{H_1, ..., H_r\}$, resulting in a new population for the next iteration $S_{i+1} = H_r(...H_2(H_1(P_i)))$ (Deb, 2011).

[31] proposed a model that optimizes the mixing proportions of OPC-based concrete on the basis of minimizing one economic indicator (cost) and one environmental impact indicator (GWP) while satisfying one functional indicator (28 days strength). In addition [32], optimized the proportions of FA and GGBS-based ternary BCC on the same basis. The added value in the latter was the inclusion of slump and carbonation as well as strength as functional indicators. However, the functional parameters prediction models were assumed to have linear performance by Ref. [32] and only included strength by Ref. [31].

Alternatively, the current study develops an open access novel tool – Opt-bcc – for the optimization of the sustainability score of

Table 1
Summary of ML models published between 2013 and 2022 to predict functional properties of blended cement concrete.

Ref.	Compressive strength						Slump						Carbonation/Chloride penetration					
	OPC	FA	GGBS	SF	LP	CC	OPC	FA	GGBS	SF	LP	CC	OPC	FA	GGBS	SF	LP	CC
Rajeshwari & Mandal, 2013	•	•																
[14]	•	•	•															
[15]	•	•	•															
[16]	•			•														
[17]	•	•	•															
[18]	•	•																
[19]	•	•																
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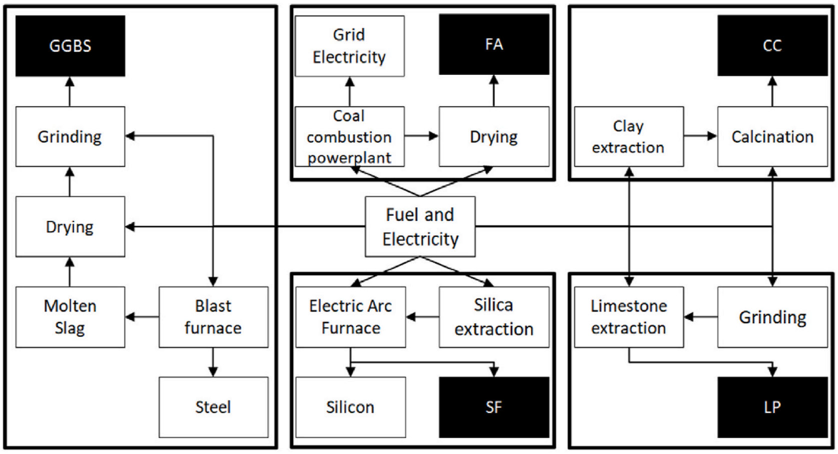

Fig. 2. The production processes for FA, GGBS, SF, LP and CC.

Table 2
The average values for the GWP and market price per unit mass of OPC versus the SCMs under study.

Inventory data for each impact indicator per unit mass (kg)	GWP		Market Price	
	kg CO_2 eq		£	
	mean	st.dev	mean	st.dev
OPC	8.96E-01	2.27E-01	8.72E-02	3.71E-03
FA	6.61E-03	3.77E-04	3.62E-02	3.77E-03
GGBS	3.06E-02	2.89E-04	3.70E-02	2.89E-03
SF	5.58E-02	3.17E-03	5.74E-01	3.17E-02
CC	3.52E-01	2.87E-02	5.20E-02	9.33E-03
LP	1.21E-01	2.21E-02	3.52E-03	1.87E-03

blended cement concrete based on the framework of the Genetic algorithms (GA). GA are classic meta-heuristic algorithms based on genetics and natural selection that look into the feasible region to find better solutions through iterations that satisfy the objective function within the boundary constraints. Even though these are commonly deployed as the preferred optimization and search techniques for a wide range of applications [33], have not yet been used for optimizing the sustainability of concrete mixes with SCMs. The optimized mixes obtained by this approach are compared against other optimization models from the literature, reaching significant improvements in terms of both economic cost and environmental impact.

2. Materials and methods

2.1. BCC mixes

The basis upon which these five promising aforementioned SCMs are utilized by partially replacing OPC is their sustainability potential. Fig. 2 is showing the process of the production of FA, GGBS, SF, LP and CC as by-products and the steps needed to prepare them as SCM. When compared with the energy and emissions involved in producing OPC (especially the inevitable direct carbon emissions due to calcination), the processing of these SCMs carries relatively minimal energy use. This is an indicator of the minimal costs and environmental impact of these materials making SCM-based BCCs more sustainable than OPC-based concrete. Throughout the next subsections, the functional, environmental and economic properties of each of these BCC types are discussed in detail.

2.2. Sustainability assessment of BCC

2.2.1. Environmental impact of BCC

Using global warming potential (GWP) as an indicator, an extensive literature search [6,7,34–43] [44–47] concluded that an average of 0.87 kg of CO2-eq. are attributed to the production of OPC. Meanwhile, as seen in Table 2, the average for FA, GGBS, LP and CC are 75%, 85%, 85% and 75% less. Hence, the higher the replacement ratio is of OPC with any of the five SCMs except SF, the higher the savings are in terms of environmental impact [48]. It is worth noting that an economic allocation of 2, 1 and 3% of the upstream processes impact was calculated as per the literature recommendations for FA, GGBS and SF respectively [49,50].

The low environmental impact could be understood examining the production processes of each SCM. As seen in Fig. 2.

- SF is obtained as a by-product from silicon manufacturing and does not require further processing. At a temperature of approximately 2000 °C, the reduction of high-purity quartz to silicon produces silicon dioxide vapor, which oxidizes and condenses at low temperatures to produce silica fume [51]. FA are the residual, unburnt particles, of coal being burnt for electrical or heating purposes which is captured by bag filters or through electrostatic precipitators [52]. Although it is ready to be bagged, capturing FA happens in humid conditions which requires a minor process of drying before its ready for use. GGBS is obtained after molten slag, which is a superficial layer produced by iron oxides inside the blastfurnace at almost 1400 °C, is dumped and quickly cooled by water jetting or quenching [53]. GGBS is then in need of drying and mechanical grinding to be ready for use as an SCM, but both processes also are minimal in terms of energy use. Aside from the minimum processing energy in case of FA and GGBS, the fact that the three SCMs are by-products from industrial processes means that using them in concrete is also saving these inert materials from being landfilled, which is an environmental impact incentive [54].

- LP and CC are not by-products, rather primary materials. LP is crushed and ground from natural limestone, which is mainly composed of the skeletal fragments of organisms and can be formed from marine organisms, lacustrine and evaporite depositional environments [32]. In comparison with OPC, LP only requires energy for quarrying and grinding, which is minimal [55]. CC is manufactured by calcining naturally available kaolinite clay in a temperature range of (700–800 °C), which is also considerably less than the temperature required for OPC production. Additionally, limestone and clay are abundant materials worldwide which reduces the potential for resources depletion [56].

At the same time, the following points provide the partial pushback against the environmental gains from the use of SCMs. First, according to the EU directive 2008, FA, GGBS and SF ought to be considered as by-products not as waste [35]. This means that they are to be allocated a percentage of the environmental burden of their original production process, which are coal combustion, steel production and glass manufacturing, respectively [57]. In addition, there is also an issue with the availability of SCMs for BCC applications. The supply of GGBS and FA worldwide is diminishing. Most of the steel production worldwide is shifting towards electric arc furnaces (EAF) rather than blast furnace ones because it requires less energy and cost [58]. For this fact, the EAF production technique took over 55% of the market in the US by 2006 [59]. FA will also face a difficulty in sourcing due to the general trend of retiring coal-fired power plants worldwide. In the US, approximately 40% of coal-fired power plants have closed in the last five years and the Netherlands is expected to reach that target by 2030 [1].

2.2.2. Economic impact of BCC

It is favourable to search for methods to lower the use of OPC even further especially in developing countries with pressing economic demands. A recent investigation identified the use of SCM as the most favourable cost reduction levers for the industry [60]. A literature review showed that, apart from SF, replacing OPC with FA, GGBS, LP or CC would yield decreases in the cost of the resulting concrete of more than 50%, as seen in Table 2.

2.2.3. Functional properties of BCC

The summary of the literature surveyed on the use of different SCM replacements on the resulting functional properties of interest of the BCC is that.

- Regarding slump, FA and GGBS are known to increase it while CC and SF drastically decrease it [61].
- Generally, replacements up to 30% of most SCMs (70% in case of GGBS and 15% for LP) would maintain, if not enhance, the 28 days compressive strength of the resulting BCC [48].
- Partial replacement of OPC with SCMs inevitably enhances the microstructure of the binder matrix when it comes to durability against chloride penetration [62].
- Although SCM additions to concrete yield a denser microstructure, there is an evident unanimous agreement within the published articles that BCC has a lower resistance to carbonation compared with OPC concrete [63].

3. Optimization of BCC mixes

The main objective of this study is to optimize the mixing proportions of binary and ternary blended cement concrete mixes incorporating FA, GGBS, SF, LP and CC as SCMs with regards to the ECO_2 sustainability index score. Any optimization process is an attempt to find the optimum solution for an objective function within a set of constraints. The objective function of this case study is the ECO_2 index calculation. The process of assessing the sustainability of a concrete mix using ECO_2 requires primarily the user to input, besides the scenario assumptions and inventory data, the functional properties of the mix in order to compare the latter with the functional requirements. Hence, as a starting point, a non-linear regression model was used to predict, for any combination of the five SCMs under study, the slump, strength, chloride resistivity and natural carbonation for the resulting BCC. The *Pre-bcc* model, which was published recently by the authors, could predict the aforementioned parameters for the boundary replacement % of each SCM with an average statistical accuracy (R-value) of 0.95 on the test set evaluated average [13]. The model is also available for open-access use through this link: https://bcc-regression.online/login/?next=/predict/.

3.1. Objective function

The first step in optimizing the mixing proportions of BCC, which is the objective of this study, is to select the relevant scenario for the ECO_2 calculation. A scenario defines the boundaries that dictate the life cycle assessment (LCA) impact calculations. The ECO_2 index is calculated as a weighted average between the normalized economic score (Z') and the normalized ecological score (Y) as in equation (1) below.

$$ECO_{2_i} = \mathrm{Y}_i \bullet w_y + Z_i^{'} \bullet w_z \tag{1}$$

$$Z_i' = \frac{max(Z_i) - Z_i}{max(Z_i) - min(Z_i)} \tag{2}$$

$$Z_i\ (€ / \mathrm{m}^3) = \sum_{j=1}^{n} \left(\frac{Market\ price}{kg} \bullet W_{j,i} \right) \bullet N_i \tag{3}$$

The normalized economic score Z' is calculated as per equation (2), while the absolute economic score Z is calculated based on the market price from Table 1 of each constituent j (CEMI, FA, etc.) as per equation (3). $W_{j,i}$ is the mass per unit volume of that constituent (j) in this mix (i) and N is the durability correction factor. This is not to be confused with w_y and w_z, which are the user-defined weights for the ecological and economic impacts for this scenario. The factor N was devised within the ECO_2 sustainability assessment framework to capture the potential deficiency in the durability of a concrete mix compared to the project specification. If the scenario defined for the ECO_2 sustainability calculation is to be purposed for plain or fiber reinforced concrete, N is assumed as 1 because the concrete is expected to sustain its service life (Garcia-Segura et al., 2013). On the other hand, in a reinforced concrete scenario, the concrete element could fail to fulfil the required service life due to corrosion of the steel reinforcement. Hence, the functional unit that is used to quantify the environmental and economic impacts is rightfully multiplied by N. The minimum value of N however is set within the ECO_2 methodology as 1 so as not to reward the undesirable prolonged durability of the concrete alternative beyond the required service life. Steel reinforcement corrosion could mainly be a result of either carbonation or chloride penetration depending on the exposure conditions [64]. The ultimate limit state design against steel corrosion according to the EN:1992-1-1 is to specify a minimum concrete cover that resists the potential carbonation and chloride penetration within the specified service life without major repair or reconstituting (Toutlemonde et al., 2021). Accordingly, N is calculated as per equation (4), where $c_{max\text{-}x}$ is the largest value for the minimum concrete cover among all studied concrete alternatives against the exposure condition x, $c_{min\text{-}x}$ is the lowest value for the minimum cover and $c_{i,x}$ is the minimum concrete cover for alternative i under study against the same exposure condition. F_n is a volume correction factor that translates the percentage of the concrete cover to the potential loss in concrete volume. Surely, the value of F_n varies depending on the geometry of the concrete element and its type (column, beam, slab), so it is left as a user-defined variable. All concrete covers are rounded up to the nearest 5 mm.

$$N_i = 1 + F_n * \frac{C_{i,x} - C_{min-x}}{C_{max-x} - C_{min-x}} \tag{4}$$

According to EN:1992-1-1, there are two critical combinations of exposure classes to design the minimum concrete cover against. The first is a combination of the carbonation exposure (XC1) where concrete is in cyclic contact with water (rain, snow, condensation etc.) and dry air (depending on outdoors conditions) and chloride penetration of (XD1/XS1) where due to limited/non-permanent concrete saturation the chlorides diffusion is relatively slow and the reinforcement corrosion develops less rapidly. The second is a combination of the carbonation (XC2) where concrete is immersed so the carbon dioxide propagation is low and (XD3/XS3) in which, due to concrete saturation when the chlorides are brought, their diffusion is rapid. The EN:1992-1-1 follows a service life prediction model based on Fick's 2nd law to calculate the required cover to protect against chloride penetration depending on $D_{(t)}$ which is the apparent diffusion coefficient for chlorides at time t (Izquierdo et al., 2001). However, due to the limitation of the database, the *Pre-bcc* regression model could only predict the concrete mix's resistivity against chloride penetration. Hence, the minimum required concrete cover for each alternative "i" would be calculated only based on the resistance to carbonation as per equation (5) where t is the required service life and K_{ni} is the natural carbonation rate of alternative i (mm/sqrt(year)) predicted by the *Pre-bcc* model assuming an atmospheric carbon concentration of 0.05%.

$$C_i = K_{ni}\sqrt{t} \tag{5}$$

The normalized ecological score Y_i is the normalized score for the Global Warming Potential (GWP) of each of the studied alternatives/mixes as shown in equations (6) and (7). GWPj/kg for example is the value per kg for constituent j of mix i which is found in Fig. 1 and W_i is the mass per unit volume of this constituent j in this mix i the mass of the binder multiplied by the ratio between the binder the constituent j and N was defined earlier

$$Y_i = \frac{max\ (Y_{GWPi}) - Y_{GWP\,i}}{max(Y_{GWP_i}) - min(Y_{GWP_i})} \tag{6}$$

$$\frac{Y_{GWPi}}{m^3} = N_i\ .\ \sum_{j=1}^{n} \left(\frac{GWP_j}{kg} . W_i \right) \tag{7}$$

Two scenarios were defined for the optimization problem. The first is assuming a plain concrete application meaning that N is equals to 1. The second scenario was assumed to be used for reinforced applications subjecting N to change based on the resistance of each alternative to carbonation for a required service life of 50 years and the minimum chloride penetration resistivity was defined as a minimum of 1200 coulombs. The minimum project requirements for both scenarios were a 100 mm slump in order to achieve a minimum class of S3 and a minimum mean 28 days compressive strength. Due to the variability in the possible strength classes according to the project requirement for the concrete element in use, eight sub-scenarios were defined for each of the two main scenarios explained (20, 40, 60 and 80 MPa).

Table 3
The specific gravity of BCC mix constituents.

Water	CEMI	FA	GGBS	SF	CC	LP	Coarse	Fine	SP
1	3.15	2.25	2.91	2.25	2.61	2.65	2.61	2.71	1.22

Table 4
Preferred range for each of the BCC mix constituents relative to the total binder content.

	Binder	Water	CEMI	FA	GGBS	SF	LP	CC	Coarse	Fine	SP
	kg/m^3	Ratio of constituent to Binder									
minimum	200	0.25	0.3	0	0	0	0	0	0.5	0.5	0
maximum	600	0.8	1	0.5	0.7	0.15	0.2	0.5	5.5	5.5	0.02
step	25	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.005

Table 5
The element notation for the generated chromosomes of the GA.

Element	**Domain**	**Meaning**
p_1	{0,1}	whether cement 42.5 or cement 52.5
p_2	{0,1,2,3,4}	the index of the first SCM from the index set $A = \{FA, GGBS, SF, LP, CC\}$
p_3	{0,1,2,3}	the index of the second SCM from the set $A - A[p_2]$
p_4	[0.25,0.8]	the water to binder ratio
p_5	[0.3,1]	hint for CEMI to binder ratio
p_6	[0,1]	hint for the factor of [min,max] to use for the first SCM defined by p_2
p_7	[0,1]	hint for the factor of [min,max] to use for the second SCM defined by p_3
p_8	[0.4,0.52]	the ratio Fine aggregate/(Coarse aggregate + Fine aggregate)
p_9	[2.5,6.5]	the term (Coarse aggregate + Fine aggregate)/Binder
p_{10}	[0,0.02]	SP to binder ratio

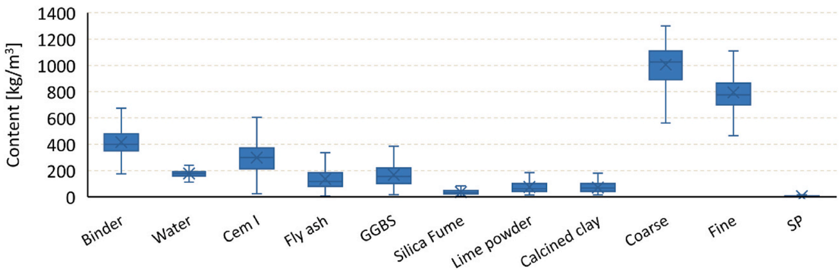

Fig. 3. Input variables data distribution from the Pre-bcc database.

3.2. Constraints

The objective of the optimization problem is hence achieving the mix with the highest ECO_2 score while satisfying certain constraints as follows. First, a mix contains a varying percentage of the following components: CEM I (Grade 42.5 or 52.5), FA, GGBS, SF, LP, CC, coarse aggregates fine aggregates and superplasticizer (SP). Logically, the first constraint is that the summation of the volume of all mix constituents in a unit volume of concrete must also equal 1.0, where ρ is the specific gravity of all components and W_i is the mass per unit volume summarized in Table 3 [65,66].

$$\frac{W_{CEMI}}{\rho_{CEMI}} + \frac{W_{FA}}{\rho_{FA}} + \frac{W_{GGBS}}{\rho_{GGBS}} + \frac{W_{SF}}{\rho_{SF}} + \frac{W_{CC}}{\rho_{CC}} + \frac{W_{LP}}{\rho_{LP}} + \frac{W_{Coarse}}{\rho_{Coarse}} + \frac{W_{Fine}}{\rho_{Fine}} + \frac{W_{SP}}{\rho_{SP}} = 1.0 \tag{8}$$

The second constraint is concerning the practicality of the mixes. The difference in the cement strength class affects the strength of the resulting mix. Hence, either the cement strength class 42.5 is used or the 52.5 one and not a combination of both. Also, the mixes are either binary or ternary, which means that a maximum of only three binder types is allowed to be used, one cement type and a combination of two more of any of the five SCMs (FA, GGBS, SF, LP and CC). The third and final constraint is regarding the best practice when it comes to concrete mixes. The literature shows that the preferred ratio between the fine aggregates to the total weight of the aggregates should be kept between 0.40 and 0.52 [32].

3.3. Optimization approach

The previous information proves that there are several challenges that are specific to the optimization process under study. First,

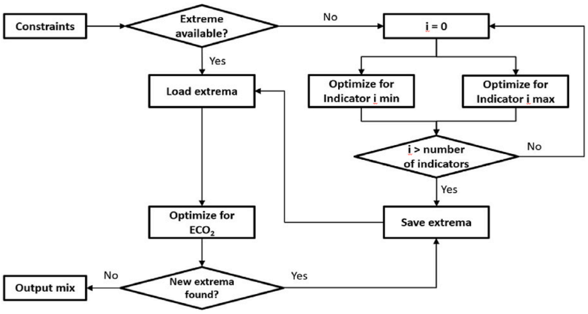

Fig. 4. A flow chart showing the population generation within the *Opt-bcc* algorithm.

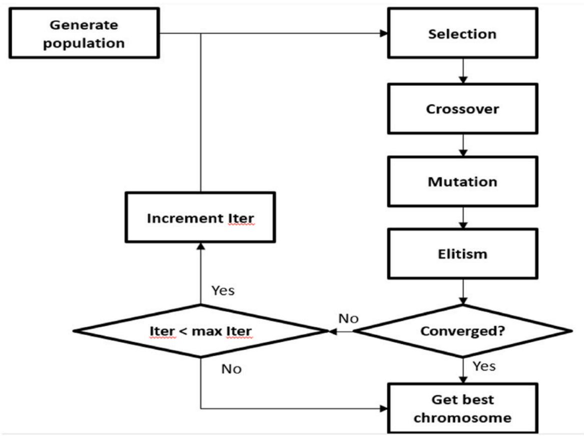

Fig. 5. A flowchart showing the *Opt-bcc* GA operators.

the optimized mix is selected out of what is called the search space and in order to define this search space there need to be certain limits that govern the selection of each of the mixing proportions (*W*). The range in which each of the constituents' falls was obtained from the input database used in developing the *Pre-bcc* regression model and is shown in Table 4. In order to clarify the variability across the specified range, Fig. 3 reports the distribution of all input variables. Each box sets the first and third quartiles with an additional line along the second quartile marking the median. The cross inside the box represents the mean of the distribution. Minimum and maximum values are depicted with whiskers. The database is available for public use under the following link (https://sites.google.com/aucegypt.edu/pre-bcc-db/home). The first challenge then is that the step size by which the search space is formed is too small causing a 3.15×10^{21} wide space within the 10 dimensions ruling out the possibility of using a simple approach such as grid search. The second challenge is concerning the nature of the constraints, which require the use of the regression learners developed in the *Pre-bcc* regression model for strength, slump, carbonation and resistivity. The use of those functions which are non-linear, non-convex, and not differentiable rules out any attempt at turning the constrained optimization into non-constrained optimization and using differentiable techniques. The third and final challenge is concerning the analysis of results. Although the ECO_2 score is a single objective function, it is in fact a weighted linear formulation of multiple objective functions. This means that an analysis of the results requires considering multi-decision metrics.

In order to address these, the general approach was the use of Evolutionary, especially Genetic Algorithms (GA) as opposed to gradient-based methods. It was also decided to first use the optimization algorithm subject to the same constraints in order to find the extrema (normalization constants), then use those as the normalization constants. At the same time, during ECO_2 optimization, the new mixes are checked for providing new maxima or minima for any of the eight indicators, and the normalization constants are updated accordingly. This approach is shown in Fig. 4 below.

4. The *Opt-bcc* optimization implementation

4.1. Optimization operators

A typical GA would include a mechanism for the generation of the population that complies with the set constraints and three main operators: selection, crossover and mutation. For the *Opt-bcc* optimization GA, the following operators were designed as shown in the flowchart in Fig. 5.

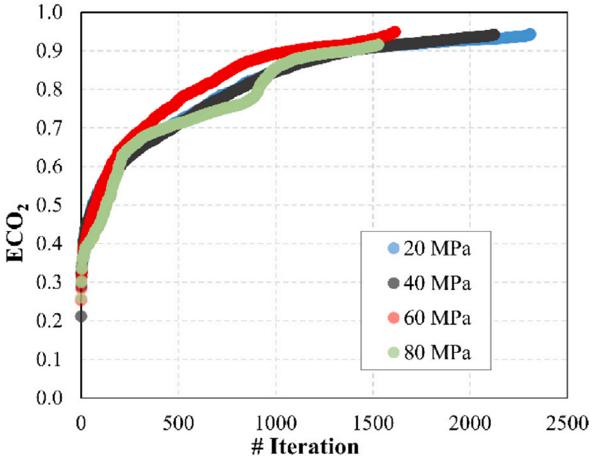

Fig. 6. ECO_2 evolution during the optimization process for each strength class.

- Generation: One advantage of EA is that the individual generation can be used to only consider mixes that comply with the constraints. In order to do this, *Opt-bcc* generates an individual (chromosome) $p = (p_1 - p_{10})$ where the attributes p_i are as shown in Table 5.
- Evaluation: Since the same algorithm is used for both generating the extrema (normalization factors), and for optimization, the evaluation function is different between the two cases;
  1. ECO_2 optimization: this is the ECO_2 score for the mix generated by the individual.
  2. Search for extrema: d is $+1$ for maxima and -1 for minima. Recall that Y, Z are the absolute versions of the two component terms of the ECO_2 score.
- Selection: The selection operator is used to enhance the overall population score by only selecting half of the population and cloning them. The method used here is tournament selection with a tournament size of 3. Hence, elements of 3 are randomly selected and the highest score of each is chosen. This strategy allows the algorithm to widen the search space rather than a greedy best individual selection strategy.
- Crossover: The crossover operator takes pairs of individuals $u, v \in P_g$ within the population at generation g with a probability of c_x , and a randomly chosen string of attributes are swapped for the two individuals. The value for c_x used for ECO_2 was 0.7 for optimization and 0.6 for extrema generation.
- Mutation: The mutation operator randomly chooses individuals at a probability of c_m, and within that, the attributes are randomly changed at a rate c_r according to Gaussian distribution. The value for c_x used for ECO_2 was 0.1 for optimization and 0.03 for extrema generation. The value for c_r was constant at 0.05.
- Elitism: This operator combines the best of the parent population (from the previous generation), and the offspring (resulting from the operators above) to ensure that the performance is monotonically increasing.

4.2. Constraints handling and termination criteria

The constraint handling was implemented using the DEAP Delta-Penalty function, evaluating a point where the constraint was not met as 0, i.e., $J_i(G(p)) \notin [l_i, u_i] \Rightarrow F(p) = 0$. Given the evaluation function $F(p)$ defined above, this is equivalent to a hard barrier at those points within the search space. Finally, the *Opt-bcc* GA terminates when the evaluation of the best element of the population does not change for seven iterations. The optimization process is a search through the space of different concrete mixes. The constraints outline the forbidden vs navigable regions of this space, defined by certain characteristics of the mix, namely the slump, strength, natural carbonation rate and resistivity of the mix. Since empirical values for those characteristics are only available for a subset of the search space, the regression learners developed in the *Pre-bcc* were utilized to evaluate the characteristics for any mix in the search space. The *Pre-bcc* regression learners are cascade learners trained on a dataset compiled from different sources using a variant of boosting. The dataset and the regression training are documented in a publication by the author [13].

5. Results and discussions

5.1. Scenario 1

The first scenario ran was for plain concrete, where the durability functional parameters are of no impact on the ECO_2 score calculation. The ECO_2 score was assumed to have an equal (50%) weight for the ecological and economic impacts. For each strength class (20, 40, 60 and 80 MPa), a sub-scenario was prepared. Fig. 6 depicts the ECO_2 score evolution obtained by the different mixes evaluated throughout the optimization process that comply with the 4 strength class constraints. As shown, the ECO_2 score consistently increases during the search process, converging in the optimum at scores above 0.9. The plateau region near the final convergence of the optimization model suggests that there are a large number of different concrete mixes that can reach comparable high-

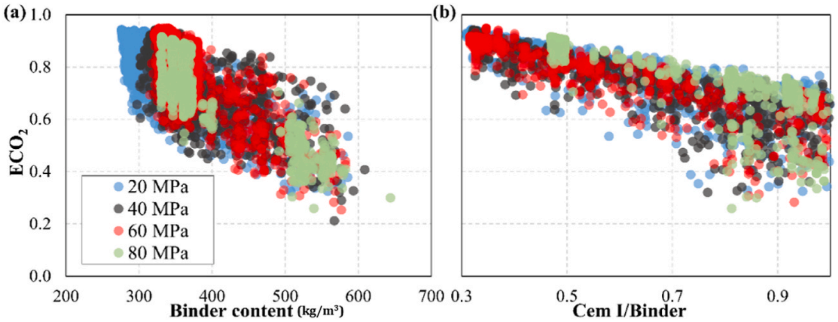

Fig. 7. Influence of (a) Binder content and (b) CEMI/Binder ratio on ECO_2 for each strength class in scenario 1.

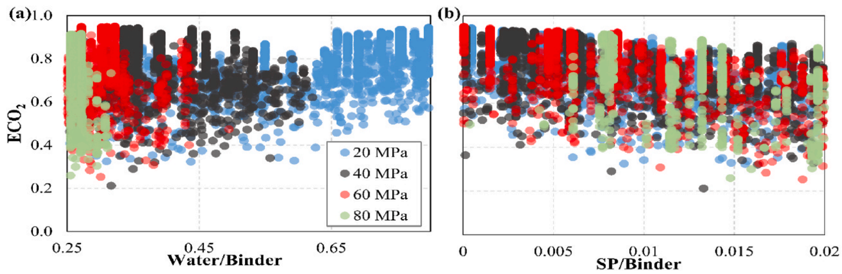

Fig. 8. Influence of (a) Water/Binder and (b) SP/Binder ratio on ECO_2 for each strength class in scenario 1.

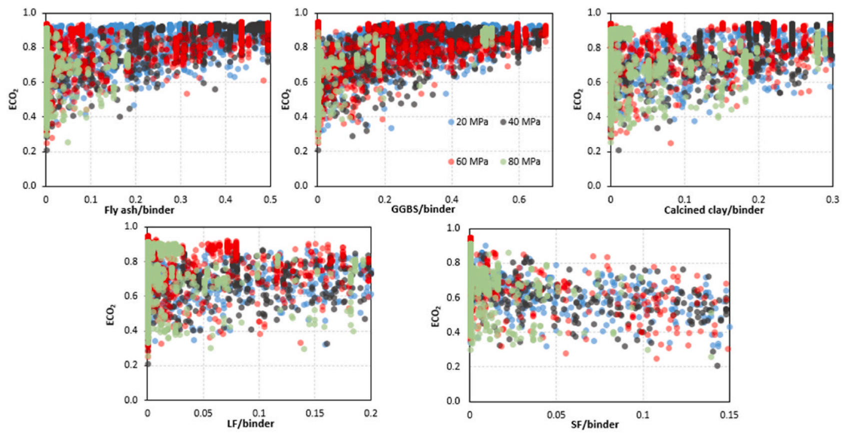

Fig. 9. The optimization results for the influence of replacing OPC with all five SCMs on the ECO_2 score.

sustainability performances. Consequently, the discussion presented here is not focussed on the identification of the most optimized mixture. Instead, the large number and wide range of mixes evaluated during the search process (between 1529 and 2310 for each sub-scenario) is used here to enable the assessment of the coherence of the model for plain concrete applications and deduce general insights for sustainable mix design.

The results shown in Fig. 7 depicts the influence of the (a) total binder content and (b) CEMI/binder ratio on the ECO_2 score for each strength class. Fig. 7a shows that the sustainability of the mixture (ECO_2) increases with the reduction on the total binder content. As expected, the ECO_2 score increases with the reduction of the cement to binder content, highlighting the positive impact of mineral additions on the sustainability of concrete. The CEMI/binder ratio seems to follow a trend of decreasing as the strength requirements increase (in Fig. 7b). In this case, high-strength mixtures require a minimum CEMI/binder ratio above 0.5, which is in agreement with [67].

The water/binder ratio (Fig. 8a) depicts a bow tie-shaped data distribution where the maximum ECO_2 scores are placed in the lowest and highest water/binder ratios evaluated. The strength requirement gradually limits the maximum water/binder ratio allowed for the strength class 40 MPa (0.60), 60 MPa (0.45) and 80 MPa (0.32). It is clear that the optimum water/binder ratios for mixes with target strength above 20 MPa is concentrated below 0.45 suggesting a serious revision to current construction practices where the

Table 6
Benchmark values for the price and carbon footprint of plain optimized blended cement concrete mixes.

Unit/m^3		20 MPa		30 MPa		40 MPa		50 MPa		60 MPa		70 MPa		80 MPa	
		Avg	st dev	Avg	st dev	Avg	st dev	Avg	st dev	Avg	st dev	Avg	st dev	Avg	st dev
Price	€	38.3	1.2	43.5	3.1	44.1	3.0	48.7	5.3	51.8	2.9	52.2	5.4	56.0	5.2
GWP	kg CO_2 eq	113.3	11.6	132.6	24.7	137.3	19.8	155.2	36.4	163.0	19.1	173.6	34.1	201.4	26.3

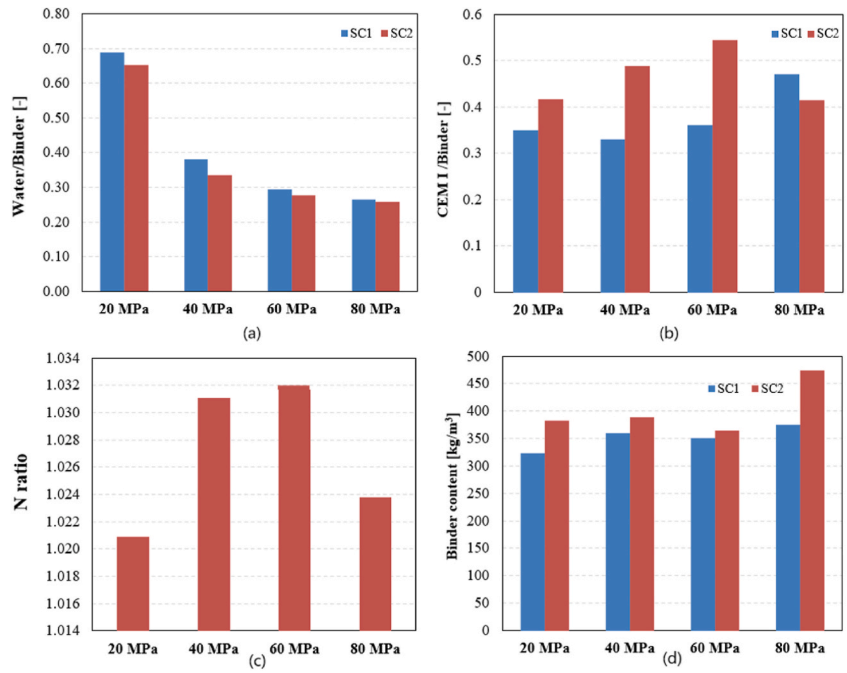

Fig. 10. A comparison between the water/binder ratio (a), CEMI/binder ratio (b) and binder content (kg/m^3) (d) of each strength class between scenarios 1 and 2. (c) Shows the N values of the optimum mixes for scenario 2.

common W/B ratio is usually higher. On the other hand, as seen in Fig. 8 (b), the superplasticizer (SP) content does not seem to be a key factor for the sustainability of the mix, as all contents obtained a wide range of possible ECO_2 scores. However, it is visible a slight reduction of the average sustainability of the mixes with the increase of SP/binder ratio, especially for SP contents above 1%. The model also captures the lack of viability of obtaining high-strength mixtures (80 MPa) without a minimum SP usage.

As a summary, it is clear that the addition of silica fume as an SCM beyond minimal dosages does not yield the most sustainable concrete mixes across the boundary condition specified due to its high cost and environmental impact. The data displayed in Fig. 9 below also shows that the type of SCM replacement (whether it is fly ash, GGBS or calcined clay) and their combination is not a limiting factor for achieving high mix sustainability as much as the %replacement. Finally, based on a global average of the ECO_2 scores >0.75, the data in Table 6 presents an appropriate benchmark for the GWP and cost of each strength class of plain concrete as per the specified boundary conditions.

5.2. *Scenario 2*

The second scenario on the other hand is assuming a 50-year-old building service life for reinforced concrete. Hence, it was decided that the optimal BCC mixes should satisfy the boundary conditions of resisting the deterioration of the concrete elements against carbonation and chloride penetration. The minimum required resistivity against chloride penetration is 1200 coulombs and for carbonation, the exposure class is assumed to be XC3 and F_n is assumed as 0.1 (the concrete cover is assumed to comprise 10% per unit volume of concrete). Similar to scenario 1, a sub-scenario was prepared for the four strength classes evaluated (20, 40, 60 and 80 MPa). As explained in section 5.1, the results shown below are not directed to identify the optimum mixes for the specified set of boundaries. Instead, the trends obtained by averaging the global values of the different mix design parameters for mixes with ECO_2 score >0.75. The values for scenario 2 are compared to the plain concrete scenario to verify the coherence of the model when durability requirements are introduced and conclude a judgement over the role of durability performance of concrete on its sustainability potential.

Fig. 10 represents the average binder contents of all valid mixes explored during the optimization process for Scenario 1 and 2. First, in a similar trend to that of scenario 1, it could be clearly noticed that the higher the strength requirement, the lower the water: binder ratio should be and as seen in Fig. 10 (a) the added durability requirements decreases the ratio, though slightly, even further.

Table 7
A comparison between the optimized ratio of the different constituents of the BCC using the *Opt-bcc* model and [31,32].

Strength	30			40			50		
Model	ECO_2	[31]	[32]	ECO_2	[31]	[32]	ECO_2	[31]	[32]
B	300	330	380	305	360	455	335	417	515
W	215	188	167	155	170	167	115	160	167
CEM-I	90	330	140	90	360	140	100	417	155
FA	90	0	200	75	0	200	150	0	200
GGBS	0	0	40	0	0	115	0	0	160
CC	120	0	0	140	0	0	85	0	0
Coarse	1085	895	1024	1161	1125	983	1199	1125	939
Fine	742	945	683	775	742	655	805	701	640
SP	0.79	0.52	4.95	1.87	1.85	5.90	0.77	1.61	6.74
Price/m^3	37	52	49	40	57	52	41	61	56
GWP/m^3	116	312	148	122	1	151	123	392	167
N. Price	1	0	0.21	1	0	0.28	1	0	0.27
N. GWP	1	0	0.84	1	0	0.87	1	0	0.84
N. CED	1	0	0.72	1	0	0.77	1	0	0.75
ECO_2	1	0	0.49	1	0	0.55	1	0	0.53

Second, in terms of water to CEM I replacement rate, it is clear that on the contrary to the trend in Scenario 1, the increase in strength requirement for Scenario 2, seems to reduce the allowable limit of integrating SCMs. As shown in Fig. 10 (b), except for the 80 MPa strength class, it is also clear that with the added durability requirement, the CEM I component of the binder is 10–30% higher than that in scenario 1. The observation follows the established knowledge of the inferior durability performance of blended cement concrete mixes [63]. However, it is worth noting that across all strength classes, the optimum mixes achieving the durability requirement unanimously scored a higher N value than 1 as seen in Fig. 10 (c). This means that the shorter service life for blended cement concrete in comparison to OPC concrete which might lead to repairs/maintenance and/or replacement of the concrete cover does not take away from the environmental and economic gains of using SCMs. This is a significant finding of the model, that brings in a debatable perspective to the priorities of sustainable concrete technology strategies. As opposed to the common belief that the longer the service life of a building, the more sustainable it is, the results show that the minimal environmental impact attributed to the repair and maintenance of a concrete structural element due to the potential loss of concrete cover caused by corrosion related deterioration in the case of blended cement concrete mixes is lower than the initial environmental impact and cost associated with using OPC concrete. Finally, it is the belief of the authors that, although the optimization algorithm shows a slight increase in the minimum required binder content for each strength class in both scenarios as shown in Fig. 10 (d), that this is not enough to support the correlation between both variables. Specific studies showed that there is no clear correlation between the binder content of a concrete mix design and the target strength and durability properties [10,68,69].

5.3. Comparing against other models

In order to validate the significance of the novel optimization model, the results were compared against those presented by both the models presented by Refs. [31,32]. The cost and GWP were used to assess the economic and environmental impact of each alternative as per the ECO_2 inventory data and assessment process aforementioned. Since both models from the literature assume a plain concrete scenario, the comparison against the *Opt-bcc* GA model depended on the selected optimized concrete mixes from scenario 1. The values for the mixing proportions used to represent the optimum mix for each strength class were obtained as the global average of mixes with ECO_2 scores >0.9. As seen in Table 7 below, for each strength class (sub-scenario), the mix design resulting from the *Opt-bcc* optimization model proves to be cheaper and of less environmental impact than the ones proposed by Refs. [31,32] by at least 70% and 30% respectively. The results are seen as valid because the same inventory data, assumptions and calculation process was used for all. The reason behind the enhanced performance of the *Opt-bcc* optimization model could be the fact that the strength and slump regressors allowed the accurate prediction of the mixes within the boundary conditions that include the lowest possible binder content and water: binder ratio. Also, the availability of calcined clay as an SCM, which is proven to enhance the functionality of the mixes while minimizing the environmental and economic impact.

5.4. Web-based optimization software

For validation purposes, an open-access web-based tool was also created to allow users to optimize BCC mixes for a selected scenario utilizing the ECO_2 based framework explained in earlier sections. The *Opt-bcc* tool, developed under the name of the GA model, is available online at https://bcc-regression.online/optrequest/. Upon registering with a valid username and password, the user is allowed to start a "new request" for an optimization project. The user first of all specifies if the optimization should run a reinforced concrete one by ticking the relevant box or else a plain concrete scenario is ran by default. Hence, the user selects the sub-scenario(s) which are to be included in the optimization. If the user chooses to change the inventory data upon which the ECO_2 calculation manually by simply changing the values in the table, a message would come up asking the user to wait for an email notification that the scenarios were finished before logging in to check them. Otherwise, if the user agrees to the values included in the inventory database shown in the original table, once they click submit request, the result would show up under the specified label in the home page. An

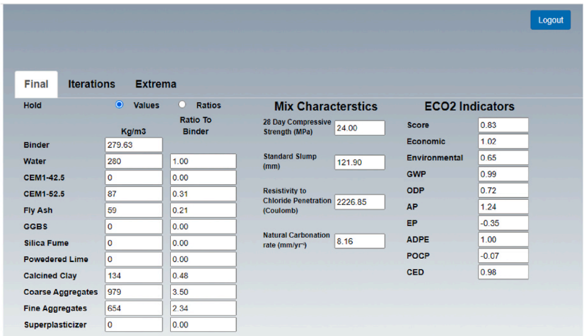

Fig. 11. An example of the optimized mixes output by the Opt-bcc web-tool.

example of a previous optimization for a reinforced concrete scenario with a minimum 28 days compressive strength requirement of 20 MPa is shown in Fig. 11.

6. Conclusions

The paper presents a novel GA optimization model, *Opt-bcc*, which is available for open-access use through https://bcc-regression.online/optrequest/. The paper also presents a set of contributions that could be summarized as follows.

- A genetic algorithm was built to optimize the mixing proportions of BCC mixes with the objective of minimizing their environmental and economic impact against performance-based specifications. The new *Opt-bcc* optimization model generated BCC mixes that achieve up to 70% less environmental impact and cost compared to established optimization models from the literature.
- The ECO_2 algorithm establishes the basis, out of the hundreds of possible combinations, for benchmarks for the GWP and market price of a concrete unit volume for specific strength and durability requirements.
- The optimization scenarios ran in this study showed that regardless of the % of SCM replacement and the type of SCM used to replace the OPC, the optimal sustainable BCC mixes depend highly on decreasing the total binder content. It is noticeable that the higher the strength, surely the water to binder ratio decreases. Also, the minimum binder content is slightly increased, but it is all in the range of 300–360 kg/m^3.
- The lower durability performance of BCC compared to OPC does not take away from the environmental and economic merits of using SCMs. In reinforced concrete scenarios, the ability to replace the OPC with SCM from is marginally reduced from an average of 60–70% to only 40–50%.

One of the limiting factors of the paper is that the underlying database used for the ECO_2 index calculation contains average values with significant standard deviations for the inventory data. Hence, it is recommended that users enter their own inventory data based on primary sources and re-run the optimization scenarios. Also, the fact that the service life prediction is only carried out for carbonation due to the limited database for chloride penetration diffusion coefficient for the SCMs under study. Hence, further work is being done to expand the *Pre-bcc* regression model capability and include a wider boundary condition to the optimization algorithm. Moreover, the current computational capacity for the web-based tool is limited, so the simulation results could only be generated after hours of inputting the data by the user. However, it is in the future plans of the researchers behind this manuscript to enhance the speed of simulation to generate the results real time.

Author Statement

Conceptualization, H.H.; Methodology, H.H.; Software, A.T.; Validation, A.d.l.F; N.T.; Formal analysis, A.T.; T. I; Investigation, H. H.; T. I; Resources, N.T.; Data curation, H.H.; A.T.; T.I.; Writing—original draft preparation, H.H.; Writing—review and editing, A.d.l.F; N.T.; Visualization, H.H; T.I.; Supervision, A.d.l.F; N.T.; Project administration, A.d.l.F, Funding acquisition, A.d.l.F.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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