- Technical Paper -

APPLICATION OF RESPONSE SURFACE METHODOLOGY AND UNCERTAINTY ANALYSIS FOR EXPLORATORY ANALYSIS OF CONCRETE MATERIAL SUSTAINABILITY

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ABSTRACT

This paper presents an exploratory type of concrete sustainability analysis by using response surface methodology and uncertainty analysis to cater continuous variables such as water-binder ratio and percentage of replacement materials. Integrating both analytical tools enables the determination of local maximum or minimum points, as well as numerical optimization to locate desirable points based on pre-defined concrete sustainability criteria. This integrated approach provides more comprehensive information that can guide decisions on the design of sustainable concrete.

Keywords: concrete sustainability, response surface methodology, uncertainty analysis

1. INTRODUCTION

Defining the sustainability of concrete material quantitatively is important for the industry to select decisions and actions that are contributory to global sustainable development. Because of the multidimensional nature of concrete sustainability, it is often analyzed similar to a multicriteria decision problem (or multicriteria analysis). Multicriteria analysis consists of methodologies that condense the information of various indicators into a composite value (or sustainability score) [1], summarizing the behavior of the system of interest. The method is usually used to make quantitative comparisons to rank or select the best in a set of alternatives or decisions (e.g., a set of concrete mixes) and is considered as the appropriate tool to perform assessments of sustainability [2]. There are two caveats, however, with the use of multicriteria analysis: methodological multiplicity and its limited exploratory power.

The first caveat refers to the menu of available multicriteria methods in literature – each with differing structural assumptions – to operationalize sustainability evaluations. Depending on the method subscribed to by the analyst, different conclusions about the sustainability of the system of interest may result [3]. As a consequence, it is difficult to make distinct pronouncements about the sustainability of a particular concrete material under this methodological variability, as each result represents only one possibility. The first caveat, however, can be resolved by incorporating uncertainty analysis (UA) into the multicriteria analysis, which details how methodological multiplicity relates to the output of sustainability evaluation.

On the other hand, conventional multicriteria analysis is very restrictive, as it only investigates limited number of points (i.e., a number of concrete mixes). Its exploratory power diminishes – the second caveat – when involving continuous variables (i.e., range of water-binder (W/B) ratio). Multicriteria analysis, for example, only ranks a number of concrete mixes in order based on the sustainability score so that the relatively "best" alternative(s) can be selected directly by decision makers. Since only few mixes are included in this ranking, there is a possibility that the true maximum (or minimum), or the optimum sustainability score, within the continuum of the analytical domain is missed.

In this paper, to tackle the two major caveats mentioned, the use of an additional analytical tools is introduced – the application of UA in combination with the response surface methodology (RSM) – to extend the concrete sustainability evaluation to an exploratory type of analysis. RSM is an appropriate approach to perform exploratory investigations because of its model fitting capability, while UA handles methodological uncertainty. The results of the multicriteria analysis with UA for a number of concrete mixes are used as inputs to RSM to form mathematical models that illustrate a continuous trend of sustainability scores within the domain of the variables investigated. Further, the RSM models allow making numerical inferences of the values of any point within the analytical domain, including the determination of optimum values, therefore, making concrete sustainability evaluation not only robust but also exploratory.

2. METHODS

Figure 1 shows the general analytical method employed in this paper. The multicriteria analysis for sustainability evaluation is first subjected to uncertainty analysis (Phase I). The output of phase I is then used for response surface modeling (Phase II), wherein the empirical equations of the desired responses are generated (Phase III). These equations are then used for

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numerical optimization (Phase IV). The following subsections further detail Phases I and II, while Phases III and IV are demonstrated in Section 3.

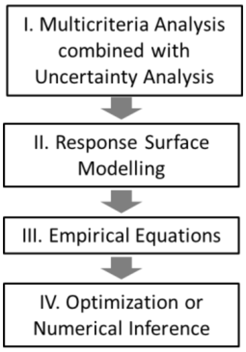


Figure 1 General analytical method

2.1 Multicriteria Analysis

Multicriteria analysis is comprised of four primary stages: (1) formation of the sustainability indicator set, (2) normalization of indicator values, (3) indicator weighting, and (4) aggregation (see also Figure 2). Indicators set formation defines the sustainability criteria upon which different alternatives are compared. The indicators in this set are then normalized to remove the differences in their units and scales. Each indicator is then associated with weight to signify their relative importance. Finally, they are aggregated to a single score (Y) for ease of interpretation by different stakeholders.

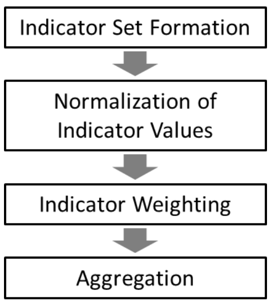


Figure 2 Stages of multicriteria analysis

While the multicriteria analysis seems straightforward, each stage, however, can be performed using different methods (some commonly used methods are listed in Table 1) – the first caveat. Due to space limitations, Table 1 only includes the brief description of each method, and the reader is referred to the appropriate literatures for an extensive explanation of each methods.

Figure 3 maps all the possible methodological combinations of the methods listed in Table 1 to calculate the sustainability score (*Y*). From this map, an analyst, for example, could perform sustainability evaluation following a single path, i.e., SI1-R-EW-LN, or alternatively SI2-S-PCA-GM. Each methodological combination that can be formed from Figure 1 is said to be unique because essentially the underlying assumptions of the different methods are non-equivalent, and each path will likely produce differing *Y* values. This implies that there is not a single unique methodological combination for performing sustainability evaluation. However, due to the lack of framework and standards for guiding the selection of methodological combination, it is appropriate to assume that each combination can be considered legitimate for evaluating concrete sustainability, giving rise to *methodological uncertainty*. Additionally, From a deterministic (single-valued) point of view, the changing values of Y due to methodological uncertainty could be a source of conflict and confusion among stakeholders when selecting the superior alternative from a set of concrete mixes.

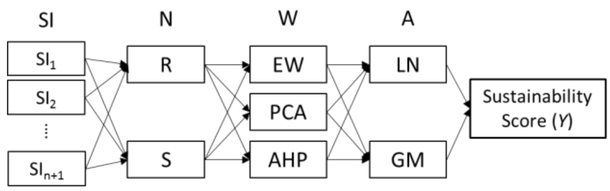


Figure 3 Map of methodological combinations

Table 1 Multicriteria analysis applicable methods

Analysis Stage	Methods	Brief Description [4]
Sustainability Indicators Set Formation (SI)	Inclusion/Exclusion of '*n*' indicators	Forming *n+1* sets of indicators by dropping indicators one-at-a-time (OAT) (see, e.g., [5]).
Normalization of Indicator Values (N)	Distance to a Reference (R)	Relative distance (ratio) of value of an indicator from the reference value [5].
	Standardization (S)	Normalizing disparate indicator values by statistical standardization [5], i.e., use of z-score and t-score.
Indicator Weighting (W)	Equal Weighting (EW)	Equal weights are assigned to indicators.
	Principal Component Analysis (PCA)	Weights are derived by performing PCA, which takes the variability and correlation of indicators in the data set. PCA can summarize a set of indicators while preserving the maximum possible proportion of the total variation in the original data set (see [5] for extensive discussion)
	Analytic Hierarchy Process (AHP)	The weights of each indicators are determined by comparing them against each other either by qualitative or quantitative means [5].
Aggregation (A)	Linear (LN)	Weighted summation of the normalized indicator values [5].
	Geometric (GM)	Aggregating indicators by geometric mean (multiplicative) [5].

Table 2 Mix proportion and the summary statistics of the sustainability scores of concrete mixes

Alternatives	Mix Proportion (kg/m^3)						Sustainability Score Statistics				
	W	C	FA	S	NA	RA	Minimum	Average	Maximum	Variance	SD
Control	171	342	0	746	1015	0	20.34	21.75	23.46	0.533	0.730
WB30-RA0	135	225	225	659	1067	0	44.52	47.07	51.89	2.275	1.508
WB30-RA50	135	225	225	659	533	478	47.16	50.33	55.62	4.112	2.028
WB30-RA100	135	225	225	659	0	957	47.21	50.78	55.58	3.476	1.864
WB375-RA0	135	180	180	721	1095	0	50.67	53.17	57.76	1.571	1.253
WB375-RA50	135	180	180	721	548	491	52.66	53.40	54.07	0.167	0.409
WB375-RA100	135	180	180	721	0	982	53.69	55.97	57.78	0.732	0.855
WB45-RA0	135	150	150	772	1103	0	48.14	53.45	56.91	3.996	1.999
WB45-RA50	135	150	150	772	552	500	52.31	56.33	58.31	2.107	1.452
WB45-RA100	135	150	150	772	0	999	51.26	57.75	60.85	4.314	2.077

2.2 Uncertainty Analysis (UA)

The presence of methodological uncertainty implies that the result of sustainability evaluation is not single-valued, but, rather a random variable. Ignoring this randomness (i.e., using a single path for sustainability evaluation) means a less robust analysis, which could lead to a biased decision. To deal with the randomness of Y, UA is introduced to the sustainability evaluation to perform two main functions: to identify the main sources of uncertainty, and to propagate the uncertainties from the source to the output (i.e., Y values) [4]. The main sources of uncertainty, as implied in Section 2.1, are the stages of the multicriteria analysis due to methodological multiplicity. To propagate the uncertainties from these stages, multiple sustainability evaluations must be performed by using all possible methodological combinations mapped in Figure 1, and returning the sustainability score of each concrete mix alternatives per evaluation. The values of Y for each evaluation have been rescaled from 0 to 100 to neutralize the scale effect of the non-equivalent methods. A distribution of Y values can then be obtained, which is used to create its probability density function (PDF) – the output of UA. Several statistics can then be computed from the PDF, such as measures of central tendency, measures of variability, and the probabilities. The following discussions, however, focus only on the minimum (Y_{min}), average (Y_{ave}), and maximum (Y_{max}) sustainability scores, as well as the standard deviation (*SD*) of Y, because these are the minimum requirements for making statistical inferences about the behavior of an exploratory point in the analytical domain.

2.3 Response Surface Methodology

Model fitting in RSM consists of a series of mathematical and statistical techniques to devise an empirical equation [8] – a series of polynomial terms – of the response of interest (or the dependent variable, i.e., sustainability score) as a function of the factors (or independent variables, i.e., W/B and recycled aggregate replacements). This response model can be represented graphically as a surface, hence the name "response surface." Since the response is defined mathematically, numerical (or graphical) optimization is possible. RSM was performed using the Design Expert 11 software.

Four response surfaces can be devised based on the PDFs generated from the results of UA by using the minimum (Y_{min}), average (Y_{ave}), maximum (Y_{max}) and standard deviation (*SD*) values of each concrete mix. Y_{min}, Y_{ave}, and Y_{max} define the range of the possible sustainability scores within the analytical space, while *SD* estimates the variability of Y.

2.4 Data

The data used to demonstrate how to perform exploratory RSM investigation under methodological uncertainty was sourced from [8], which investigates two experimental variables or factors: (1) effect of replacing natural aggregates with low-grade recycled aggregates (RA) at various percentages (0%, 50%, 100%), and (2) the effect of varying W/B (0.30, 0.375, 0.45). The mix proportion is reproduced in Table 2 for convenience. Ten concrete mixes (including the control) created from the combinations of RA and W/B were evaluated for sustainability by multicriteria analysis. In the source paper, time dependent values (i.e., compressive strength, Young's modulus, and air permeability) were reported at several curing periods (i.e., 28 and 91 days). In this paper, however, the analysis is limited to the 28-day curing period value of the time dependent properties as this is the standard minimum curing period required to define concrete quality. The nomenclature used to identity the concrete mixes in the source paper is also adopted here for direct referencing of values.

On the other hand, the indicators used for sustainability evaluation were referred from [8]. In summary, 18 sustainability indicators (Table 3) were utilized, which reflect a combination of mechanical

Table 3 List of sustainability indicators

Indicator Name	Unit
Primary raw materials consumption	kg/m^3
Water consumption	kg/m^3
Recycled materials content	kg/m^3
CO_2 emissions	kg-CO_2/m^3
SOx emissions	kg-SOx/m^3
NOx emissions	kg-NOx/m^3
Particulate matter emissions	kg-PM/m^3
Compressive strength	MPa
Young's modulus	N/mm^2
Cost of raw materials	Monetary
Cost of recycled materials	Monetary
Global warming potential	Tons CO_2 eq.
Photochemical ozone creation potential	kg-C_2H_4 eq.
Acidification potential	kg-SO_2 eq.
Eutrophication potential	kg-PO_4 eq./m3
Human toxicity potential	kg 1.4-Dichlorobenzene eq.
Structural safety	kN-m
Production cost	Monetary

performance, environmental emissions and impacts, and economic cost. The value of each indicator is computed for $1 m^3$ functional unit of concrete. Due to space limitations, the detailed description of each indicator is not reflected here, and the reader is referred to the source literatures ([7] and [8]).

3. RESULTS AND DISCUSSION

3.1 Multicriteria Analysis and Uncertainty Analysis

By performing multiple sustainability evaluation following the methodological combinations in Figure 3, the uncertainties from the stages of multicriteria analysis are propagated. The concrete mixes were evaluated for sustainability using 19 *sets* of indicators created from 18 indicators by alternatively dropping one indicator-at-a-time (see Table 1) to simulate the natural inconsistency of indicator sets, because in concrete sustainability, no accepted single set of indicators exists. Further, 2 normalization methods, 3 weighting approaches, and 2 aggregation rules were applied. Overall 228 methodological combinations were used for sustainability evaluation.

Figure 4 is the PDF of WB30-RA50 generated by plotting the result of 228 multicriteria sustainability evaluation simulations. Each concrete mix will have a different PDF, which graphically explains the susceptibility of its sustainability score, Y, to methodological uncertainties. The variability of Y suggests that the sustainability assessments for concrete should not be performed and presented in a deterministic manner but rather in probabilistic form to emphasize the presence of methodological uncertainties. Performing UA allows for the determination of the minimum and maximum values, which define the range of possible sustainability scores per concrete mix alternative.

The summary statistics of the sustainability scores of the 10 concrete mixes after conducting UA is reflected in Table 2. From this result, it is clear that the sustainability scores of each concrete mix are not invariant to the methodological changes. The differences in the variance imply that methodological uncertainties affect each concrete mix's sustainability score unevenly, which could be attributed to the inherent disparity of the data of indicators between alternatives. The most affected is WB45-RA100 with sustainability score ranging from 51.26 to 60.85, while the least affected is WB375-RA50. Based on the sustainability scores, however, all alternatives are better than the control mix. The statistics in Table 2 were used as inputs for RSM computations.

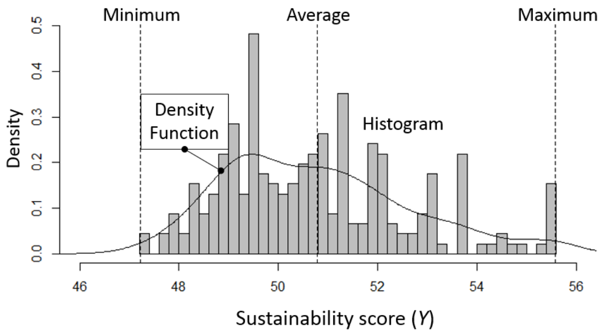


Figure 4 Distribution of Y values for WB30-RA50

3.2 Response Surface Models

The models of the concrete sustainability score responses (Y_{min}, Y_{ave}, Y_{max}) and the estimate model of the variability of sustainability scores, SD, are shown in Table 4. These models were obtained by adding (or removing) higher order terms from an initial polynomial model (usually linear) and performing f-statistic to measure the significance (p-value) of each term in the model. A term can be removed to simplify the model without substantially affecting the predicting power of the response model based on p-value (e.g., p-value > 0.05) of each term. The response model is accepted if $R^2 > 0.90$ and the adjusted $R^2 > 0.80$. Since these response models are empirical, they are valid only for the region of space being investigated (at RA = [0%, 100%] and W/B = [0.30, 0.45]), and their accuracy is dependent on the number of input points.

The response models in Table 4 allow numerical inference of the possible values of the minimum, average, maximum, and the standard deviation of the sustainability score at any point within the analytical space. They also illustrate graphically the trend of Y as a function of RA and W/B, as in Figure 5, which shows the surface generated for Y_{min}. The experimental points are reflected in the response surfaces as filled circular dots. From this surface, it is discernable that the true maximum point (marked with red square) is not part of the set of concrete mixes originally investigated. This maximum would normally be missed in point analysis. Exploratory analysis, therefore, provides the decision maker with better information so that they can select, for example, the optimum values, making their decision more robust.

Figure 6 shows the contour plots of Y_{ave}, Y_{max}, and SD. Figures 5, and 6b demarcate the theoretical limits of Y, but may wrongfully estimate the mean if both are used independently. The use of Figure 6a helps estimate the location of the mean (expected) value of Y, but is not enough to describe the

Table 4 Response surface models for sustainability scores and the standard deviation

Equation No.	Response	Equation	R^2
1	Y_{min}	$-57.969 + 0.088(RA) + 549.378(W/B) - 0.000585(RA)^2 - 694.519(W/B)^2$	0.9793
2	Y_{ave}	$-2.788 + 0.036(RA) + 251.222(W/B) - 277.630(W/B)^2$	0.9649
3	Y_{max}	$23.491 + 147.567(W/B) + 0.001848(RA)^2 - 160.723(W/B)^2 - 0.0399(RA)^2(W/B)^2 + 0.000021(RA)^3(W/B)^2 + 0.067684(RA)^2(W/B)^3$	0.9997
4	SD	$5.044 + 0.037(RA) + 0.000651(RA)^2 - 47.779(W/B)^2 - 0.005404(RA)^2(W/B) - 0.3375(RA)(W/B)^2 + 0.010347(RA)^2(W/B)^2 + 364.719(W/B)^5$	0.9927

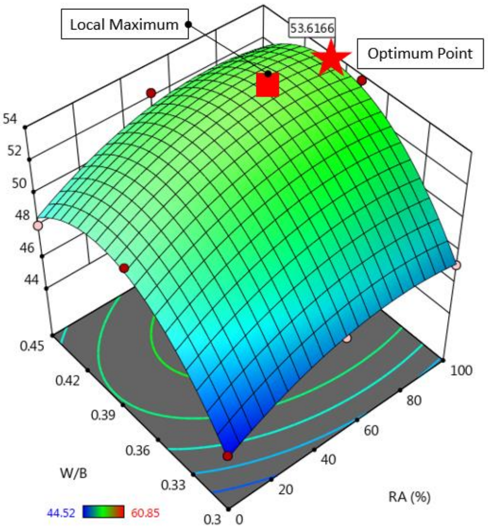


Figure 5 Surface plot of Y_{min}

randomness of the sustainability scores within the limits defined by Y_{min} and Y_{max}. Hence, Figure 6c, is also equally important to provide an estimate measure of variability, or, equivalently, the spread of the Y values from the mean. Lower SD means that the sustainability scores tend to be close to the mean, while higher SD means the sustainability scores are spread in a much wider range. However, SD alone cannot provide an estimate of Y, nor it can define the theoretical limits for Y (the minimum or maximum). Therefore, Figures 5 and 6 should be used jointly to characterize more precisely the behavior of sustainability score at a particular point as a result of methodological choices.

Important trends can also be observed using the response surfaces, directly linking the experimental variables to the behavior of the sustainability scores. In Y_{min} surface (Figure 5), for example, it is observable that increasing use of recycle aggregate is beneficial for sustainability but only up to 80% then the benefit starts to diminish. In the same surface (or alternatively using Eq. 1), increasing W/B is beneficial only up to 0.38. On the other hand, based on average (Figure 6a), both the increases in RA and W/B is beneficial for sustainability. For exploratory investigations, the surfaces generated by Eq. 1 to 4 are highly important because they provide an idea of the randomness of the sustainability score of the concrete mix behaves when the experimental variables are changed continually within the analytical domain.

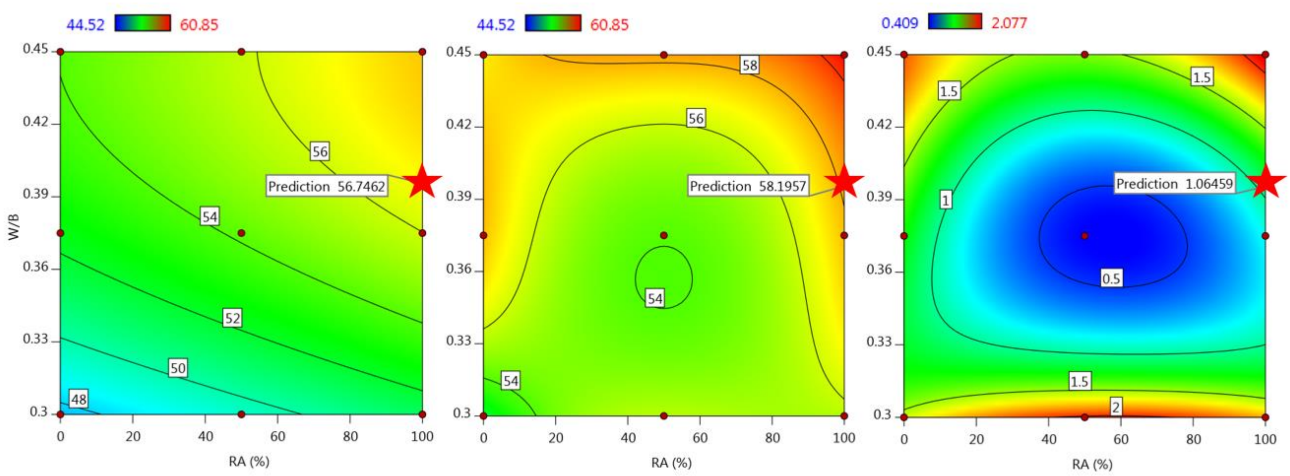
3.3 Sample Numerical Optimization

By optimizing based on predefined criteria, the most sustainable point(s) (or region in the analytical space) can be discovered. In this data set, for example, an analyst might be interested in what point(s) satisfy when maximizing the use of RA within the given range of W/B such that it produces the maximum sustainability score. A numerical optimization can be performed following these criteria because the response models are numerically defined (Table 4).

The optimization criteria described previously are only applied to Y_{min}, Y_{ave}, and Y_{max} since they estimate the sustainability scores, while SD was used only to describe the variability of Y at the located optimum point. Table 5 summarizes the results of numerical optimization. The values within the parentheses indicate the optimum values to obtain a maximum Y, while maximizing RA content within the range of W/B; otherwise, those without parentheses are the equivalent values of Y_{min}, Y_{ave}, Y_{max}, and SD when the optimum values of RA and W/B are substituted to Eq. 1 to 5.

Table 5 shows that, for the same optimization criteria, the optimum points will likely differ. In this case, however, optimizing on Y_{ave} and Y_{max} located the same optimum point at RA = 100% and W/B = 0.45. Using this location, the equivalent minimum sustainability score is 51.5544, which is lower than the optimum value when using Y_{min} with a score of 53.6166. To eradicate the possibility of obtaining a Y value less than the optimal minimum value, optimizing using Y_{min} surface (or Eq. 1) is more desirable.

The optimization result (location and value) for Y_{min} is marked with a 'star' in Figure 5 and 6, showing that the desired criteria is achieved by using RA = 100% and W/B = 0.3955. The response models infer the following statistics for this point: minimum =



(a) (b) (c)

Figure 6 Contour plots of (a) Y_{ave}, (a) Y_{max}, and (c) SD

Table 5 Summary statistics of the sustainability scores of concrete mixes

Response used for Optimization	Numerical Values			RA (%)	W/B	SD
	Y_{min}	Y_{ave}	Y_{max}			
Y_{min}	(53.6116)	56.7462	58.1957	(100)	(0.3955)	1.0646
Y_{ave}	51.5544	(57.6450)	60.7875	(100)	(0.4500)	2.0770
Y_{max}	51.5544	57.6450	(60.7875)	(100)	(0.4500)	2.0770

53.6166, average = 56.7462, maximum = 58.1957, and SD = 1.0646. From these statistics, it is possible to estimate the distribution and PDF (similar to Figure 4) of this point by using, for example, a truncated normal distribution, as illustrated in Figure 7, without again performing multicriteria analysis and uncertainty analysis. In this case, the normal distribution was selected because of its simplicity for this purpose, but other statistical distributions can also be applied (e.g., beta distribution) to obtain the idealized behavior of the sustainability score.

The estimation of this PDF is important because of the following reasons: (1) it provides the range and the random behavior of Y values at the point of interest, (2) it can help guide future design of experiments and validate the experimental results and, (3) it produces quantitative information on locations without actual experimental data, which may be either too costly or takes longer time to obtain to support immediate decisions.

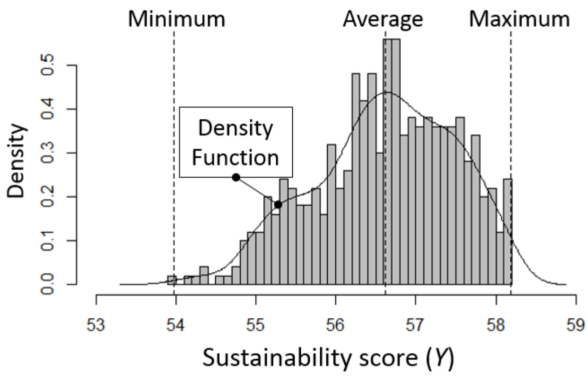


Figure 7 Estimated sustainability scores using truncated normal distribution

4. CONCLUSIONS

The above analyses led to the following conclusions:

(1) Multicriteria analysis alone is not a robust exploratory method for problems involving variables with continuous domain, such as those considered in concrete mix design (i.e., RA and W/B) as it only investigates pre-selected points within the experimental domain.

(2) The application of response surface methodology, together with uncertainty analysis, illustrates more distinctively and continually the behavior of the concrete sustainability score within the experimental domain, leading to the discovery of important points, such as the local maximum or minimum.

(3) Numerical optimization is possible with RSM, which is important to locate point(s) that meet pre-determined sustainability criteria for concrete sustainability to guide future experimentations and support actions needing immediate decisions.

(4) The combination of multicriteria analysis, uncertainty analysis, and response surface methodology makes the quantitative concrete sustainability evaluation robust.

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