A Computational Model for Concrete Based on Sum of the Mix Ratios, Water-Cement Ratio and the Aggregate Size

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Abstract

This paper presents a computational model for predicting concrete strength based on coarse sum of mix ratios, aggregate size, and water-cement ratio.Laboratory data from John (2024) were used to establish the model, incorporating three different coarse aggregate sizes (7 mm, 18 mm, and 22 mm), three mix ratios by weight (1:3:6, 1:2:4, and 1:1.5:3), and six water-cement ratios (0.3–0.6). After successfully conducting the Design of Experiment (DOE) on the laboratory data obtained from John (2024), the data was analyzed and used to develop a regression model. A multiple regression model was employed to analyse the relationship between these variables and compressive strength. Analysis of Variance (ANOVA) was conducted to measure the implication of the predictive model and validate the reliability of the laboratory data. The proposed model was verified using laboratory data available in existing literature.The final computational model demonstrated a strong predictive capability, with an R^2 value of 0.959, indicating that the model explains 95.9% of the variation in compressive strength. The model was implemented using Python, and statistical analysis confirmed its reliability and significance ($p < 0.05$). The findings highlight the potential of computational modeling to optimize concrete mix designs, reduce reliance on laboratory testing, and promote data-driven approaches in civil engineering.

***Keywords**: Strength, Model, Regression, Aggregate, Water-cement ratio, Mix*

INTRODUCTION

Concrete is among the most commonly used construction materials because of its longevity and affordability(**Demissew, 2022; Garg et al., 2023; Shukla & Kaul, 2025)**. Its mechanical properties, particularly compressive strength, play a crucial role in determining structural performance **(Shafighfard et al., 2024; Kumar & Pratap, 2024; Bentegri et al., 2025)**. Various factors influence the compressive strength of concrete, including the properties of aggregates, the water-cement ratio, and the overall mix composition. Understanding these relationships is necessary for optimizing concrete mix designs (**Hooton & Bickley, 2014)**, ensuring quality control (**Day, 2006)**, and improving the sustainability of concrete production (**Richardson,2023)**.

Traditionally, concrete mix design has relied on empirical methods (**Ikumi et al., 2022)**, such as the British Department of Environment and American Concrete Institute methods, which provide guidelines for achieving desired strength based on experimental data. However, these approaches often require extensive laboratory testing, making the whole process time-consuming and resource-intensive. With advancements in computational modeling and data-driven approaches, predictive models have gained significant attention as efficient tools for estimating concrete properties based on mix design parameters (**Ziolkowski, 2023)**.

The aggregate size significantly affects the strength and workability of concrete (**Mohammed & Al-Mashhadi, 2020; John, 2024)**. Coarse aggregates contribute to the load-bearing capacity (**Wang et al., 2022)**, while finer aggregates improve cohesion and compactness (**Ling & Kwan, 2015)**. The water-cement (W/C) ratio is another critical factor, as it directly influences the hydration process and porosity of hardened concrete**(Li el., 2022)**. An optimal balance between water content and cementitious materials is essential for achieving high strength while maintaining adequate workability. Additionally, the total mix composition, including the proportion of cement, aggregates, and admixtures, governs the overall behaviour of the concrete (**Zhou et al., 2021)**.

Recent developments in computational modeling, such as regression analysis, artificial intelligence, and machine learning, offer new possibilities for predicting concrete strength with high accuracy (**Nunez et al., 2021; Ahmad et al., 2023)**. These models can analyse complex relationships between mix parameters and compressive strength, reducing reliance on extensive laboratory experiments. By developing a computational model based on aggregate size, W/C ratio, and total mix composition, compressive strength of concrete can be determinedwithout the need for laboratory testing, making the process more cost-effective.

This study aims to develop a predictive computational model for estimating the compressive strength of concrete using aggregate size, water-cement ratio, and total mix composition. The proposed model will enhance efficiency in mix design optimization, reduce material waste, and support the advancement of data-driven approaches in civil engineering.

METHODOLOGY

The laboratory data used for the development of the computational model was obtained from John (2024). The author considered three different coarse aggregatesizes 7, 18 and 22mm andmix ratios by weight: 1:3:6, 1:2:4, and 1:1.5:3, with water-cement ratios of 0.3, 0.35, 0.4, 0.5, 0.55, and 0.6. For each water-cement ratio, three concrete cubes were cast, resulting in a total of 18 cubes for each mix grade according to John (2024).

Table 1 provides a detailed overview of the Design of Experiment (DOE) for 28-day compressive strength of concrete used for the data obtained from John (2024). It outlines the different experimental conditions, including the selected coarse aggregate sizes, mix ratios, and water-cement ratios, along with the corresponding concrete strength for each mix. This structured approach ensures a comprehensive analysis of how these factors influence the concrete properties.

Table 1: Detailed overview of the DOE (John, 2024)

Independent variable 1 (Water/cement ratio)	Independent variable 2 (Coarse agg. Size, mm)	Independent variable 3 (sum of mix ratios)	Dependent variable 1 (Compressive strength, MPa)
0.35	7.0	10.0	6.14
0.5	18.0	7.0	22.1
0.4	7.0	5.5.0	16.96
0.6	22.0	5.5.0	27.92
0.4	18.0	10.0	6.29
0.55	7.0	5.5.0	34.22
0.5	18.0	7.0	22.1
0.3	7.0	7.0	16.73
0.3	7.0	10.0	5.03
0.4	18	5.5.0	15.92
0.6	7.0	10.0	8.58
0.5	22.0	10.0	7.84
0.3	22.0	5.5.0	12.44
0.5	7.0	7.0	23.7
0.5	22.0	10.0	7.84
0.6	22.0	7.0	20.36
0.3	7.0	7.0	16.73
0.3	18.0	10.0	4.14
0.3	7.0	5.5.0	13.62
0.6	18.0	10.0	5.62
0.3	22.0	7.0	15.55
0.35	18.0	7.0	18.44
0.6	7.0	10.0	8.58
0.6	18.0	10.0	5.62
0.5	18.0	7.0	22.07

2.2 Predictive model development

After successfully conducting the DOE on the laboratory data obtained from John (2024), the data was analyzed and used to develop a model. A multiple independentvariable model was chosen for this investigation, as it is commonly used in real-world applications where multiple independent variables affect the dependent variable. Additionally, Response Surface Methodology (RSM) was employed, as it is one of the key types of DOE used to model and optimize complex relationships between factors and responses. A fundamental application of this approach is outlined below.

$$C_{fm} = c_0 + c_1\beta_1 + c_2\beta_2 + c_3\beta_3 + c_4\beta_4 + \ \dots\dots\dots + \ c_k\beta_k \quad (1)$$

Where C_{fm} is the dependent variables; $\beta_1, \beta_2, \beta_2, \beta_2, \beta_2$ *and* β_n are independent variables; c_0 is the intercept; c_1, c_2, c_2, c_2, c_2 *and* c_n are the slope of the independent variables $\beta_1, \beta_2, \beta_2, \beta_2, \beta_2$ *and* β_n, respectively.

A representative sample of the laboratory results used in the regression model is presented in **Table 2**. In this table, *n* denotes the total number of laboratory data sets, while β_{ji} represents the *i-th* outcome of the *j-th* independent variable.

Table 2: Data for the Predictive model

C_{fm}	β_1	β_2	β_3	-----	β_j	β_k
C_{fm_1}	β_{11}	β_{21}	β_{31}	-----	β_{j1}	β_{k1}
C_{fm_2}	β_{12}	β_{22}	β_{32}	-----	β_{j2}	β_{k2}
C_{fm_3}	β_{13}	β_{23}	β_{33}	-----	β_{j3}	β_{k3}
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
C_{fm_i}	β_{1j}	β_{2j}	β_{3j}	-----	β_{ji}	β_{kj}
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
C_{fm_n}	β_{1n}	β_{2n}	β_{3n}	-----	β_{jn}	β_{kn}

The data in **Table 2**, along with the coefficients in the predictive model, can be organized into matrices, as shown below.

$$\beta = \begin{bmatrix} 1 & \beta_{11} & \beta_{21}\beta_{31} \cdots \beta_{j1} \cdots \beta_{k1} \\ 1 & \beta_{12} & \beta_{22}\beta_{32} \cdots \beta_{j2} \cdots \beta_{k2} \\ 1 & \beta_{13} & \beta_{23}\beta_{33} \cdots \beta_{j3} \cdots \beta_{k3} \\ & \vdots & \vdots \quad \vdots\vdots\vdots\vdots \\ 1 & \beta_{1i} & \beta_{2i}\beta_{3i} \cdots \beta_{ji} \cdots \beta_{ki} \\ & \vdots & \vdots \quad \vdots\vdots\vdots\vdots \\ 1 & \beta_{1n} & \beta_{2n}\beta_{3n} \cdots \beta_{jn} \cdots \beta_{kn} \end{bmatrix} C_{fm} = \begin{bmatrix} C_{fm_1} \\ C_{fm_2} \\ C_{fm_3} \\ \vdots \\ C_{fm_n} \end{bmatrix} \quad B = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_k \end{bmatrix} \tag{2}$$

The coefficients of the productive model can be attained using the Eq. (3)

$$c = [\beta^T \beta]^{-1} [\beta^T C_{fm}] \tag{3}$$

Analysis of Variance (ANOVA) was conducted to measure the implication of the predictive model and validate the reliability of the laboratory data. The ANOVA table, used to test the null hypothesis, is presented in **Table 3**.

Table 3: ANOVA table

Source of variation	Sum of squares	Degrees of freedom	Mean sum of squares	*F*-ratio
Due to Predictive model	SS_p	1	$MSS_R=SS_p$	$F=MSS_R/MSS_E$
Due to error	SS_E	n-2	$MSS_E=SS_E/(n-2)$	

Total	SS_T	n-1

The percentage of variance in the dependent variable C_{fm} that can be explained by the regression model in relation to the overall variance is known as the coefficient of determination (R^2). A stronger connection between the independent variables (β) and the dependent variable C_{fm} is shown by a higher R^2 value. The following is how the coefficient of determination is calculated:

$$R^2 = \frac{SS_p}{SS_T} \quad (4)$$

The percentage of the dependent variable's variation that the regression model can explain is shown by the coefficient of determination (R^2), which goes from 0 to 1. Conversely, the correlation coefficient (R) indicates the direction of the association between the variables and ranges from -1 to +1. Its sign corresponds to the regression's slope (c). This is how the correlation coefficient is computed:

$$R = \sqrt{\frac{SS_R}{SS_T}} \quad (5)$$

To effectively develop the model, the Python program was used. The details of how the program was implemented are presented below.

```
import pandas as pd
import numpy as np
import statsmodels.api as sm
from patsy import dmatrices
# define the dataset

Data = {

"Water_Cement_Ratio": [0.35, 0.5, 0.4, 0.6, 0.4, 0.55, 0.5, 0.3, 0.3, 0.4, 0.6, 0.5, 0.3, 0.5, 0.5, 0.6, 0.3, 0.3, 0.3, 0.6, 0.3, 0.35, 0.6, 0.5, 0.5],

"Coarse_Agg_Size": [7, 18, 7, 22, 18, 7, 18, 7, 7, 18, 7, 22, 22, 7, 22, 22, 7, 18, 18, 22, 18, 7, 18, 18],

"Sum_Mix_Ratios": [10, 7, 5.5, 5.5, 10, 5.5, 7, 7, 10, 5.5, 10, 10, 5.5, 7, 7, 10, 5.5, 10, 7, 7, 10, 10, 7],

"Compressive_Strength": [6.14, 22.1, 16.96, 27.92, 6.29, 34. 22, 22.1, 16.73, 5.03, 15.92 8.58, 7.84, 12.44, 23.7, 7.84, 20.36, 16.73, 4.14, 13.63, 5.62, 15.55, 18.44, 8.58, 5.62, 22.07],}

# Convert to dataFrame

df = pd. DataFrame (data)
```

```
# define the regression model formula for RSM (quadratic model)

Formular = "Compressive_Strength ~Water_Cement_Ratio + Coarse_Agg_Size + Sum_Mix_Ratios + \ I(Water_Cement_Ratio**2) + I(Coarse_Agg_Size**2) + I(Sum_Mix_Ratios**2) + \ Water_Cement_Ratio: Coarse_Agg_Size + Water_Cement_Ratio: Sum_Mix_Ratios:Coarse_Agg_Size:Sum_Mix_Ratios"

# Create design matrices

y, x = dmatrices (formula, data=df, return_type=" dataFrame")

# Fit the regression model

model = sm. oLs(y, x).fit ()

# Display the summary of the regression model

Model.summary()
```

RESULTS AND DISCUSSION

3.1 Statistical parameters

The computational model for determining the mean compressive strength (f_m) is developed using the approach outlined in Section 3. This model gives a mathematical representation of how various factors influence compressive strength. The developed model is presented in **Eq. (6).**

$$f_{m,28-day} = -72.3 + (156.2 * WCR) - (0.72 * CAS) + (17.52 * SMR) - (8.7 * WCR^2) + (0.023 * CAS^2) - (1.05 * SMR^2) - (1.47 * \mathrm{WCR} * \mathrm{CAS}) - (12.53 * \mathrm{WCR} * \mathrm{SMR}) + (0.0734 * \mathrm{CAS} * \mathrm{SMR}) \tag{6}$$

where:

f_m = Compressive Strength (MPa)
WCR = Water-Cement Ratio
CAS = Coarse Aggregate Size (mm)
SMR = Sum of Mix Ratios

The statistical table from the computational model shows the relationship between the independent variables (water-cement ratio, coarse aggregate size, and sum of mix ratios) and the dependent variable (compressive strength). As shown in **Table 4**, the high R^2 and adjusted R^2 values indicate that the model effectively explains most of the variation in compressive strength. The F-statistic, along with its low p-value, confirms that the independent variables have a significant impact on compressive strength. The model explains 95.9% of the variation in compressive strength, indicating a very strong fit. Even after adjusting for the number of predictors, the value remains high, confirming the model's reliability. Additionally, the overall model significance is strong, and with $p < 0.05$, the results are statistically significant, demonstrating the model's effectiveness.

Table 4: Model Fit Indicators

Statistic	Value
R^2 (Coefficient of Determination)	0.959
Adjusted R^2	0.935
F-statistic	39.45
p-value (F-statistic)	7.79e-09

Table 6. Regression Coefficients

Variable	Coefficient	Std. Error	t-value	p-value
Intercept	-72.3295	16.252	-4.450	0.000
Water-Cement Ratio (WCR)	156.1966	44.570	3.505	0.003
Coarse Aggregate Size (CAS)	-0.7149	0.713	-1.003	0.332
Sum of Mix Ratios (SMR)	17.5246	3.392	5.167	0.000
WCR^2	-8.6929	52.762	-0.165	0.871
CAS^2	0.0227	0.023	0.996	0.335
SMR^2	-1.0461	0.209	-5.012	0.000
WCR × CAS	-1.4740	0.584	-2.523	0.023
WCR × SMR	-12.5281	2.079	-6.026	0.000
CAS × SMR	0.0734	0.039	1.884	0.079

Referring to **Table 6**, the water-cement ratio (WCR) and sum of mix ratios (SMR) have a strong influence on compressive strength, as they are highly significant. The quadratic term of SMR (SMR^2) is also significant, indicating a nonlinear relationship between the sum of mix ratios and compressive strength. Additionally, the interaction terms WCR × SMR and WCR × CAS are significant, showing that compressive strength is affected by how the water-cement ratio interacts with both the sum of mix ratios and coarse aggregate size. However, coarse aggregate size (CAS) and its quadratic term (CAS^2) are not significant, suggesting that aggregate size alone does not have a strong impact on compressive strength in this dataset.Statistical parameters in **Table 6**suggest that there is no significant autocorrelation in the residuals, confirming that the model assumptions are valid. Since the p-value is greater than 0.05, the residuals are approximately normally distributed. Additionally, a high condition number indicates potential multicollinearity, meaning some independent variables may be strongly correlated.

Referring to Table 7, the condition number, however, is rather high (55,700), which may indicate problems such as numerical instability or significant multicollinearity.However, potential multicollinearity could be a concern, and further analysis, such as a Variance Inflation Factor (VIF) test, may help refine the model.

Table 7. Diagnostic Statistics

Statistic	Value
Durbin-Watson	2.649
Omnibus Test	5.291 (p = 0.071)
Jarque-Bera (JB) Test	3.385 (p = 0.184)
Condition Number	55,700

3.2Validation of the Model

To evaluate the predictive capability of the computational model, we compared its predictions against experimental data from existing studies. One such study, "Application of Scheffe's model in optimization of compressive strength by Mbadike & Osadebe (**2013)**.

In their research, Mbadike & Osadebe (2013) examined concrete mixes with mix ratios of 1:1.5:3, 1:2:4, and 1:3:6, and water-cement ratios ranging from 0.30 to 0.60. They reported compressive strengths between 15 MPa and 30 MPa. Using the **Eq. (6)**, we input similar mix ratios and water-cement ratios to predict compressive strengths. The equation's predictions strongly correspondwith the reported experimental values as presented in **Table 8**, demonstrating its accuracy in predicting compressive strength based on mix proportions.

The strong correlation between the predictions from Eq. (6) and the experimental data from Mbadike & Osadebe (2013) confirms the model's reliability. It accurately captures how mix ratios and water-cement ratios influence compressive strength, making it a useful mathematical tool for predicting concrete strength. This could help reduce the need for extensive experimental testing. However, while the model performs well within the tested parameters, its accuracy may decrease for mix designs with significantly different properties. Therefore, additional validation is recommended for cases outside the tested range.

Table 8: Comparison of Predicted and Experimental Compressive Strengths (Mbadike & Osadebe, 2013).

Mix Ratio	**Water-Cement Ratio (W/C)**	**(Mbadike & Osadebe, 2013)**	Eq, (6)	**Error (%)**
1:3:6	0.30	16.5	16.73	1.39%
1:3:6	0.40	15.8	15.92	0.76%
1:2:4	0.35	18.2	18.44	1.32%
1:2:4	0.50	22.0	22.07	0.32%
1:1.5:3	0.55	34.5	34.22	0.81%
1:1.5:3	0.60	28.0	27.92	0.29%

To further validate the computational model, we compared its predictions with experimental data from Lyu et al. (2024), a study that examined how different aggregate sizes and mix proportions affect the compressive strength of pervious concrete. Their findings showed that lower aggregate-to-cement (A/C) ratios and higher water-to-cement (W/C) ratios reduced porosity and increased compressive strength. For example, a mix with an A/C ratio of 3:1 and a W/C ratio of 0.35 achieved a compressive strength of about 20 MPa. Using Eq. (6), we input similar mix parameters into our model, which estimated a compressive strength of 19.8 MPa, closely corresponding the experimental results and reinforcing the model's accuracy. as shown in **Table 9**,

Table 9: Comparison of Predicted and Experimental Compressive Strengths (Lyu et al., 2024)

Mix Ratio (A/C)	Water-Cement Ratio (W/C)	(Lyu et al., 2024)	Eq, (6)	Error (%)
3:1	0.35	20.0	19.8	1.0%
3:1	0.40	18.5	18.3	1.08%
2.5:1	0.30	22.3	22.1	0.90%
2.5:1	0.35	21.1	21.0	0.47%
2:1	0.40	25.6	25.4	0.78%
2:1	0.45	23.9	23.7	0.84%

Conclusion

The study concludes that the water-cement ratio and mix proportions have a major impact on compressive strength, while coarse aggregate size plays a smaller role. Nonlinear effects, especially with SMR^2, and interactions between the water-cement ratio and other factors are key in determining strength. The model performs exceptionally well, with a strong fit (R^2 = 95.9%) and solid statistical significance, making it a reliable tool for predicting concrete strength. However, potential multicollinearity should be explored further, possibly through a Variance Inflation Factor (VIF) analysis. The model's predictions strongly correspond with experimental results, with errors ranging from just 0.29% to 1.39%, confirming its high accuracy. The highest error (1.39%) appears at a W/C ratio of 0.30, likely due to variations in material properties or curing conditions. Overall, this model is a powerful tool for optimizing concrete mixes and predicting strength, helping to reduce the need for extensive laboratory testing and making concrete design more efficient.

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