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MODELLING THE PERMEATION PROPERTIES OF SELF-COMPACTING CONCRETE INCORPORATING SPOROSARCINA PASTEURII

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ABSTRACT

The face of concreting has been revolutionized with the development of self-compacting concrete, the introduction of Microbial Induced Calcite Precipitation (MICP) in concrete as well as the use of secondary cementitious materials in concrete, as it helps to improve the pore characterization of the concrete by the filling of the pore spaces and hence enhance its porosity and durability. The use of these 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 the porosity characterization of the concrete 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. In this research linear optimization models for predicting the water absorption and sorptivity of the Bio- self-compacting concrete incorporating sporosarina Pasteurii at different bacterial cell density and nutrient content with respect to age of concrete were developed for these concrete properties at 7 and 28 days with the bacterial concentration and calcium calcite content as the independent variables and water absorption and sorptivity as dependent variables; and the developed models validated using experimental data in DataFit Software. Results obtained showed that the developed linear models which took the quadratic form y(x)=a_1+a_2 x+a_3 x^2+⋯+a_n x^(n-1) were adequate for the prediction and optimization of the water absorption and sorptivity of the bio- self-compacting concrete.

Keywords: DataFit Software, Model Validation, Permeation Properties, Self-compacting concrete, sporosarcina pasteurii

1. INTRODUCTION

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 [1]. The concrete so produced is sufficiently cohesive, flows without segregation or bleeding and has very reliable quality. Self-compacting concrete has low yield stress, high deformability, moderate viscosity, and high stability characteristics that enhance its property in both a fresh and hardened state. Despite the many advantages inherent in the use of, and ground breaking researches on Self-Compacting Concrete there is no limit to improvements that can be brought about on this very important construction material, hence the introduction of new materials and technologies into SCC to help improves its properties. One such improvement is the introduction of Microbial induced calcite precipitation (MICP), which has been used successfully by researchers in enhancing concrete properties such as Compressive Strength [2], Concrete durability [3] remediation of cracks [4], water absorption [5], surface consolidation [6] and Rebar corrosion inhibition [7] amongst other applications.

One property of SCC that can be improved upon is its pore characterization or porosity, measured using the ability of the concrete to resist the ingress of water and other solutions into its matrix. The use of secondary cementitious materials, fillers and microbial induced calcite precipitation has been shown to improve the porosity of SCC [8]. The use of modelling, as a statistical tool in the optimization of concrete properties is well documented, with Artificial Neural Networks [9], Random Surface [10], Gene Expression Programming [11], Random Forrest and Python machine learning [12] being the most utilized optimization and predictive modelling tools employed in concrete technology. This work is aimed at developing optimization models for predicting and optimizing the water absorption and properties of Bio Self-Compacting Concrete incorporating *sporosarcina Pasteurii* at different bacterial cell densities and nutrient content by developing using the bacterial concentration and nutrient content as the independent variables.

2. METHODOLOGY

2.1. Experimental Data

The data used for the predictive modelling as well as the model validation was obtained from experimental programs for water absorption and sorptivity at 7 and 28 days respectively. The water absorption and sorptivity tests were carried out to determine the effect of varying concentrations of *sporosarcina pasteurii* (corresponding to McFarland turbidity scale of 0.5, 4.0 and 8.0) and calcium lactate (nutrient) content of 0.5%, 1.0% and 2.0% by weight of cementitious content on the porosity of the Bio-SCC [8].

The Sorptivity test was carried out using the procedure outlined in [13] to determine the susceptibility of the unsaturated concrete to the penetration of water through capillarity by determining the increase in the mass of the specimen resulting from absorption of water as a function of time when only one surface is exposed to water. The test was carried out at 7 and 28 days for each mix to evaluate the short and long-term effects of the SCM, filler and bacteria as well as nutrients on the rate of water absorption through interconnected capillary poles. A total of and 90 discs cut from 30 cylinders were used for the determination of sorptivity for Bio-SCC.

The water absorption test was carried out to determine, in line with the provisions of [14,15], the change in water absorption capacity of the specimens with age after being submerged for 24 hours. The test was carried out at 7 and 28 days to monitor the change in water absorption capacity of the SCC with changing varying bacterial dosage and calcium lactate concentration at fixed SCM and filler quantities. For each mix, three 50x50x50mm^3 cubes were used and the average value taken. A total of 90 cubes were used in the determination of water absorption of normal and Bio self-compacting concretes.

2.2. Modelling of Bio Self-Compacting Concrete Properties

Predictive models were developed using linear regression analysis for the optimization of the strength, water absorption and sorptivity of the Bio-SCC at different ages. 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 linear models were developed at 99% confidence levels, with the model equation taking the quadratic form $y(x) = a_1 + a_2x + a_3x^2 + \cdots + a_nx^{n-1}$, with the number of observations equal to 10. The dependent variable, y, were the water absorption, sorptivity, compressive and tensile strengths respectively while the independent variables are the bacterial density (x_1) and the calcium lactate content (x_2) respectively. Model equations were developed for optimization of the water absorption, sorptivity, compressive strength and tensile strength at 7 and 28 days curing. In all cases, the models were developed at 99% confidence levels and the model plots given accordingly.

2.2.1. Model Validation

The models developed from the experimental data from DataFit software were validated using the 28 days' properties of the self-compacting concrete. The, water absorption and sorptivity data at 28 days curing were inserted into the DataFit software and the model predicted values obtained. The percentage error was also calculated using the software and the residual normal probability plot showing the deviation of the calculated Y values from the actual experimental values for each of the self-compacting concrete properties determined. Both the modelling and model optimizations were carried out using the DataFit software.

3. RESULTS AND DISCUSSION

3.1. Water Absorption Model Development

The water absorption data given in table 1 as obtained from the experimental program for the 7 and 28 days water absorption was used to develop the regression model for water absorption by solving the variables in the DataFit software. X_1, X_2, Y_1 and Y_2 represent the bacterial concentration, calcium lactate content, 7 days' water absorption and 28 days' water absorption respectively.

Table 1. Water Absorption values for Model Development

X_1 (cfu/ml)	0	1.5E-008	1.5E-008	1.5E-008	1.2E-009	1.2E-009	1.2E-009	2.4E-009	2.4E-009	2.4E-009
X_2 (%)	0	0.5	1.0	2.0	0.5	1.0	2.0	0.5	1.0	2.0
Y_1 (N/mm^2)	6.8	6.2	6.0	5.6	5.3	5.1	4.8	4.8	4.3	3.7
Y_2 (N/mm^2)	3.4	2.9	2.4	2.2	2.0	2.0	1.7	1.7	1.5	1.2

3.1.1. Modelling 7 Days Water Absorption

The 7 days' water absorption model is determined from the model parameters presented in table 1. The values of X_1, X_2 and Y_1 are used to generate the data in table 2 and a, b, c, d and e are the model parameters.

Table 2. Regression Variable Results for 7 Days Water Absorption

Variable	*Value*	*Standard Error*	*t-ratio*	*Prob(t)*
a	6.800000005	0.720187944	9.441979781	0.00022
b	84633751.28	47025929.29	1.799725227	0.1318
c	-6.078632683	3.597005872	-1.68991459	0.15184
d	5.296126517	4.756128769	1.113537243	0.31612
e	-1.40888976	1.583582604	-0.88968505	0.41439

99% Confidence Intervals

Variable	*Value*	*99% (+/-)*	*Lower Limit*	*Upper Limit*
a	6.800000005	2.903869809	3.896130196	9.703869813
b	84633751.28	189613249.5	-104979498.2	274247000.8
c	-6.078632683	14.50348738	-20.58212006	8.424854692
d	5.29612651 677125	19.17718681	-13.88106029	24.47331332
e	-1.40888976	6.385163418	-7.794053178	4.976273657

The model equation for determining the 7 days' water absorption for a given bacterial dosage (X_1) and nutrient content (X_2), as derived from the model parameters calculated above is given as**:**

$$\boldsymbol{y = 6.8 + 84633751.278x_1 - 6.0786326x_2 + 5.29612652x_2^2 - 1.40889x_2^3} \quad \textbf{(1)}$$

Figure 1 gives the 3D plot of the regression model data for the 7 days' water absorption and shows the relationship between the calcium lactate content and bacterial concentration and their effect on the 7 days' water absorption.

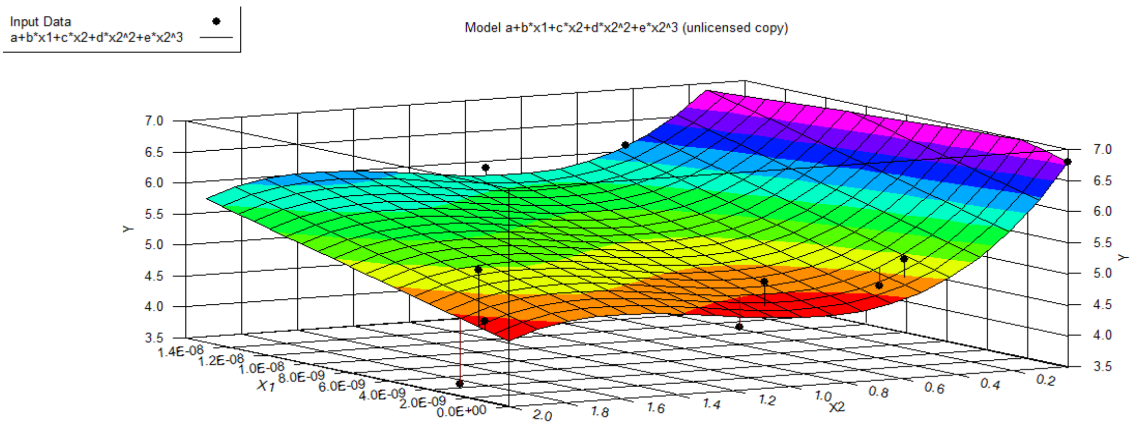

Figure 1. 3D Response Surface Model Plot for 7 Days Water Absorption

3.1.2. Modelling 28 Days Water Absorption

The model parameters for the 28 days water absorption as solved in DataFit software are presented in table 3 at 99% confidence interval where a, b, c, d and e are the model parameters.

Table 3. Regression Variable Results

Variable	*Value*	*Standard Error*	*t-ratio*	*Prob(t)*
a	3.399999993	0.408528101	8.322560888	0.00041
b	60310730.28	26689973.85	2.259677384	0.07338
c	-5.079506286	2.040410529	-2.48945309	0.0552
d	4.454366593	2.697806786	1.651106602	0.15963
e	-1.182120165	0.898217335	-1.31607365	0.24525

99% Confidence Intervals

Variable	*Value*	*99% (+/-)*	*Lower Limit*	*Upper Limit*
a	3.399999993	1.647226155	1.752773838	5.047226148
b	60310730.28	107616643.6	-47305913.28	167927373.8
c	-5.079506286	8.227139292	-13.30664558	3.147633007
d	4.454366593	10.87782674	-6.423460147	15.33219333
e	-1.182120165	3.621702118	-4.803822283	2.439581952

The model is deduced from the model parameters presented in table 2 at 99% confidence level and it takes the form:

$$\boldsymbol{y = 3.4 + 60310730.28x_1 - 5.0795x_2 + 4.45436659x_2^2 - 1.18212x_2^3} \quad (2)$$

Figure 2 gives the response surface 3D plot of the model and shows the interaction between the bacteria concentration, the nutrient content and the water absorption of the bio-SCC at 28 days curing. It shows the mutual interaction effect of the bacteria concentration and the nutrient content.

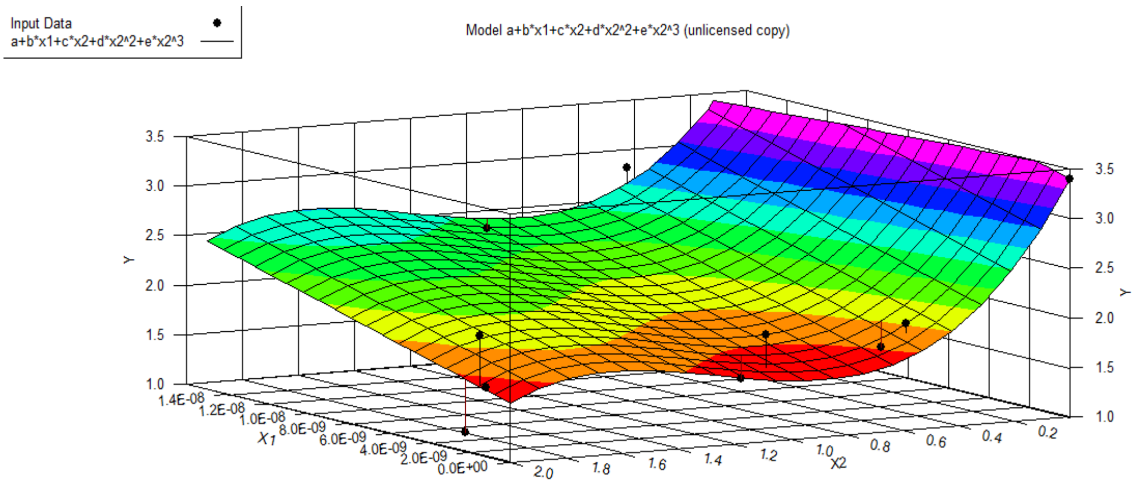

Figure 2. 3D Model Plot for 28 Days Water Absorption

3.2. Sorptivity Model Development

The sorptivity model equations for the Bio-SCC at 7 and 28 days curing are obtained by fitting the data in table 4 into the software and deriving the model data to obtain the model equations, Y_1, Y_2, X_1 and X_2 given in table 4 represents the 7 days' Sorptivity, 28 days' sorptivity, bacterial concentration and calcium lactate content respectively.

Table 4. Sorptivity 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_1 (N/mm^2)	0.103	0.098	0.073	0.071	0.067	0.053	0.050	0.048	0.045	0.041
Y_2 (N/mm^2)	0.0713	0.0437	0.0406	0.0402	0.0339	0.0326	0.0319	0.0307	0.0303	0.0278

3.2.1 Modelling 7 Days Sorptivity

The regression variable result, standard error, t-ratio and prob(t) values at 99% significant value for the sorptivity at 7 days curing are given in table 5.

Table 5. Regression Variable Results for 7 Days Sorptivity

Regression Variable Results

Variable	*Value*	*Standard Error*	*t-ratio*	*Prob(t)*
a	0.103	1.35E-02	7.607465506	0.00062
b	2306216.426	884074.3145	2.608622814	0.04775
c	-0.135148568	6.76E-02	-1.99856794	0.10213
d	9.54E-02	8.94E-02	1.06645523	0.33498
e	-2.05E-02	2.98E-02	-0.68878931	0.52161

99% Confidence Intervals

Variable	*Value*	*99% (+/-)*	*Lower Limit*	*Upper Limit*
a	0.103	5.46E-02	4.84E-02	0.15759194
b	2306216.426	3564676.044	-1258459.617	5870892.47
c	-0.135148568	0.272661505	-0.407810074	0.137512937
d	9.54E-02	0.360525747	-0.265169836	0.455881658
e	-2.05E-02	0.120039286	-0.14054517	9.95E-02

The 3D model equation for the 7 days sorptivity is derived from the model data in table 5 as

$$y = 0.1030 + 2306216.4264x_1 - 0.1351486x_2 + 9.5355911x_2^2 - 2.0505884x_2^3. \quad (3)$$

The relationship and interaction between the dependent and independent variables for the 7 days sorptivity data is shown in response surface in figure 3.

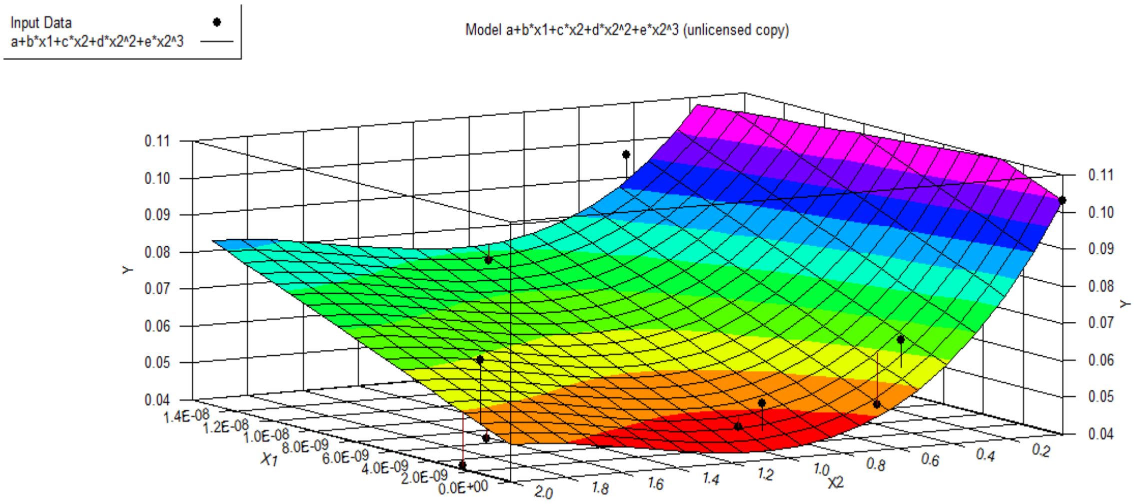

Figure 3. Model 3D Response Surface Plot for 7 Days Sorptivity

3.2.2. Modelling 28 Days Sorptivity

The relevant sorptivity data presented in table 4 is used to generate the regression variable results used in the model development for 28 days sorptivity modelling. The variables a, b, c, d and e are the model constants. The model data are generated at 99% confidence level and the result is given in table 6.

Table 6. Regression Variable Results for 28 Days Sorptivity

Regression Variable Results

Variable	*Value*	*Standard Error*	*t-ratio*	*Prob(t)*
a	7.13E-02	4.49E-03	15.89158049	0.00002
b	743149.415	293122.1588	2.535289103	0.05219
c	-0.136027389	2.24E-02	-6.070274115	0.00175
d	0.131029483	0.029628615	4.422396552	0.00688
e	-3.64E-02	9.86E-03	-3.690916496	0.01413

99% Confidence Intervals

Variable	*Value*	*99% (+/-)*	*Lower Limit*	*Upper Limit*
a	7.13E-02	1.81E-02	5.32E-02	8.94E-02
b	743149.415	1181897.856	-438748.4413	1925047.271
c	-0.136027389	9.04E-02	-0.226381798	-4.57E-02
d	0.131029483	0.119465537	1.16E-02	0.25049502
e	-3.64E-02	3.98E-02	-7.62E-02	3.37E-03

The 3D model equation for the 28 days sorptivity is derived from the model data in table 6 as:

$$y = 7.13\text{E} - 02 + 743149.415048x_1 - 0.13602739x_2 + 0.13103x_2^2 - 3.64097\text{E} - 02x_2^3 \qquad (4)$$

The relationship and interaction between the dependent and independent variables for the 28 days sorptivity data is shown in figure 4.

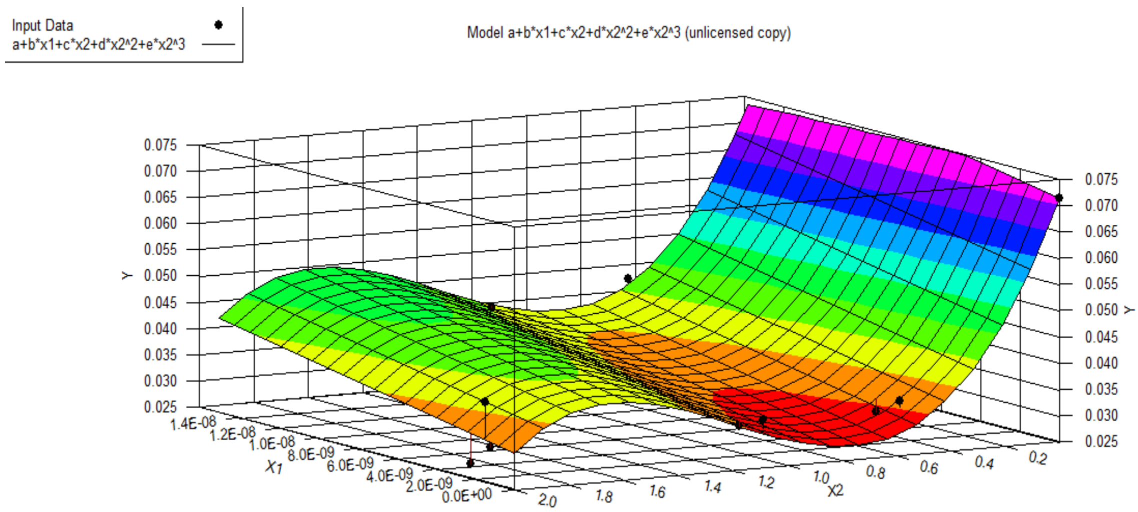

Figure 4. Model 3D Response Surface Plot for 28 Days Sorptivity

3.3. Model Validation

3.3.1 Water Absorption Model Validation

The 28 days water absorption model for a given value of bacteria concentration and calcium lactate content is given in equation 4. This model equation is validated using DataFit modelling software and the predicted 28 days water absorption values from the model, the percentage error and residual values are given in table 7 while the Residual Normal Probability Plot is given in figure 5.

Table 7. Model Validation for 28 Days Water Absorption

X_1	X_2	Y	Calc. Y	Residual	% error	abs residual
0	0	3.4	3.4	7.23E-09	2.13E-07	7.23E-09
1.50E-08	0.5	2.9	2.7	0.169265568	5.836744	0.169265568
1.50E-08	1	2.4	2.5	-0.09740109	-4.05838	0.09740109
1.50E-09	2	2.2	1.7	0.50804143	23.09279	0.50804143
1.20E-09	0.5	2	1.9	0.101553646	5.077682	0.101553646
1.20E-09	1	2	1.7	0.334886988	16.74435	0.334886988
1.20E-09	2	1.7	1.7	0.026134649	1.537332	0.026134649

2.40E-09	0.5	1.7	2	-0.27081923	-15.9305	0.27081923
2.40E-09	1	1.5	1.7	-0.237485888	-15.8324	0.237485888
2.40E-09	2	1.2	1.7	-0.534176081	-44.5147	0.534176081

The water absorption model has minimum and maximum residuals of 7.231e-9 and 0.50804 respectively with an average percentage error of 13.5%, which gives the model a 86.5% chance of predicting the 28 days water absorption. However, a study of the normal probability plot in figure 5 shows that the model ought to be sufficient for predicting the water absorption as the points lie close to the line of best fit. Generally, if the points on a residual plot show no pattern, that is, the points are randomly dispersed, we can conclude that a linear model is an appropriate model. If the points show a curved pattern, such as a U-shaped pattern, we can conclude that a linear model is not appropriate and that a non-linear model might fit better. The points all lie close to the line of best fit as shown in figure 5.

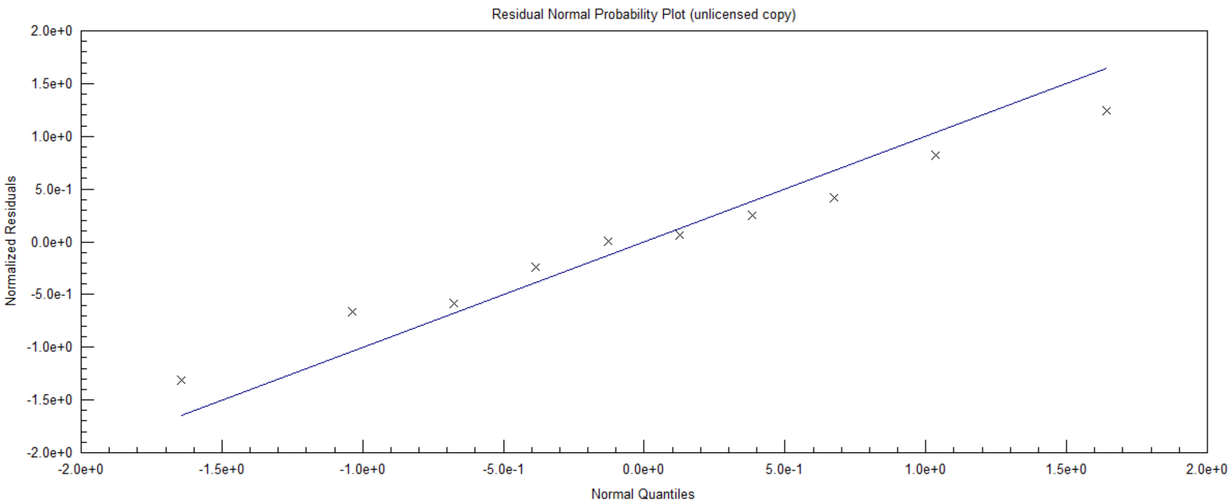

Figure 5. Residual Normal Probability Plot for Water Absorption

Table 8 gives the fit model statistics properties for the validated model, showing the acceptable limits for each property.

Table 8. Fit Model Statistics Properties for 28 Days Water Absorption

Regression Statistics	*Value*	*Limit*
Multiple R	0.989252418	1.0
R Square	0.978620346	1.0
Adjusted R Square	0.853620346	1.0
Standard Error	0.308446851	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

It can be seen that the model has a correlation coefficient of 97.8% and an adjusted coefficient of 85.4% 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.

3.3.2. Sorptivity Model Validation

The 28 days sorptivity model equation given in (4) is validated using DataFit software and other statistical measures. The predicted values from the model, the residual values and the percentage error are given in table 9 while figure 6 gives the plot of the residual probabilities.

Table 9. Model Validation for 28 Days Sorptivity

X_1	X_2	Y	$Y_{calc.}$	Residual	% error	ABS residual
0	0	0.0713	0.0713	1.23E-10	1.72E-07	1.23E-10
1.50E-08	0.5	0.0437	0.0426	0.00106029	2.426282	0.001060285
1.50E-08	1	0.0406	0.041	-0.0004397	-1.08304	0.000439715
1.50E-09	2	0.0402	0.0332	0.00699909	17.41066	0.006999087
1.20E-09	0.5	0.0339	0.0324	0.00151575	4.47123	0.001515747
1.20E-09	1	0.0326	0.0309	0.00181575	5.569776	0.001815747
1.20E-09	2	0.0319	0.033	-0.001078	-3.37921	0.001077969
2.40E-09	0.5	0.0307	0.0333	-0.002576	-8.39098	0.002576032
2.40E-09	1	0.0303	0.0317	-0.001376	-4.54136	0.001376032
2.20E-09	2	0.0278	0.0337	-0.0059211	-21.299	0.005921118

A comparison of the data in table 9 and the residual probability plot in figure 6 shows that there is both a positive and negative difference between the actual experimental and the Y values predicted by the model, but in all cases the data points lie close to the curve. The average percentage error of 6.86% and a minimum and maximum residual values of -0.0059 and 0.007 respectively indicate that the model can be used to predict the 28 days' sorptivity with more than 93% accuracy for values of X_1 and X_2.

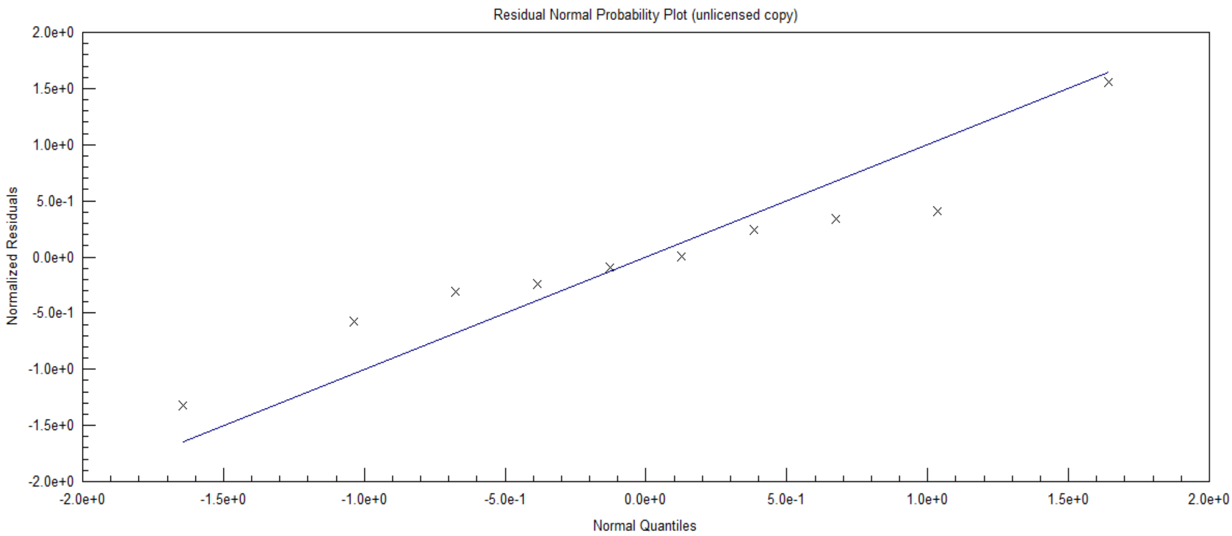

Figure 6. Residual Normal Probability Plot for 28 Days Sorptivity

Table 10 gives the fit model statistics properties for the validated model, showing the acceptable limits for each property. It can be seen that the model has a correlation coefficient of 99.0% and an adjusted coefficient of 86.6% 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. Thus, for a desired target Sorptivity, the bacteria concentration and nutrient content can be determined that will satisfy the said sorptivity, taking cognizance of other parameters in the concrete.

Table 10. Fit Model Statistics Properties for 28 Days Sorptivity

Regression Statistics	*Value*	*Limit*
Multiple R	0.99543	1.0
R Square	0.990881	1.0
Adjusted R Square	0.865881	1.0
Standard Error	0.003531	Close to 0
Observations	10	

Mean Absolute Error (MAE)	0.02	Close to 0
Nash-Sutcliffe Efficiency	0.053	≤1.0
Root Mean Square Error	0.001	Close to 0

4. CONCLUSION

DataFit Software has been successfully applied to model the permeation properties of Bio self-compacting concrete at different ages. The model equations, developed at 99% confidence level, have been shown to be capable of optimizing a particular property of SCC using bacteria concentration and nutrient content as the independent variables. Both the prediction and optimization of the SCC properties can be carried out using modelling tools in the software.

The use of predictive models developed at 99% confidence level for optimizing self-compacting concrete properties at different levels using bacterial density and calcium lactate concentration as independent variables is recommended since no particular bacterial concentration or calcium lactate content optimizes all the properties of self-compacting concrete. However, for higher model accuracy, non-linear models could be developed using the software.

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AUTHORS CONTRIBUTION

This work was carried out in collaboration among all authors.

ONFLICT OF INTEREST

The Authors wish to acknowledge the Head of Department of Civil Engineering, Ahmadu Bello University Zaria for allowing the use of the Structures Laboratory for this research. Also, Joseph Sarwuan Tarka University is appreciated for sponsoring this research through the Tertiary Education Trust Fund (TETFund) intervention.

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