

SUSTAINABLE CONCRETING: OPTIMIZATION MODELLING OF THE STRENGTH PROPERTIES OF BIO-SELF COMPACTING CONCRETE INCORPORATING *SPOROSARCINA PASTEURII*, CALCINED CLAY AND LIMESTONE POWDER

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ABSTRACT

*Sustainable concreting is prerequisite for infrastructural development in developing countries so as to meet up with the sustainable development goal of adequate mass housing and other critical infrastructure. Thus, research is ever ongoing aimed at developing cheaper and more durable concrete via the incorporation of bio-based by-products in concrete to improve its properties, as well as optimizing the quantities of these secondary materials for maximum and optimal concrete production. One such revolutionary concrete that is yet to find full application in the developing world is self-compacting concrete, because of the cost and attendant environmental effects. There is thus a need to arrive at optimal materials quantities that can maximize concrete properties without recourse to many trial and error experimentations that are both time and resources consuming. The application of modelling tools in concrete technology aids in the optimization of concrete constituents for optimal self-compacting concrete performance. This research uses optimization techniques to optimize the bacteria dosage as well as model the Compressive and Tensile strength properties of a calcined clay and Limestone powder blended ternary self-compacting concrete using *sporosarcina pasteurii* as Microbial induced calcite precipitation agent and calcium lactate as nutrient source. The Bacteria was incorporated into the concrete at a bacterial content of 1.5×10^8 cfu/ml, 1.2×10^9 cfu/ml and 2.4×10^9 cfu/ml corresponding to the McFarland turbidity scale of 0.5, 4 and 8 while the nutrient (calcium lactate) content was 0.5, 1.0 and 2.0% by weight of cement for each bacterial content. The Compressive strength and tensile strengths at 28 days were determined and the results used for both the model development, strength optimization and model validation, with the strengths as the dependent variable (y) and the bacterial content corresponding to a McFarland scale of and calcium lactate content as the independent variables, X_1 and X_2 respectively. The results show an improvement in the compressive strength from 32N/mm^2 to 45.2N/mm^2 at the optimal bacterial and nutrient content of 1.2×10^9 cfu/ml and 0.5% respectively, and tensile strength from 4.01N/mm^2 to 5.0N/mm^2 . Also, the non-linear regression models proved adequate for optimizing the bacterial content for optimal self-compacting concrete performance.*

Keywords: *Optimization Modelling, Sustainable Concreting, Sporosarcina pasteurii, Self-Compacting Concrete*

1. INTRODUCTION

One of the critical needs of the society, especially in the developing world is the need for mass infrastructure and housing which can only be achieved if the needed construction materials are available locally and are cheap as compared to the conventional materials. This will ensure sustainability and also have a positive impact on the environment. Thus, research is ever ongoing aimed at developing cheaper and more durable concrete via the incorporation of bio-based by-products in concrete to improve its properties, as well as optimizing the quantities of these secondary materials for maximum and optimal concrete production. One such revolutionary concrete that is yet to find full application in the developing world is Self-compacting concrete, because of the cost and attendant environmental effects associated with its production and use (Taku et al., 2023). These challenges can however be mitigated by the incorporation of alternate cementitious and other materials into the self-compacting concrete to improve its properties and reduce the cost of its production. Self-Compacting Concrete (SCC) is a high-performance concrete that is characterized by its ability to spread into heavily reinforced areas under its own weight without the need of external vibration, and has excellent deformability and high resistance to segregation. The use of this revolutionary concrete however requires the optimization of the constituents and/or additives to concrete in order to maximize the properties thereof. There is thus a need to arrive at optimal materials quantities that can maximize concrete properties without recourse to many trial and error experimentations that are both time

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and resources consuming. The application of modelling tools in concrete technology aids in the optimization of concrete constituents for optimal self-compacting concrete performance.

The production of Self Compacting Concrete (SCC) requires large quantities of cement which would make it very expensive, unsustainable and environmentally unfriendly, as compared to Normal Vibrated Concrete. This is because cement is the most expensive and environmentally unfriendly component of concrete and thus contributes more to the cost of construction than the other materials. Other properties of SCC that can be improved upon include its compressive and Tensile strength, pore characteristics and durability characteristics (Mahoutian & Shekarchi 2015, Chen et al, 2020). The pore characteristics or porosity of SCC can be improved by incorporating calcite precipitating bacteria into SCC, since it has been successfully applied in normal vibrated concrete (NVC) (Alisha, et al., 2020, Elyamani, et al. 2014). However, since different bacterial concentrations have varying effects on concrete properties, there is a need to optimize the bacterial dosage and nutrient, that when used in conjunction with other additives in SCC, will maximize the strength properties of the concrete (Raid, et al 2022).

Modelling, as a statistical tool has been used successfully in the predictive modelling and optimization of self-compacting concrete properties by determining optimal materials content that will optimize particular properties of concern (Vijay & Murmu, M., 2018): Modelling techniques that have been successfully used in SCC to optimize bacteria content and other constituents include Artificial Neural Networks, Random Surface Methodology,, Gene Expression Programming, and Random Forrest and Python machine amongst others (Serraye et al., 2022, Mondal & Ghosh 2021, Algaifi, et al., 2021, Rajakarunakaran, et al., 2022). The use of modelling tools (software) not only helps to reduce the number of trial and errors required to optimize specific concrete properties but also help to reduce materials costs and time. Al-Husseini & Al-Mussawy (2015) and Amartey et al., (2024) successfully used DataFit Software by Oakland Technologies to model various concrete properties with good results. This research draws up quadratic models that can be used to optimize the bacterial and nutrient contents requirement for optimal strength performance of self-compacting concrete blended with Calcined clay as cement replacement material and Limestone powder as filler using DataFit software as the modelling tool.

2. MATERIALS AND METHODS

2.1 Bacteria Isolation and Inoculation

The bacteria isolation and inoculation were carried out using the method provided in Bhaskar (2016). The prepared media is cotton flogged and sterilized in an autoclave at a temperature of 1100C for 10 minutes, allowed to cool completely before inoculation of the bacteria. The ureolytic bacteria (*sporosarcina pasteurii*) was isolated from fresh soil by sub culturing in 1L of sterilized nutrient broth and the media incubated at 350C in an orbital shaker for 10days at 125rpm. The bacteria growth was determined in terms of optical density by measuring the rate of absorbance at a wavelength of 500nm. The isolate was purified using the streak plate technique on nutrient agar and the bacteria isolate identified. The quantification of the bacteria was carried out by using spectrophotometer. A blank solution of 0.5ml was placed in the spectrophotometer at a wavelength of 500nm and the reading taken. The blank solution was replaced by the bacteria solution of 0.5ml at the same wavelength and the concentration of the bacteria measured using the relation $y=8.59 \times 10^7 z + 1.3627$ where y is the bacterial concentration per ml and z is the reading at OD600. After the media have cooled, the conical flask is labeled using a masking tape then a standardized inocular of the bacterial isolate is be inoculated. A standardized inocular is a bacterial suspension which its turbidity is compared with that of the McFarland turbidity standard which ranges from scale 0.5 to 9, with each scale representing a bacteria cell density. After inoculating the media with the standardized bacteria, the conical flasks were incubated in an Incubator at a temperature of 370C for 24 hours before use. For this research, the bacterial cell density used corresponded to a McFarland turbidity scale of 0.5, 2.0 and 4.0.

2.2 Determination of Compressive and Tensile Strength

The experimental program was carried out using ten mixes designated S0 to S9. S0 was used as the control mix since it contained neither bacteria nor nutrient and S1 to S9 had different nutrient contents and bacterial cell density. A total of 90 number 100x100x100 cubic millimeter cubes (for compressive strength) and 70 number 100x200 cubic millimeters cylinders (tensile strength) were used to get the strength values for the model development and validation. The water to cementitious material ratio was kept constant at 0.53 for all the mixes. S1 to S3 contain 1.5×10^8 cfu/ml of bacterial at 0.5, 1.0 and 2.0% calcium lactate respectively, while S4 to S6 and S7 to S9 contained 1.2×10^9 cfu/ml and 2.4×10^9 cfu/ml respectively with the nutrient content of 0.5, 1.0 and 2.0% calcium lactate as a percentage of cement used accordingly.

The compressive strength at different ages was determined using the procedure set out in BS EN 12390-3(2009) to evaluate the effect of the varying bacterial cell density and percentage nutrient content on the 7- and 28-days' strength of the self-compacting concrete incorporating calcined clay and limestone powder as SCM and filler respectively. The tensile strength of the Bio-SCC was also determined in line with the procedure outlined in BS EN 12390-6(2009), to determine the load under which cracking develops.

2.3 Modelling of Bio Self-Compacting Concrete Properties

The modelling and model validation was carried out using DataFit Software 9.1.32 developed by Oakland Technologies Ltd and is a scientific and engineering tool that helps to simplify the task of data plotting, regression analysis (curve fitting) and statistical analysis. Its main features include, but not limited to Intuitive graphical interphase, open data base connectivity, multi-variant linear and non-linear regression, variable selection (data mining), predefined regression models, user defined regression variables, Robust solver using the Levenberg-Marquardt method, different solution options, automatic solution ranking and solution logging.

Predictive models were developed using non-linear regression analysis for the optimization of the strength, of the Bio- SCC at curing age of 28 days. These models were developed using DataFit (version 9.1.32), an optimization modelling software developed by Oakdale Engineering. The model calculations, model equations and model plots were carried out using the software. The models were developed at 99% confidence levels, with the model equation taking the form of Eq. 1 as follows.

$$y(x) = a_1 + a_2x + a_3x^2 + \dots + a_nx^{n-1} \quad (1)$$

With the number of observations equal to 10. The dependent variable, y, is the compressive and tensile strengths while the independent variables are the bacterial density (x_1) and the calcium lactate content (x_2) respectively, while a_1, a_2, \dots, a_{n-1} are constants. For the two-variable model, the polynomial model takes the form of Eq. 2 as follows:

$$y = a - bx_1 + cx_2 - dx_2^2 + ex_2^3 \quad (2)$$

2.3 Model Validation

The models developed from the experimental data were validated using the data of the 28 days' compressive and tensile strengths of the self-compacting concrete. The model validation was carried out using DataFit software. Also, the functionality of a predictive model is hinged on the ability of such a model to be validated by confirming that it achieved the purpose for its development, by comparing the model simulations to the independent experimental data set. Other indicators that can be used to validate a model, according to (Zeybek, 2018) include Mean Absolute Error (MAE), Nash Sutcliffe Efficiency (NSE) and Root Mean Square Error (RMSE).

The Mean absolute error of a regression model with respect to a test set is the mean of the absolute values of the individual prediction errors over all instances in the test set and is defined as the average of the absolute difference between the observed and the predicted values in the test sample.

$$MAE = \frac{\sum_{i=1}^n |M_i - P_i|}{n} \quad (3)$$

where M_i and P_i are the absolute experimental and predicted values and n is the number of variables.

The Nash-Sutcliffe Efficiency measures the efficiency of a model by evaluating the degree to which the observed and simulated data fit the 1:1 line, and ranges from 0 to 1. According to Lin, et al., (2017), models with NSE values above 0.5 are satisfactory while those greater than 0.65 and 0.75 are good and indicate high quality respectively.

The NSE is given by

$$NSE = 1 - \frac{\sum_{i=1}^n (P_i - P_{iavg})^2}{\sum_{i=1}^n (M_i - M_{iavg})^2} \quad (4)$$

Where M_i, M_{iavg}, P_i and P_{iavg} are the i^{th} experimental value, average experimental value, i^{th} predicted value and the average predicted value respectively and n is the number of samples.

The Root Mean Square Error is used to evaluate the quality of prediction models and it estimates how well the model can predict the target value. It is given as

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (P_i - M_i)^2}{n}} \quad (5)$$

where M_i and P_i are the absolute experimental and predicted values and n is the number of variables.

3 RESULTS AND DISCUSSION

3.1 Compressive Strength Development and Modelling

Table 1 gives the compressive strength at 28 days curing age of the Bio-SCC, where Y_1 represents the compressive strength at age of 28 days, while the bacterial cell density and percentage of calcium lactate are represented as X_1 and X_2 respectively. For the sake of the modelling, the compressive strength is the dependent variable while the bacteria concentration and calcium lactate (nutrient) used for the concrete production are the independent variables.

Table 1: Compressive Strength values for Model Development

X_1 (cfu/ml)	0	1.5×10^{-8}	1.5×10^{-8}	1.5×10^{-8}	1.2×10^{-9}	1.2×10^{-9}	1.2×10^{-9}	2.4×10^{-9}	2.4×10^{-9}	2.4×10^{-9}
X_2 (%)	0	0.5	1.0	2.0	0.5	1.0	2.0	0.5	1.0	2.0
Y (N/mm ²)	32	40.5	36.6	34.7	45.2	43.7	42.3	40.3	37.5	35.8

It can be seen that the concrete develops more compressive strength as it ages from 0 to 7 and 7 to 28 days, with the maximum strength obtained at an optimal bacterial content of 1.2×10^{-9} cfu and calcium lactate content of 0.5%. However, there is an optimal bacterial content and calcium lactate concrete that produced the maximum compressive strength. According to Dinesh, et al. (2017), surface healing and inner matrix healing takes place simultaneously as the age of the concrete increases. The production of calcium calcite and subsequent surface healing progresses with age as long as the bacteria remains active since the surface is constantly in contact with water and there is available nutrient for MICP. It is therefore no wonder that all properties of concrete that are related to the surface will be maximized at the highest bacteria and nutrient concentrations. However, for properties related to the inner matrix healing like strength, there exists an optimal bacterial cell density and percentage nutrient content that maximizes the properties. This is because at higher calcite precipitation due to higher bacterial content and activity, the surface pores are blocked, leading to lower availability of water inside the mortar matrix for further bacterial activity.

The model for optimizing the constituents for optimal concrete compressive strength was developed using the model data presented in Table 2 which was obtained by solving for Y as the dependent variable while X_1 and X_2 were taken as the independent variables. The model was developed at 99% confidence level.

Table 2: Model Data Table for 28 Days Compressive Strength

Variable	Value	Standard Error	t-ratio	Prob(t)
a	32.0000000176132	3.10660759080525	10.30062507	0.00015
b	-296144193.164094	165903546.605611	-1.78503835	0.13432
c	46.1596621756695	15.3508601208864	3.006975623	0.02986
d	-52.8929954480893	20.4524624558887	-2.58614314	0.04907
e	15.8360939275015	6.84185367986713	2.314591143	0.06851

The model equation for determining the 28 days' compressive strength for a given bacterial dosage (X_1) and nutrient content (X_2), as derived from the model parameters calculated above is given as

$$y = 32.0 - 296144193.164x_1 + 46.15967x_2 - 52.89299545x_2^2 + 15.83609393x_2^3 \tag{6}$$

Figure 1 gives the surface response plot showing the interaction between the bacteria concentration, the nutrient content and the compressive strength at 28 days curing. Y is the compressive Strength in N/mm² while X_1 and X_2 are the bacterial cell concentration in cfu/ml and the calcium lactate content in percentage. The curved nature of the response surface shows a positive interaction within and between the factors and the response (Reji & Kumar, 2023). Generally, the different colors represent different levels of the response, in this case the compressive strength. The cooler colors (blue and green) represent areas of lower strength, while the warmer colors indicate areas of high strength/ interactions (Awolusi et al., 2019). Thus, the levels of interactions of the factors with the response (compressive strength) can be easily identified using the response surface plot.

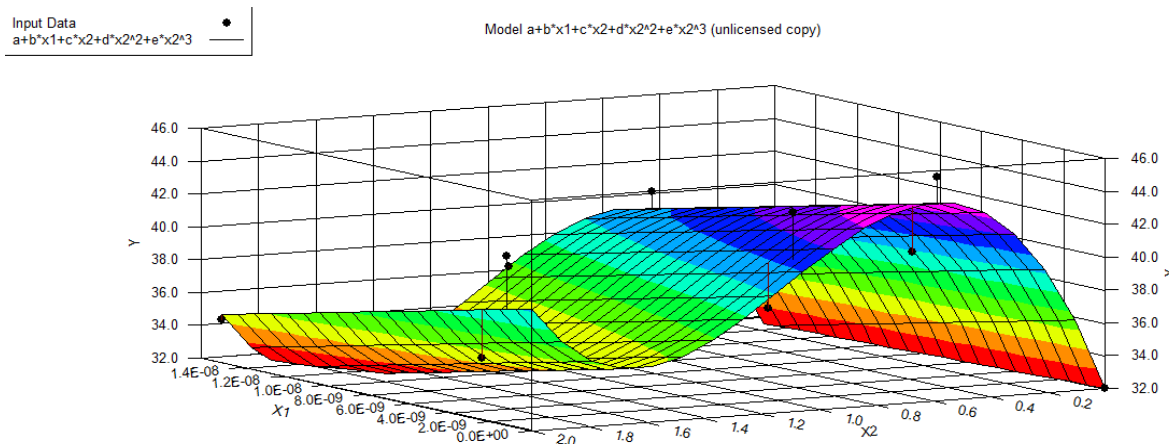


Figure 1: 3D Model Plot for Compressive Strength at age of 28 Days

3.2 Model Validation for Compressive Strength

The model developed was used to calculate strength values for the given independent values and the result compared with the experimental values for the 28 days compressive strength. Table 3 gives the predicted values from the model, the percentage error and the residual values for the 28 days compressive strength.

Table 3: Predicted Model Values 28 Days Compressive Strength

X ₁	X ₂	Y	Calc. Y	Residual	% error	Abs. residual
0	0	32	32			
1.5x10 ⁻⁸	0.5	40.5	39.39	1.106069	2.73103434	1.106068913
1.5x10 ⁻⁸	1	36.6	36.66	-0.0606	-0.1655677	0.060597775
1.5x10 ⁻⁸	2	34.7	34.99	-0.29393	-0.8470637	0.293931099
1.2x10 ⁻⁹	0.5	45.2	43.48	1.719279	3.80371471	1.719279047
1.2x10 ⁻⁹	1	43.7	40.75	2.952612	6.75655002	2.952612359
1.2x10 ⁻⁹	2	42.3	39.08	3.219279	7.61058874	3.219279035
2.4x10 ⁻⁹	0.5	40.3	43.13	-2.82535	-7.0107889	2.825347921
2.4x10 ⁻⁹	1	37.5	40.39	-2.89202	-7.7120389	2.892014609
2.4x10 ⁻⁹	2	35.8	38.73	-2.92535	-8.1713629	2.925347933

The data in Table 3 shows that there is both a positive and negative difference between the actual experimental and the Y values predicted by the model, but in most cases the percentage error falls within ±5% of the actual, with the average percentage error of 3.7% which shows that the model can be used to predict the 28 days' compressive strength with more than 95% accuracy for values of X₁ and X₂. Similarly, the model can be used to the optimal values of the independent variables that can give a particular required strength. Also, Figure 2 gives the normal probability plot with R² value of over 95% the 28 days' strength of the SCC can be optimized using the model.

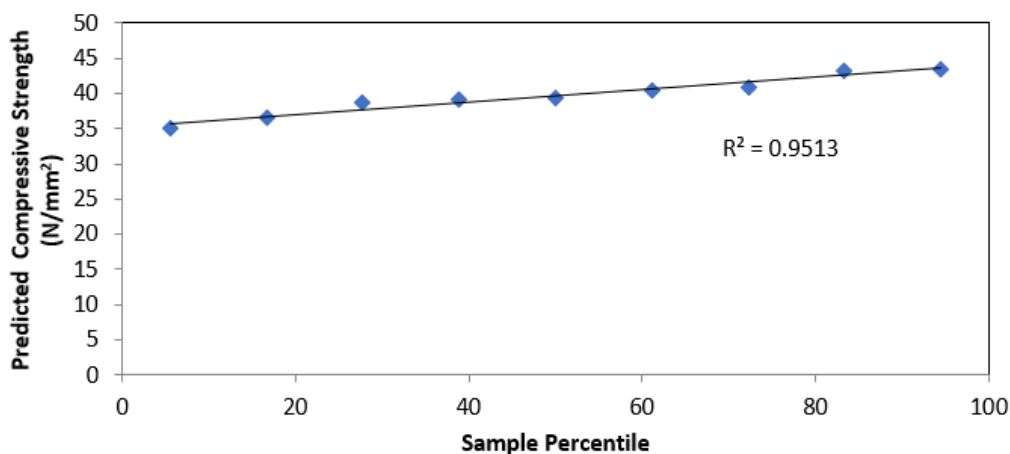


Figure 2: Normal Probability plot for Compressive Strength Model

Table 4 gives the fit model statistics properties for the validated model. It can be seen that the model has a correlation coefficient of 99.5% and an adjusted coefficient of 87.9% with MAE, NSE and RMSE values all falling within the specified limits. It can thus be said that based on the performance indices examined, the model satisfies the prediction model conditions. This is in line with Mondal & Ghosh (2021), and Amartey et al (2024). Thus, for a desired target compressive strength, the bacteria concentration and nutrient content can be determined that will satisfy the said strength, taking cognizance of other parameters in the concrete.

Table 4: Fit Model Statistics Properties

Regression Statistics	Value	Limit
Multiple R	0.994973	1.0
R Square	0.989972	1.0
Adjusted R Square	0.878861	1.0
Standard Error	0.12377	Close to 0
Observations	10	
Mean Absolute Error (MAE)	0.01	Close to 0
Nash-Sutcliffe Efficiency	0.049	≤1.0
Root Mean Square Error	0.001	Close to 0

3.3 Tensile Strength Development and Modelling

The tensile strength of the bio-SCC was determined at 28 days age of the concrete and Table 5 gives the result of the experimental program to determine the tensile strength of the BIO-SCC where Y_1 is the strength in tension at 28 days ages and X_1 and X_2 bacterial cell density and calcium lactate content, respectively.

Table 5: Tensile Strength values for Model Development

X_1 (cfu/ml)	0	1.5E-8	1.5E-8	1.5E-8	1.2E-9	1.2E-9	1.2E-9	2.4E-9	2.4E-9	2.4E-9
X_2 (%)	0	0.5	1.0	2.0	0.5	1.0	2.0	0.5	1.0	2.0
Y_2 (N/mm ²)	4.01	4.5	4.3	4.1	5.5	5.1	4.5	4.0	4.4	4.2

The strength development pattern for the tensile and compressive strengths are similar due to the fact that the two are related (Weber & Thiele, 2019). Also, for a given value of X_1 , the tensile strength is Maximized with X_2 at 0.5%, with the highest value of Y_1 obtained at X_1 value of 1.2E-9 cfu/ml.

The values of Y_1 , X_1 and X_2 were plotted into DataFit to obtain the model data presented in table 6 from which the model equation is developed as given in equation 7;

$$y = 4.01 - 28120008.92044x_1 + 2.97520412x_2 - 3.041870764x_2^2 + 0.83101069067x_2^3 \tag{7}$$

Table 6: Model Data Table for 28 Days Tensile Strength Model Development

Variable	Value	Standard Error	t-ratio	Prob(t)
a	4.01000001	0.520782112	7.699957	0.00059
b	-28120008.92	27811558.73	-1.01109	0.35837
c	2.975204122	2.573370832	1.156151	0.29986
d	-3.041870764	3.428587709	-0.88721	0.4156
e	0.831010691	1.146947243	0.724541	0.50121

The 3D response surface graph for the tensile strength model showing the interaction between the dependent variable (y) and the independent variables X_1 and X_2 is presented in Figure 3. Y is the tensile Strength in N/mm² while X_1 and X_2 are the bacterial cell concentration in cfu/ml and the calcium lactate content in percentage.

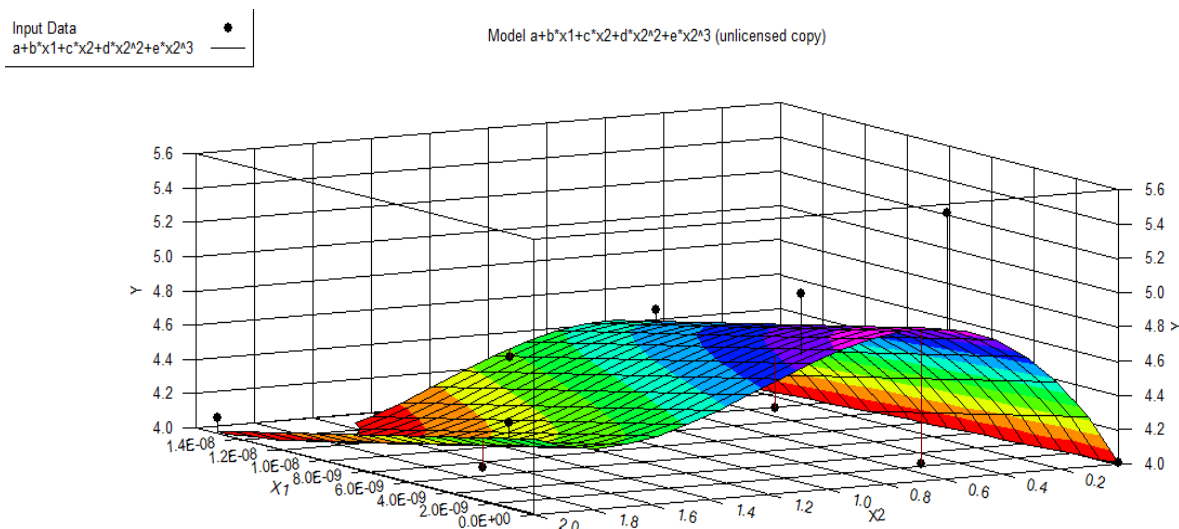


Figure 3: 3D Model Plot for 28 days Tensile Strength Development

3.4 Tensile Strength Model Validation

The model equation presented in (2) is validated using DataFit software by inputting the 28 days’ tensile strength values and solving for the predicted or model values.

Table 7 gives the predicted data from the model using software as well as the absolute residuals and percentage error with the average percentage error from the prediction of 5.66% showing that there is a 95% chance of the model predicting the tensile strength correctly. Also, the average absolute residual of 0.261 indicates a good model with the maximum residual value of 0.69 showing that the experimental and calculated “y” values are close.

Table 7: Predicted Model Values 28 Days Tensile Strength

X ₁	X ₂	Y	Calc. Y	Residual	% error	Abs. residual
0	0	4.01	4.01	-9.8E-09	-2.4E-07	9.7599E-09
1.5E-08	0.5	4.5	4.419211	0.080789	1.79532	0.080789418
1.5E-08	1	4.3	4.352544	-0.05254	-1.22195	0.052543924
1.5E-08	2	4.1	4.019211	0.080789	1.970473	0.080789412
1.2E-09	0.5	5.5	4.807267	0.692733	12.59515	0.692733295
1.2E-09	1	5.1	4.7406	0.3594	7.047058	0.359399953
1.2E-09	2	4.5	4.407267	0.092733	2.06074	0.092733289
2.4E-09	0.5	4	4.773523	-0.77352	-19.3381	0.773522694
2.4E-09	1	4.4	4.706856	-0.30686	-6.97400	0.306856037
2.4E-09	2	4.2	4.373523	-0.17352	-4.13149	0.173522700

Also, the model statistics properties shown in Table 8 shows that the model has a correlation coefficient of 99.6% and an adjusted coefficient of 86.8% with MAE, NSE and RMSE values of 0.01, 0.049 and 0.001 respectively all falling within the specified limits for a good model, indicating a good model.

Table 8: Fit Model Statistics Properties for Tensile Strength Modelling

Regression Statistics	Value	Limit
Multiple R	0.996329397	1.0
R Square	0.992672268	1.0
Adjusted R Square	0.867672268	1.0
Standard Error	0.41020317	Close to 0
Observations	10	
Mean Absolute Error (MAE)	0.01	Close to 0
Nash-Sutcliffe Efficiency	0.049	≤1.0
Root Mean Square Error	0.001	Close to 0

The model can thus be used to predict the tensile strength as well as optimize the bacteria dosage and nutrient content that will give a required target tensile strength, all other parameters being taken into consideration. The normal probability plot is given in Figure 4.

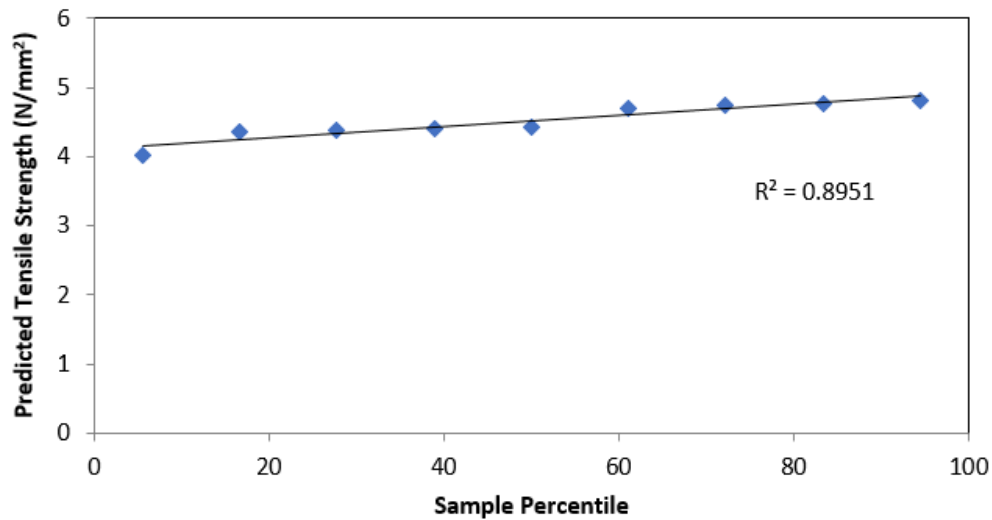


Figure 4: Normal Probability plot for Compressive Strength Model

4. CONCLUSIONS

Based on the findings of the study, it can be concluded that:

- the incorporation of *Sporosarcia pasteurii* in self-compacting concrete improved the compressive strength from 32N/mm² to 45.2N/mm² and tensile strength from 4.01N/mm² to 5.0N/mm² at the optimal bacterial and nutrient content of 1.2e-9cfu and 0.5% of cementitious content respectively. Thus it can be inferred that the use of MICP bacteria improves the overall performance of self-compacting concrete with respect to strength and durability characterization.
- DataFit software was used successfully to develop 3D optimization quadratic regression models for optimizing bacterial dosage and calcium lactate content that can maximize the strength properties of a ternary Bio-SCC with the compressive and tensile strengths optimization models of the Bio-SCC at age 28 days developed as $y = 32.0 - 296144193.164x_1 + 46.15967x_2 - 52.89299545x_2^2 + 15.83609393x_2^3$ and $y = 4.01 - 28120008.92044x_1 + 2.97520412x_2 - 3.041870764x_2^2 + 0.83101069067x_2^3$ respectively.
- Sustainable concreting can be ensured through, amongst other means, the optimization of concrete properties by optimizing the material content of the concrete

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