THE ACCURACY OF SCHEFFE'S THIRD DEGREE OVER SECOND-DEGREE, OPTIMIZATION REGRESSION POLYNOMIALS

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ABSTRACT

Pozzolanas are materials containing reactive silica and/or aluminum. When the material is mixed with lime in powdered form and in the presence of water, it will set and harden like cement. Rice Husk Ash (RHA) is a form of natural pozzolana. It *is found locally in abundance in Nigeria and in many other parts of the world. Udeala (2003), produced a mix containing RHA with* 45 *per cent slaked lime. This work uses Scheffe's* (1958), *simplex theory to optimize the compressive strength of concrete made from RHA pozzolan based on* (4,2) *and (4,3) simplex lattices. The strengths predicted by the models are in good agreement with their corresponding experimentally observed values. The accuracy of strength predicted by the third degree polynomial is about* 21 *per cent higher than that of the second-degree polynomial. This implies that, except for need of high accurate results, the use of higher order polynomial, that is cumbersome and time wasting, is not necessary. With the models, any desired strength of hardened concrete, given any mix proportions,* is *easily evaluated. The computer programs are written in BASIC language.*

KEYWORDS

Rice-Husk-Ash, Optimization, Simplex Lattice, Compressive Strength.

INTRODUCTION

Rice Husk Ash (RHA) is an agro-waste material,found in abundance in Nigeria, India and in many other parts of the world. RHA is one of the natural Pozzolanas containing reactive silica and/or aluminum. When the material is mixed with lime in powdered form and in the presence of water, it will set and harden like cement [1]. The Indian ITDG [2], has it that Greeks and the Romans were the first civilization known to have used pozzolanas in lime mortars. The strength and other properties arc affected by lime-pozzolan ratio.

Many of the desirable characteristics of concrete are qualitatively related to its compressive strength [3]. Also the compressive strength is the most convenient to measure and is used as a criterion of the over all quality of the hardened concrete [4]. Compressive strength ($Ó_c$), is calculated using the following equation:

$$Ó_c = \frac{P}{A} \quad (1)$$

where

P is crushing load and A is the cross-sectional area of the concrete cube or cylinder.

Scheffe's Optimization Theory

Strength of concrete depends on the adequate proportioning of its ingredients. Scheffe [5], developed an optimization theory that is used to optimize the strength of concrete.

The simplex

According to Jackson, [6] "simplex is the structural representation (shape) of the line or planes joining the assumed positions of the constituent materials (atoms) of the mixture".

H. Scheffe [5], considered experiments with mixtures of which the property studied depends on the proportions of the components but not their quantities in the mixture. An obvious example of such a study is the relationship between the compressive strength of concrete and the proportion of w/c (water-cement), cement, sand and coarse aggregate.

If a mixture has a total q components and Xi, be the proportion of the components (ingredients) of the ith component in the mixture such that

$X_i \geq 0$ (i =1-4) (2)

Then, if we assume the mixture to be a unit quantity then the sum of all the proportions of the components must be unity. That means that

$X_1 + X_2 + X_3 + X_4 = 1$

Or

$$\sum_{i=1}^{4} X_i = 1 \qquad (3)$$

where in this case,

X_1 is proportion of water/cement (w/c) ratio

X_2 is proportion of cement

X_3 is proportion of sand

X_4 is proportion of crushed stone.

Thus, the factor space is a regular (q-l) dimensional simplex

Simplex Lattice

For a 4-component mixture, we have a tetrahedron simplex -lattice. Taking a whole factor space in the design. We will have (q.m) simplex lattice whose properties are defined as follows.

(a) The factor space has uniformly spaced distribution of points

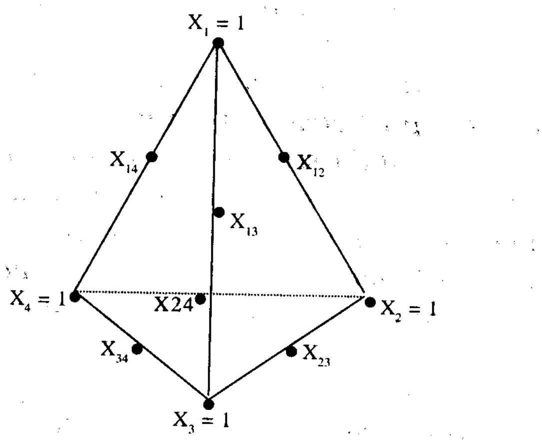
(b) The proportions used for the factor has m + 1 equally spaced values from 0 to 1, that is

$X_1 = 0.\frac{1}{m}, \frac{2}{m} \ldots 1$ and all possible mixtures with these proportions for the factor. Scheffe [5], also showed that the number of points in (q, m) lattice is given by $\frac{q(q+1)\ldots(q+m-1)}{m!}$ (4)

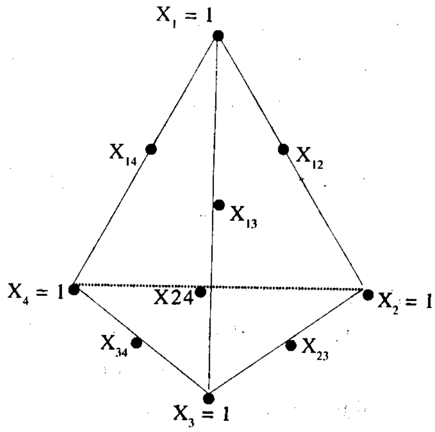
where m is a digit number.

This implies that for a (4.2) lattice, the number of points (coefficients) = $\frac{4(4+1)}{1x2}$ = 0

And for a (4,3) lattice the coefficients are 20 (see fig.la and b).



a. (4, 2)



b. (4, 3)

***Fig. 1:** The simplex lattices.*

Legend: Y_i, Y_{ij}, (I = 1 – 4 and j = 2 - 4), the 'response', represents the expected compressive strength to concrete.

DESIGN POINTS

The criterion of eqn. 3 makes is impossible to use the normal mix ratios such as 1 : 2 : 4 at a given water/cement ratio. Therefore, a transformation of the actual components, i. e. the ingredient proportion is necessary. The transformed proportion X_i (i = 1 – 4) for each experimental point are called "Pseudo - component" for actual components Z, the pseudo – components X is given by X = A_Z

Where A is the inverse of Z matrix. Similarly the inverse transformation from pseudo – components to actual components is expressed as

Z = BX

Where B is the inverse of A, matrix.

The pseudo – components and the actual component selected for the design points are shown in Table 1 and 2

Table 1 Actual (Z_i) and Pseudo (X_i)-components for Scheffe's (4,2) simplex Lattice

N	X_1	X_2	X_3	X_4	Response	Z_1	Z_2	Z_3	Z_4
1	1	0	0	0	Y_1	0.88	0.86	0.85	0.84
2	0	1	0	0	Y_2	1	1	1	1
3	0	0	1	0	Y_3	2.8	2.0	2.5	2.2
4	0	0	0	1	Y_4	4.5	4	3.5	3.0
5	*1/2*	*Y2*	0	0	Y_{12}	0.87	1	2.4	4.25
6	*1/2*	0	*Y2*	0	Y_{13}	0.865	1	2.65	4.0
7	*1/2*	0	0	112	Y_{14}	0.86	1	2.5	3.75
8	0	*1/2*	*1/2*	0	Y_{23}	0.855	1	2.25	3.75
9	0	*1/2*	0	*1/2*	Y_{34}	0.85	1	2.1	3.5
10	0	0	*1/2*	*1/2*	Y_{34}	0.845	1	2.35	3.25

Table 2 Actual (Z_i) and Pseudo (X_i) Components for Scheffe's (4,3) simplex Lattice

Expt	X_1	X_2	X_3	X_4	Response symbol	X_1	X_2	X_3	X_4
1	1	0	0	0	Y_1	*0.88*	*0.8*	*0.85*	0.84
2	0	1	0	0	Y_2	1	1	1	1
3	0	0	1	0	Y_3	2.8	2.0	2.500	2.200
4	0	0	0	1	Y_4	4.5	4.0	3.500	3.000
5	2/3	2/3	0	0	Y_{112}	0.873	1	2.53	4.330
6	1/3	2/3	0	0	Y_{I22}	0.867	1	2.266	4.167
7	2/3	0	1/3	0	Y_{113}	0.870	1	2.700	4.167
8	1/3	0	2/3	0	Y_{113}	0.860	1	2.600	3.833
9	2/3	0	0	1/3	Y_{114}	0.867	1	2.600	4.000
10	1/3	0	0	2/3	Y_{I44}	0.853	1	2.400	3.500
11	0	2/3	1/3	0	Y_{223}	0.857	1	2.170	3.830
12	0	1/3	2/3	0	Y_{233}	0.853	1	2.330	3.667
13	0	2/3	0	1/3	Y_{224}	0.853	1	2.067	3.667
14	0	1/3	0	2/3	Y_{244}	0.847	1	2.133	3.333
15	0	0	2/3	1/3	Y_{334}	0.847	1	2.400	3.334

Expt	X_1	X_2	X_3	X_4	Response symbol	X_1	X_2	X_3	X_4
16	0	0	1/3	2/3	Y_{344}	0.843	1	2.300	3.167
17	1/3	1/3	1/3	0	Y_{I23}	0.862	1	2.400	3.996
18	1/3	1/3	0	1/3	Y_{I24}	0.859	1	2.331	3.830
19	1/3	0	1/3	1/3	Y_{I34}	0.856	1	2.498	3.663
20	0	1/3	1/3	1/3	Y_{234}	0.849	1	2,230	3.497

The Simplex Canonical Polynomials
Response

The properties studied in the assumed polynomial are real-valued functions on the simplex. They are termed responses. In our study the target strength is the response. Scheffe [5] assumed that a polynomial function of degree m, in the q (q = 4) variables X_1 X_2,….,Xq subject to eqn.3 will be called a (g, m) polynomial and that it will be of the form:

$$Y=b_o + \sum_{i=1}^{q} b_i x_i + \sum_{1\le i\le q,}\sum_{1\le j\le q} b_{ij} + \sum_{1\le i\le q, 1\le j\le q, 1\le k\le q} b_{ijk}X_iX_jX_k + \sum bi_1i_2 \dots i_nX_{i1}X_{x2}\dots X_{in} \quad (7)$$

b is a constant coefficient.

He also showed that the number of coefficients in eqn 7 is given by $C^n_{q+n\ -1}$ but eqn 7 must be subject to the condition of eqn.3, hence b_i values are not unique.

let

X_q = 1- Sx_i. (8)

Substituting the values of X_q into eqn. 7 The number of coefficients b_i will reduce to C^n_q + n-1 or q(q+1)…(q+n-1)

where n is a digit number. This implies that the number of the coefficients equal to a (q,n) lattice. The implication here, therefore, is that the values of a (q,n) polynomial can be assigned arbitrarily on a (q,n) lattice and values on the simplex (eqn 3) are then uniquely determined. The reduced form of equation 7 for a (4,2) and (4,3) simplex lattices are:

Y_{42}= $á_1X_1$+$á_2X_2$+$á_3X_3$+$á_4X_4$+$á_{12}{}^{X}{}_{I}{}^{X}{}_{2}$ +$á_{13}X_1X_3$+$á_{14}X_1X_4$+$á_{23}$ X_2 X_3 +$á_{24}X_2X_4$ +$á_{34}X_3X_4$ (9)

$Y_{43} = \propto_1{}^{X}{}_1 + \propto_2X_2 + \propto_3X_3 + \propto_4X_4 + \propto_{12}X_IX_2 + \propto_{13}X_1X_3 + \propto_{14}X_IX_4 + \propto_{23}X_2X_3 + \propto_{24}X_2X_4 + \propto_{34}X_3X_4 + \gamma_{12}X_IX_2(X_I\text{-}X_2) + \gamma_{13}X_IX_3(X_I - x_3) + \gamma_{14}X_1X_4\ (X_1\text{-}X_4) + \gamma_{23}X_2X_3(X_2\text{-}X_3) + Y_{24}X_2X_4\ (X_2\text{-}X_4) + Y_{34}X_3X_4(X_3\text{-}X_4) + \propto_{123}X_IX_2X_3 + \propto_{124}X_IX_2X_4 + \propto_{134}X_1X_3X_4 + \propto_{234}\ X_2X_3X_4$ (10)

It was shown [6], that the following relations hold:

$á_i = y_i$ (11a)

And for (4,2) polynomial,

$á_{ij} = 4y_{ij} - 2y_i\ 2y_j$ (11b)

While for a (4,3) polynomial,

$\propto_{12} = \frac{9}{4}(y_{112} + y_{113} - y_1 - y_2)$ (12a)

$\propto_{13} = \frac{9}{4}(y_{113} + y_{122} - y_1 - y_3)$ (12b)

$\propto_{14} = \frac{9}{4}(y_{114} + y_{144} - y_1 - y_4)$ (12c)

$\propto_{23} = \frac{9}{4}(y_{223} + y_{233} - y_2 - y_3)$ (12d)

$\propto_{24} = \frac{9}{4}(y_{224} + y_{244} - y_2 - y_4)$ (12e)

$\propto_{34} = \frac{9}{4}(y_{334} + y_{344} - y_3 - y_4)$ (12f)

$\gamma_{12} = \frac{9}{4}(3y_{112} + 3y_{122} - y_1 + y_2)$ (13a)

$\gamma_{13} = \frac{9}{4}(3y_{113} + 3y_{133} - y_1 + y_3)$ (13b)

$\gamma_{14} = \frac{9}{4}(3y_{114} + 3y_{144} - y_1 + y_4)$ (13c)

$\gamma_{23} = \frac{9}{4}(3y_{223} + 3y_{233} - y_2 + y_3)$ (13d)

$$\gamma_{24} = \frac{9}{4}(3y_{224} + 3y_{244} - y_2 + y_4) \quad (13e)$$

$$\gamma_{34} = \frac{9}{4}(3y_{334} + 3y_{344} - y_3 + y_4) \quad (13f)$$

$$\propto_{123} = 27y_{123} - \frac{27}{4}(y_{112} + y_{122} + y_{113} + y_{133} + y_{223} + y_{233}) + \frac{9}{4}(y_1 + y_2 + y_3) \quad (14a)$$

$$\propto_{124} = 27y_{124} - \frac{27}{4}(y_{112} + y_{122} + y_{114} + y_{144} + y_{224} + y_{244}) + \frac{9}{4}(y_1 + y_2 + y_4) \quad (14b)$$

$$\propto_{134} = 27y_{134} - \frac{27}{4}(y_{113} + y_{133} + y_{114} + y_{144} + y_{334} + y_{344}) + \frac{9}{4}(y_1 + y_2 + y_4) \quad (14c)$$

$$\propto_{234} = 27y_{234} - \frac{27}{4}(y_{223} + y_{233} + y_{224} + y_{244} + y_{334} + y_{344}) + \frac{9}{4}(y_1 + y_3 + y_4) \quad (14d)$$

where $\propto$ is response, and Y is experimentally observed values.

Materials and Methods

The main material for this research is the Rice Husk Ash (RHA)-slaked lime mix.

The mix ratios used for the simplex design points were as a result of preliminary research findings about the concrete made from the pozzolan.

a. the RHA was used as supplied.

b. aggregates:

i. sand

The sand was collected from River Benue, Makurdi- Nigeria and prepared according to the standards specified by BS 1017:[8] parts 1 and 2 and BS 882: [9]. The grading was carried out to BS 812: 103:[10]. The sand belongs to zone C [11]

ii. coarse aggregate (crushed stone)

The crushed granite chippings were collected from Kwande, Benue State-Nigeria. The maximum size of aggregate used was 20mm.

Compressive Strength

Preliminary work showed that the optimum water- cement ratio is 0.86. Batching of the ingredients was done by weight. The concrete cubes were cast according to BS 1881-108: [12]. The cubes were sprayed with water after 24 hours. They were then demoulded after 3 days (72 hours) and transferred to the curing tank at room temperature for 56 days. The cubes were tested for compressive strength on removal from the curing tank using compression machine to the requirements of BS 1881-115: [13].Eqn 1 is used to calculate the compressive strength of the cubes in N/mm^2

Results and Analysis

Compressive strength test results base on Scheffe's (4,2) simplex lattices.

The results of the compressive strength test results, based on Scheffe's (4,2) simplex lattices are shown in Table 3.

Table 3: Compressive Strength Test Results Based on Scheffe's (4,2) Simplex Lattices

Expt. No.	Replication	Response Y_i N/mm^2	Response	ΣY_i	y N/mm^2
1	1A 1B	1.8 1.8	Y_1	3.6	1.8
2	2A 2B	1.9 2.0	Y_2	3.9	2.0
3	3A 3B	0.4 0.4	Y_3	2.4	1.2
4	4A 4B	0.5 0.4	Y_4	0.9	0.5
5	5A 5B	0.4 0.3	Y_{12}	0.7	0.4
6	6A 6B	1.8 1.7	Y_{12}	3.5	1.8

Expt. No.	Replication	Response Y_i N/mm^2	Response	ΣY_i	y N/mm^2
7	7A 7B	2.6 2.6	Y_{14}	5.2	2.6
8	8A 8B	2.8 2.6	Y_{23}	5.4	2.7
9	9A 9B	3.1 3.4	Y_{24}	6.5	3.3
10	10A 10B	1.8 1.7	Y_{34}	3.5	1.8

Legend: $\mathbf{y} = \frac{\sum_{i-1}^{m} y_i}{m_i}$

The Regression Equation

Based on eqn. 11 and table 3, the coefficients of the (4,2) polynomial of eqn 9 are determined as follows:

$\propto_1 = 1.8$, $\propto_2 = 2.0$, $\propto_3 = 0.4$, $\propto_4 = 0.5$

$\propto_{12} = 4*0.4-2*1.8-2*2.0 = -6.0$

Similarly,

$\propto_{13} = 2.8$, $\propto_{14} = 5.8$, $\propto_{23} = 6.0$, $\propto_{24} = 8.2$ and $\propto_{34} = 5.4$

Thus, from equation 9, we have

$$Y = 1.8x_1 + 2.0x_2 + 0.4x_3 + 0.5x_4 - 6.0x_1x_2 + 2.8x_1x_3 + 5.8x_1x_4 + 6.0x_2x_3 + 8.2x_2x_4 + 5.4x_3x_4 \quad (15)$$

Eqn 15 is the mathematical model for the optimization of the compressive strength of the Rice Husk Ash pozzolan concrete, based on Scheffe's (4, 2) polynomial.

Compressive strength test results based on Scheffe's* (4,3) *simplex lattices.

The results of the compressive strength test results, based on Scheffe's (4,3) simplex lattices are shown in Table 4.

Table 4 Compressive Strength Test Results, based on Scheffe's (4.3) simplex Lattice.

Expt. No.	Response (y) N/mm^2	Response Symbol	Expt. No.	Response (y) N/mm^2	Response
1	1.82	Y_I	11	1.07	Y_{223}
2	2.00	Y_2	12	1.60	Y_{233}
3	1.21	Y_3	13	2.00	Y_{224}
4	0.60	Y_4	14	1.80	Y_{244}
5	0.98	Y_{I12}	15	2.12	Y_{334}
6	1.78	Y_{122}	16	1.62	Y_{344}
7	1.78	Y_{113}	17	2.60	Y_{123}
8	0.53	Y_{133}	18	3.36	Y_{124}
9	1.07	Y_{144}	19	2.42	Y_{134}
10	1.24	Y_{114}	20	3.52	Y_{234}

The Regression Equation

Based on equations 11a,12, 13, 14, and Table 4, we have the values of the coefficients of eqn 10 as shown below:

$\propto_1$=1.82, $\propto_2$=2.00, $\propto_3$=1.21, $\propto_4$=0.60, $\propto_{12}$= -2.39,
$\propto_{13}$= -1.62, $\propto_{14}$= -0.25, $\propto_{23}$= -1.22, $\propto_{24}$= -2.70, $\propto_{34}$= 4.34,
γ_{12}= -5.00, γ_{13}=7.07, γ_{14}= -3.89, γ_{23}= -5.36, γ_{24}= -1.80,
γ_{34}= 2.00, $\propto_{123}$=40.59, $\propto_{124}$=53.48,$\propto_{134}$=25.25, and $\propto_{234}$=*43.27*

Thus, the regression equation is given by

$$\hat{y} = 1.82x_1 + 2.0x_2 + 1.21x_3 + 0.6x_4 -2.39x_1x_2 - 1.62x_1x_3 -0.25x_1x_4 - 1.22x_2x_3 + 2.7x_2x_4 + 4.34x_3x_4 - 5.0x_1x_2(x_1-x_2) + 7.07x_1x_3(x_1-x_3) - 3.89x_1x_4(x_1-x_4) - 5.36x_2x_3(x_2-x_3) - 1.8x_2x_4(x_2-x_4) + 2.0x_3x_4(x_3-x_4) + 40.59x_1x_2x_3 + 53.48x_1x_2x_4 + 25.25x_1x_3x_4 + 43.27x_2x_3x_4$$

Eqn 16 is the mathematical model for the optimization of the compressive strength of the Rice Husk Ash pozzolan concrete, based on Scheffe's (4, 3) polynomial.

Computer output

The outputs from executed programs based on the two model equations are shown below.

An executed program for the compressive strength based on Scheffe's(* 4,2) *-lattice polynomial

Desired strength 3.0

Counter	xl	x2	x3	x4	y	zl	z2	z3	z4
1	0.000	0.390	0.080	0.530	3.001	0.849	1.000	2.157	3.430
2	0.000	0.400	0.100	0.500	0.000	0.849	1.000	2.160	3.450
3	0.000	0.420	0.120	0.460	3.000	0.850	1.000	2.161	3.480
4	0.000	0.440	0.130	0.430	3.000	0.850	1.000	2.160	3.505

The maximum value of strength predictable by this model is 3.4131 N/sq.mm

An executed program for the compressive strength based on Scheffe's(* 4,3) *-lattice polynomial

Desired strength 3.5

Counter	X1	x2	x3	x4	v	z1	z2	z3	z4
1	0.350	0.130	0.280	0.240	3.499	0.859	1.000	2.473	3.795
2	0.350	0.170	0.100	0.380	3.499	0.858	1.000	2.414	3.745
3	0.350	0.260	0.030	0.360	3.501	0.860	1.000	2.374	3.800
4	0.350	0.290	0.020	0.340	3.501	0.860	1.000	2.365	3.825
5	0.350	0.360	0.020	0.270	0.499	0.861	1.000	2.349	3.895
6	0.360	0.250	0.270	0.120	3.501	0.862	1.000	2.449	3.925

The maximum value of strength predictable by this model is 4.134676 *N/sq.rnm*

CONCLUSION

The research showed that the Rice Husk Ash (RHA) produced an average compressive strength of 3.2 *N/mm*^{2} (32.6 kg/cm^2).This meet the minimum standard strength requirements (IS 4098-[14].

The model equations were tested for adequacy using the student's t-test and the Fisher test on 10 controlled design points each. The strengths predicted by the models are in good agreement with the corresponding experimentally observed results. With the models, any desired strength of hardened concrete, given any mix proportions, is easily evaluated. Conversely, the various mix proportions, matching any stipulated strength, are also easily obtained using simple BASIC computer programs (see appendix A). The accuracy of strength predicted by the third degree polynomial is about 21 per cent higher than that of the second-degree polynomial. This implies that, except for the need of high accurate results, the use of higher order polynomial.ass cumbersome and time wasting is not necessary.

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APPENDIX A

Program for Scheffe's model

```
10 REM A GW BASIC V2.02 program that computes the proportions of concrete mixes to a desired strength.
20 REM Scheffe's model
30 COUNT = 0
40 GOSUB 100
50 END
100 REM procedure begins
110 YMAX = 0
120 PRINT
130 PRINT "A Model for Computation of Concrete Mix Proportions to Desired Strength"
140 PRINT
150 INPUT "Desired Strength"; YIN
160 GOSUB 600
170 FOR Xl = 0 TO 1 STEP .01
180 FOR X2 = 0 TO I-Xl STEP .01
190 FOR X3 = 0 TO l-XI-X2 STEP .01
200X4= l-XI-X2-X3
300 REM Assign Coefficients
310 Al =
320 A2 =
330 A3 =
340 A4 =
350A12=
360A13=
370AI4=
380 A23 =
390 A24 =
400A34=
410 YOUT =
Al *Xl +A2*X2+A3*X3+A4*X4tA I 2*X 1 *X2+A13*XI *X3+A14*XI
*X4tA23*X2*X3+A24*X2*X4tA34*X3*X4
420 GOSUB 700
430 IF (ABS (YIN- YOUT)<= 0.001) THEN 440 ELSE 460
440 COUNT = COUNT + l
450 GOSUB 800
460NEXTX3
470 NEXT X2
480NEXTXI
490 PRINT
500 IF (COUNT>0) THEN 510 ELSE 530
510 PRINT "The max. Value of strength predictable by this model is"; ymax;
"N/sq.mm."
520 GOTO 540
530 PRINT "Sorry! Desired strength out of range of the model"
540 RETURN
600 REM print heading
610 PRINT
620 PRINT "COUNT Xl    X2    X3    X4    Y Z1  Z2 Z3           Z4"
630 RETURN
700 REM Checkmax
710 IF YMAX<YOUT THEN YMAX = YOUT ELSE YMAX = YMAX
```

```
720 TETURN
800 REM Out results
810 Zl = 0.88*Xl +0.86*X2+0.85*X3+0,84*X4
820Z2= Xl+X2+X3+X4
830Z3 = 2.8*XI+2.0*X2+2.5*X3+2.2*X4
840 Z4 = 4.5*X 1 +4.0*X2+3.5*X3+3.0*X4
850 PRINT TAB (1); COUNT; USING "####.##"; Xl;X2;X3;X4;YOUT;Zl;Z2;Z3;Z4
860 RETURNS
```