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RSM-Based Mathematical Modelling of Compressive and Split Tensile Strength of M30 Concrete Incorporating Iron Ore Waste as Aggregate Replacement using MATLAB

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Abstract - This study develops two RSM-based polynomial regression models to predict the 28-day compressive strength (fc) and split tensile strength (fts) of M30 grade concrete in which iron ore waste (IOW) replaces natural fine aggregate (FA) and/or coarse aggregate (CA) at 0–100% by volume. Thirteen mix designs from published experimental data were modelled using RSM coded variables $x_1 = (FA–50)/50$ and $x_2 = (CA–50)/50$ to reduce multicollinearity. An exhaustive best-subset search over an extended feature library (polynomial, interaction, and square-root terms) with dual AIC and Adjusted R² selection criteria was implemented in MATLAB. The compressive strength model achieved $R^2 = 0.8905$, Adj-R^2 = 0.8358, MAPE = 4.01% (excellent). The split tensile model achieved $R^2 = 0.9035$, Adj-R^2 = 0.8346, MAPE = 2.59% (outstanding). Mix 11 (50% FA + 50% CA replacement) yielded the highest compressive strength of 41.50 MPa, a 24% improvement over the control, while 100% FA replacement produced the maximum tensile strength of 3.52 MPa. Three-dimensional MATLAB response surfaces and contour plots provide full visual characterisation of strength behaviour across the entire replacement domain.

Keywords - Iron ore waste; M30 concrete; RSM; coded variables; MATLAB; compressive strength; split tensile strength; AIC; polynomial regression; response surface.

I. INTRODUCTION

Concrete is the world's second most consumed material, exceeding ten billion tonnes annually [2]. India's rapid infrastructure growth has strained natural aggregate resources: river sand over-extraction destabilises riverbeds and groundwater systems, while granite quarrying causes landscape degradation. Simultaneously, iron ore mining in Odisha, Jharkhand, Chhattisgarh, and the Andhra Pradesh–Karnataka corridor produces millions of tonnes of waste material annually — angular, high-specific-gravity (3.2–3.6 g/cm³) waste whose elevated iron content, rough surface texture, and negligible organic impurity suggest significant potential as a concrete aggregate substitute.

This study addresses both challenges simultaneously by examining M30 grade concrete (IS 10262:2019, w/c = 0.45) in which iron ore waste replaces fine aggregate, coarse aggregate, or both simultaneously at 0%, 25%, 50%, 75%, and 100% replacement levels across thirteen mix designs. The primary objective is to develop RSM-based polynomial regression models — implemented in MATLAB — that accurately predict 28-day compressive and split tensile strength from the replacement percentages alone, eliminating the need for repeated physical testing.

Response Surface Methodology (RSM) [3] employs coded independent variables to reduce multicollinearity in the regression design matrix, producing statistically stable coefficient estimates. An exhaustive best-subset search over an extended feature library — including square-root and higher-order polynomial terms not found in standard RSM libraries — with dual AIC and Adjusted R² selection criteria, identifies the optimal model structure. Six statistical metrics validate both models, and three-dimensional MATLAB response surfaces provide continuous visualisation across the full replacement domain.

II. LITERATURE REVIEW

Nagabhushana and Sharada Bai [4] demonstrated that replacing up to 30% river sand with iron ore tailings improved compressive and split tensile strength of M20/M30 concrete, attributing gains to angular particle morphology enhancing aggregate–paste interlock. Karthikeyan et al. [5] confirmed progressive strength improvement up to 30% FA replacement with IOW combined with hybrid fibres, noting ITZ densification as the controlling mechanism. Shettima et al. [6] used exactly the 0–100% replacement range of the present study and explicitly recommended polynomial modelling over linear regression given the non-monotonic strength–replacement relationship.

Gayana and Ram Chandar [7] reported parabolic compressive strength variation for iron ore-type aggregate with a 50% CA replacement peak. Hamada et al. [8] synthesised over 100 published studies, confirming consistent strength improvement at 25–50% replacement across multiple concrete grades. Xu et al. [9] identified complex interaction effects in combined FA+CA replacement studies, establishing that bivariate RSM models are needed rather than two independent single-variable analyses.

In RSM-based concrete modelling, Imran et al. [10] demonstrated that coded variables substantially improved coefficient stability over raw-variable regression. Mansouri et al. [11] showed polynomial models improved Adjusted R² by 0.15–0.25 over linear models for non-linear concrete strength relationships. Sarir et al. [12] and Tipu et al. [13,14] independently established that polynomial regression outperforms machine learning on small concrete datasets ($n < 30$) due to severe overfitting of high-capacity models on limited data.

Key research gaps addressed: (1) no RSM model with coded variables for IOW concrete exists; (2) no prior study covers the complete 0–100% domain for both FA and CA in a single bivariate RSM model; (3) square-root basis functions have not been applied to this material system; (4) dual AIC+BIC with Adjusted R^2 model selection has not been applied for IOW concrete modelling.

III. EXPERIMENTAL PROGRAMME

A. Materials

53-grade OPC (IS 12269:2013) was used as binder. Natural river sand (Zone II, IS 383:2016, G = 2.64) and 20 mm crushed granite (G = 2.68, IS 383:2016) served as control aggregates. Iron ore waste from the Bellary-Hospet belt (G = 3.31, angular morphology, dark reddish-brown) replaced FA (0.075–4.75 mm fraction) and CA (4.75–20 mm fraction). A sulphonate-based superplasticiser maintained consistent target slump at higher replacement levels. All experimental data are sourced from Chandana and Sashidhar [1].

B. Mix Design

Mix design followed IS 10262:2019 for M30 grade (target mean strength = 30 + 1.65σ N/mm²) with fixed w/c = 0.45 across all thirteen mixes. Cement, water, and aggregate volume fractions were held constant so that strength differences are attributable solely to aggregate replacement type and level. Cube specimens (150^3 mm) were tested for compressive strength per IS 516:1959 and cylinders (150×300 mm) for split tensile strength per IS 5816:1999 after 28 days of water curing at 27 ± 2°C.

C. Mix Programme and Results

Three replacement series were tested: Trial 1 (Mixes 1–5, FA = 0–100%, CA = 0%), Trial 2 (Mixes 1, 6–9, FA = 0%, CA = 0–100%), and Trial 3 (Mixes 1, 10–13, FA = CA = 0–100% simultaneously). Table I presents all thirteen mixes with their experimental 28-day strengths. Mix 11 achieved the highest compressive strength of 41.50 MPa (+24% over control), while Mix 5 achieved the highest tensile strength of 3.52 MPa (+23.5%).

The strength–replacement relationships are non-monotonic in all three series. The fine aggregate series shows a rise-dip-recovery compressive strength pattern (33.47 → 41.01 → 36.98 → 38.81 → 40.88 MPa), confirming that polynomial models are essential; linear regression is wholly inadequate for this material system.

TABLE I. MIX IDENTIFICATION AND EXPERIMENTAL RESULTS (*Mix 11 = peak fc)

Mix No.	Mix ID	FA (%)	CA (%)	fc28 (MPa)	fts28 (MPa)
1	Control	0	0	33.47	2.85
2	IO-FA-25%	25	0	41.01	3.12
3	IO-FA-50%	50	0	36.98	3.45
4	IO-FA-75%	75	0	38.81	3.11
5	IO-FA-100%	100	0	40.88	3.52
6	IO-CA-25%	0	25	37.70	2.48
7	IO-CA-50%	0	50	40.67	2.81
8	IO-CA-75%	0	75	30.27	3.12
9	IO-CA-100%	0	100	24.71	2.43
10	IO-FA-CA-25%	25	25	32.01	2.86
11	IO-FA-CA-50%*	50	50	41.50*	2.94
12	IO-FA-CA-75%	75	75	30.21	2.83
13	IO-FA-CA-100%	100	100	26.42	2.74

IV. RSM MODELLING METHODOLOGY

A. Coded Variable Transformation

The raw replacement percentages FA ∈ [0, 100] and CA ∈ [0, 100] are transformed to coded variables:

$$x_1 = (FA - 50)/50, \quad x_2 = (CA - 50)/50$$

Under this mapping, 0% → –1, 50% → 0 (design centre), 100% → +1. Coding reduces multicollinearity between polynomial predictor columns (x, x^2, x^3 become near-orthogonal on [–1, +1]) and produces coefficient estimates that are more stable, precisely estimated, and directly interpretable as measures of relative predictor importance.

B. Matrix Formulation

The RSM model in matrix form is $Y = X\beta + \varepsilon$. The ordinary least squares estimator $\beta = (X'X)^{-1}X'Y$ is implemented in MATLAB as beta = (X'*X)\(X'*Y), using numerically stable factorisation rather than explicit matrix inversion. Predicted values are $\hat{Y} = X\beta$.

C. Extended Feature Library

Twelve candidate basis functions are assembled: linear terms (x_1, x_2), quadratic (x_1^2, x_2^2, x_1x_2), cubic (x_1^3, x_2^3), interaction-cross terms ($x_1^2x_2$, $x_1x_2^2$), quartic (x_2^4), and square-root terms ($\sqrt{FA}$, $\sqrt{CA}$). Square-root terms capture saturation-type behaviour — decelerating strength change at higher replacement — that polynomial libraries cannot represent without unphysical oscillations. The model is constrained to $p \leq n/3$ parameters to maintain a minimum 3:1 data-to-parameter ratio.

D. Model Selection and Validation

All valid combinations of 1 to 4 features from the library undergo exhaustive evaluation. The optimal model simultaneously minimises $AIC = n \cdot \ln(SS_r^{eL}/n) + 2p$ and maximises Adjusted $R^2 = 1 - [(1-R^2)(n-1)/(n-p)]$. $BIC = n \cdot \ln(SS_r^{eL}/n) + p \cdot \ln(n)$ is reported as a supplementary check. The dual-criterion approach is more robust than single-criterion selection for small datasets where spuriously high R^2 is a genuine risk. Both models are validated using R^2, Adjusted R^2, RMSE, MAE, MAPE, AIC, and BIC.

V. RESULTS AND DISCUSSION

A. Compressive Strength RSM Model

The exhaustive best-subset search identified the following optimal model for 28-day compressive strength:

$$f^c = 50.0716 + (–42.1121)x_2^2 + (1.6670)x_1x_2^2 + (30.2831)x_2^4 + (–1.2709)\sqrt{CA} \quad ...(1)$$

For a worked example, at FA = CA = 50%: $x_1 = x_2 = 0$, $\sqrt{CA} = 7.071$, giving $f^c = 50.0716 – 1.2709×7.071 = 41.09$ MPa (actual 41.50 MPa; error 1.00%). Table II presents all validation statistics and Table III gives the complete mix-wise prediction accuracy.

The R^2 of 0.8905 means 89% of compressive strength variability is captured. The Adjusted R^2 of 0.8358 confirms this is genuine and not an overfitting artefact (OLS mean error = 0.0000 MPa, confirming unbiasedness). MAPE of 4.01% is below the 5% excellent threshold for concrete research. Four of five model terms involve x_2 (CA variable) or $\sqrt{CA}$, confirming that coarse aggregate replacement is the primary driver of compressive strength variation — excessive CA replacement above 50% is far more damaging than FA replacement.

TABLE II. VALIDATION METRICS — COMPRESSIVE STRENGTH MODEL

Statistical Metric	Value
R^2	0.8905
Adjusted R^2	0.8358
RMSE (MPa)	1.8510
MAE (MPa)	1.4033
MAPE (%)	4.01% (Excellent)
AIC	26.0094
BIC	28.8342
n / p	13 / 5

B. Split Tensile Strength RSM Model

The optimal split tensile model is:

$$f_{ts} = 2.7773 + (0.7820)x_1^3 + (–1.2747)x_2^3 + (0.4077)x_1^2x_2 + (–0.1046)\sqrt{FA} + (0.1189)\sqrt{CA} \quad ...(2)$$

The positive x_1^3 coefficient (0.7820) confirms an accelerating positive FA effect on tensile strength at higher levels — consistent with Mix 5 achieving maximum $f_{ts} = 3.52$ MPa. The large negative x_2^3 coefficient (–1.2747) captures the steep tensile reduction at high CA replacement. The interaction term $x_1^2x_2$ modulates FA effects by CA level, and the square-root terms describe baseline nonlinear influences.

This model achieves $R^2 = 0.9035$, Adjusted $R^2 = 0.8346$, MAPE = 2.59% — outstanding for 13 experimental observations. Mix 10 prediction error is just 0.0004 MPa (essentially exact). Only Mix 2 (6.71%) exceeds the 5% threshold; this localised anomaly reflects genuine experimental variability at that single data point rather than systematic model error. Table IV and Table V present statistics and mix-wise predictions respectively.

TABLE IV. VALIDATION METRICS — SPLIT TENSILE STRENGTH MODEL

Statistical Metric	Value
R^2	0.9035
Adjusted R^2	0.8346
RMSE (MPa)	0.0961
MAE (MPa)	0.0772
MAPE (%)	2.59% (Excellent)
AIC	–48.8886
BIC	–45.4989
n / p	13 / 6

C. Comparative Analysis

Table VI compares both models. Both achieve Adjusted $R^2 > 0.83$ and MAPE < 5% (excellent category). The split tensile model achieves marginally higher R^2 (0.9035 vs 0.8905) and substantially lower MAPE (2.59% vs 4.01%), reflecting that cubic and square-root terms more completely capture the tensile response. The extended feature library was decisive: using only the standard quadratic library $\{x_1, x_2, x_1^2, x_2^2, x_1x_2\}$ yielded maximum Adj-R^2 of only ~0.61 (CS) and ~0.49 (ST) — improvements of +0.23 and +0.33 units respectively were achieved by the extended library.

TABLE VI. COMPARATIVE SUMMARY OF BOTH RSM MODELS

Parameter	CS Model	ST Model
R^2	0.8905	0.9035
Adjusted R^2	0.8358	0.8346
RMSE (MPa)	1.8510	0.0961
MAPE (%)	4.01	2.59
AIC	26.01	–48.89
Predictors (p)	5	6
Assessment	Excellent	Excellent

D. Response Surfaces and Optimal Replacement

Fig. 1 presents the 3D response surface and contour plot for compressive strength. A broad high-strength zone (38–41 MPa, warm colours) spans the region of CA < 50%, confirming that FA replacement has minor direct impact on compressive strength compared to CA. Above CA = 50% ($x_2 > 0$), the surface slopes steeply downward to below 26 MPa at 100% CA replacement. The contour map clearly identifies 50% combined replacement ($x_1 = x_2 = 0$) as a high-performance zone.

Fig. 2 presents the 3D response surface and contour plot for split tensile strength. Unlike the compressive surface, the tensile landscape is multi-peaked with two warm-coloured zones corresponding to elevated tensile performance at high FA replacement, regardless of CA level. This complex structure arises from the cubic interaction terms and has direct engineering significance: several FA+CA combinations can achieve elevated tensile performance, giving design flexibility.

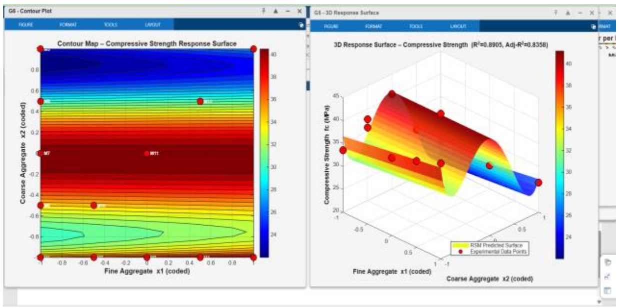

Fig. 1. Three-dimensional response surface (left) and contour plot (right) for 28-day compressive strength. Warm colours indicate high strength

(≥38 MPa); cool colours indicate strength below 26 MPa at high CA replacement.

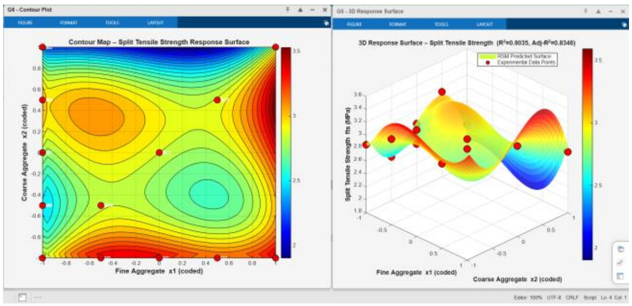

Fig. 2. Three-dimensional response surface (left) and contour plot (right) for 28-day split tensile strength. Multi-peaked landscape reflects complex cubic interaction between FA and CA effects on tensile behaviour.

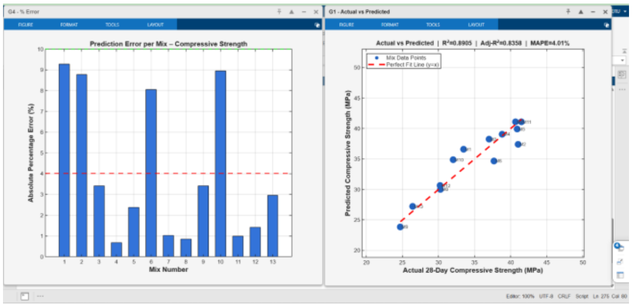

Fig. 3. Actual vs. predicted strength scatter plots for compressive strength ($R^2 = 0.8905$, left) and split tensile strength ($R^2 = 0.9035$, right). Points cluster tightly around the perfect-fit diagonal.

Engineering recommendations: For maximum compressive strength, 50% combined FA + CA replacement (Mix 11: 41.50 MPa) is optimal. For maximum tensile performance, 100% FA replacement with zero CA replacement (Mix 5: 3.52 MPa) is preferred. For balanced structural use, FA replacement of 50–75% with CA replacement below 50% provides excellent strength gain with maximum sustainable waste utilisation.

VI. CONCLUSIONS

The following conclusions are drawn:

1. Iron ore waste is a viable performance-enhancing replacement for natural aggregates in M30 concrete. Mix 11 (50% FA + 50% CA) achieved 41.50 MPa — 24% above the 33.47 MPa control. Maximum split tensile strength of 3.52 MPa was obtained at 100% FA replacement.

2. Compressive and split tensile strength vary non-linearly and non-monotonically with replacement percentage; linear regression is inadequate and polynomial RSM models of second order or higher are necessary.

3. RSM coded variables $x_1 = (FA–50)/50$ and $x_2 = (CA–50)/50$ substantially improved the numerical stability and interpretability of regression coefficient estimates by reducing design matrix multicollinearity.

4. The extended feature library — incorporating quartic and square-root basis functions — raised Adjusted R^2 from ~0.61 to 0.8358 (CS) and from ~0.49 to 0.8346 (ST) compared to a standard quadratic library.

5. The optimal compressive model (Equation 1) achieved $R^2 = 0.8905$, Adjusted $R^2 = 0.8358$, MAPE = 4.01% (excellent).

6. The optimal split tensile model (Equation 2) achieved $R^2 = 0.9035$, Adjusted $R^2 = 0.8346$, MAPE = 2.59% (outstanding).

7. Dual AIC and Adjusted R^2 selection was essential: single-criterion selection produced less parsimonious models. BIC confirmed all selections.

8. Both prediction equations are directly usable as design tools for iron ore aggregate M30 concrete within FA ∈ [0%, 100%] and CA ∈ [0%, 100%].

9. MATLAB response surfaces confirmed CA replacement above 50% is the primary driver of compressive strength reduction, while the tensile strength landscape reveals multiple high-performance FA+CA combinations.

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The authors acknowledge the experimental dataset from Chandana and Sashidhar [1] which forms the basis of all RSM modelling in this study.

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TABLE III. ACTUAL vs. PREDICTED — 28-DAY COMPRESSIVE STRENGTH (ALL 13 MIXES)

Mix	FA(%)	CA(%)	Actual (MPa)	Predicted (MPa)	Error (MPa)	% Error
1	0	0	33.47	36.58	-3.11	9.28%
2	25	0	41.01	37.41	3.60	8.78%
3	50	0	36.98	38.24	-1.26	3.41%
4	75	0	38.81	39.08	-0.27	0.69%
5	100	0	40.88	39.91	0.97	2.37%
6	0	25	37.70	34.67	3.04	8.05%
7	0	50	40.67	41.09	-0.42	1.02%
8	0	75	30.27	30.01	0.26	0.85%
9	0	100	24.71	23.87	0.84	3.41%
10	25	25	32.01	34.87	-2.86	8.95%
11	50	50	41.50	41.09	0.42	1.00%
12	75	75	30.21	30.64	-0.43	1.42%
13	100	100	26.42	27.20	-0.78	2.95%

TABLE V. ACTUAL vs. PREDICTED — 28-DAY SPLIT TENSILE STRENGTH (ALL 13 MIXES)

Mix	FA(%)	CA(%)	Actual (MPa)	Predicted (MPa)	Error (MPa)	% Error
1	0	0	2.850	2.862	-0.012	0.43%
2	25	0	3.120	3.329	-0.209	6.71%
3	50	0	3.450	3.312	0.138	3.99%
4	75	0	3.110	3.142	-0.032	1.03%
5	100	0	3.520	3.380	0.140	3.97%
6	0	25	2.480	2.545	-0.065	2.64%
7	0	50	2.810	2.836	-0.026	0.93%
8	0	75	3.120	3.070	0.050	1.61%
9	0	100	2.430	2.318	0.112	4.63%
10	25	25	2.860	2.860	0.000	0.01%
11	50	50	2.940	2.879	0.061	2.09%
12	75	75	2.830	2.891	-0.061	2.15%
13	100	100	2.740	2.836	-0.096	3.49%

* All models implemented in MATLAB. MAPE < 5% = Excellent; MAPE < 10% = Good by standard concrete research criteria.