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MIXTURE MODEL WITH INVERSE TERMS FOR WELD-METAL CHEMISTRY PREDICTION AS A FUNCTION OF SAW FLUX INGREDIENTS

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Abstract
The development of regression equations in terms of welding flux ingredients for prediction and optimisation of weld-metal quality has received much attention. However, studies that take edge effects into account are sparse. In this study, models that incorporate edge effects were proposed for the predictions of carbon, nitrogen and phosphorus contents in weld-metal using secondary data. From the study, none of the models provides an adequate fit for carbon and nitrogen content in weld-metal (R^2_{Adj} are $< 50\%$). The models showed some promise for phosphorus content ($R^2_{Adj} > 50\%$). Special cubic and full cubic with inverse terms fitted the phosphorus data better than others. Their respective (R^2_{Adj}; R^2_{Pred}) values were (81.32; 80.27%) and (81.57; 80.48%). The difference between their respective R^2_{Adj} and R^2_{Pred} are less than 0.2 as specified in the literature. Development of prediction models for carbon and nitrogen and understanding of the phenomenon of edge effects are recommended for further study.

Keywords: Edge Effects, Mixture models, Predictive ability, Response equations, Welding flux, Weld-metal.

1.0 INTRODUCTION

The type and proportions of ingredients used in welding flux formulation determine the quality of weld-metal, cost and productivity of the welding process as well as the health of the welder and other workers in the welding environment [1-4]. Also, flux ingredients, welding wire constituents and welding parameters react and interact in a very complex way. Hence, the formulation of welding flux to achieve the best balance among multiple conflicting quality attributes is not a trivial problem. As a result of the daunting problem, the traditional approach of flux formulation has been by lengthy and expensive trial-and-test experiments [5, 6]. Efforts to mitigate the drawbacks of the traditional approach have led to the development of methodologies for the development of regression equations for the prediction and optimisation of welding flux performance [5, 7-9].

In the last two decades, the use of statistical design of experiment (DoE) and development of regression models for the prediction and optimisation of welding flux quality attributes have received a lot of attention [10-14]. However, there are instances where the models fitted to the experimental data could not adequately predict some of the responses. For instance, Scheffe's Quadratic Canonical Polynomial (SQCP) used by Kanjilal et al, [7], was able to adequately predict the $O_2, Mn, Si, S, and\ Ni$ contents in the weld-metal, but they couldn't predict those of $Carbon, Phosphorus\ and\ Nitrogen$ because it is limited to modelling overall curvature. Given the importance of the roles these elements play in weld-metal quality, there is the need to identify models that can adequately predict their contents as a function of flux ingredients. Adeyeye and Oyawale [5] suggested other model forms and sequential model build-up procedure for Scheffe's canonical polynomials (SCP) and their extensions to check for (i) third order curvature (ii) asymmetric third order curvature (iii) planar and edge effects (iv) overall curvature with edge effects (v) third order curvature with edge effects and (vi) third order asymmetric curvature with edge effects. The first two approaches have been implemented recently [15 -18], while the remaining four that consider edge effects are yet to be implemented [3]. Since there exist some quality attributes that the SQCP couldn't adequately predict, other prediction and optimisation tools are required for the formulation of welding flux with optimum performance. It is unlikely that this could be efficiently achieved without appropriate prediction models for such attributes. There is therefore the need to look beyond the SQCP models. In this study, Kanjilal et al [7] work will be revisited and the efficacy of other model forms will be tested taking edge effects into account for the prediction and optimisation of weld-metal chemistry as a function of welding flux ingredients.

1.1 LITERATURE

A survey of the literature revealed that the traditional approach of welding flux formulation involves extensive experiments and application of physical science principles such as reaction kinetics and thermodynamics, plasma physics and chemistry, solution thermodynamics and slag chemistry. For instance, Baune et al. [19, 20] studied the effect of fluoride and calcite on the diffusible hydrogen content of weld-metal, while Du Plessis and Du Toit [21] investigated the effect of flux-oxidising ingredients on the diffusible hydrogen content. Farias et al, [22] studied the effects of wollastonite and quartz on fusion rate and short-circuit frequency. They observed that the intermediate-wollastonite-content flux (8% quartz and 8% wollastonite) performed better in fusion rate analysis on direct current electrode positive and direct current electrode negative. The intermediate-wollastonite-content electrode also tended to present a higher short-circuit frequency on DC. They did not give the reasons for the observed behaviours. This could be because the approach used could not identify and quantify the direction and magnitude of interaction among the process variables. One of the possible reasons for the better performance of the intermediate-wollastonite-content flux on these criteria might be due to the synergetic binary interaction effects of quartz and wollastonite. It may also be due to the ternary or even quaternary synergism of wollastonite, quartz, Mn powder and iron powder. The traditional approaches are lengthy, costly and not able to guarantee optimum flux formulation and identify the direction and magnitude of interactions among the flux ingredients. Also, the models developed through them are cumbersome and not easy to use [3, 5, 6].

The application of the physical science approach coupled with extensive experiments lacks the rigour and sophistication to model the complex reactions and interactions among the flux ingredients, welding wire and process parameters. A usual practice in such complex situations is to apply regression analysis in which some equations are fitted to experimental data. Kanjilal et al. [7-9] used the statistical design of experiment method known as mixture design coupled with regression analysis to develop regression equations for flux quality attributes as a function of flux ingredients to complement the detailed scientific approaches. Although regression analysis is not new, Kanjilal et al. [7-9] appeared to be among the earliest application of it to welding flux design. Prediction equations were developed for the prediction of mechanical, chemical and microstructural properties of weld-metal as a function of the flux ingredients. In addition to prediction, the models also gave information in terms of the direction and magnitude of binary interactions among the flux ingredients.

However, the SQCP models used by Kanjilal et al. [7], could not adequately predict the carbon, phosphorus and nitrogen contents of the weld-metal. To address this limitation, Adeyeye and Oyawale [5], suggested other model forms such as Scheffe's Full Cubic Canonical Polynomial (SFCCP) for asymmetric third order curvature and ternary interactions, and Scheffe's Special Cubic Canonical Polynomial (SSCCP) for third order curvature and ternary interactions. These models have been very useful. For example, Sharma and Chhibber [15] used SSCCP for the prediction of Cr and Ti, Sharma and Chhibber [14] used SFCCP for the prediction of change in enthalpy and specific heat. Other researchers used the SFCCP for prediction of density, specific heat and change in enthalpy and SSCCP for thermal conductivity, thermal diffusivity, grain fineness number, change of enthalpy, weight loss, thermal conductivity, thermal diffusivity and specific heat with flux ingredients as the predictor variables [14-18, 23, 24].

Adeyeye and Oyawale [5] further suggested the use of models with term of the form x_i^{-1} added to reflect the possible extreme changes in the quality attributes that sometimes occur in some mixture problems as the value of certain ingredients tend to a boundary value ($x_i \rightarrow \in_i$). This behaviour is referred to as the edge effects [25]. The sequence of model build-ups to take individual effects, binary and ternary interactions as well as the edge effects into account were also presented. Available literature reveals that these models have not been tested in real-world welding flux formulation situations [3]. There is the need to test the relevance and efficacy of these models. Adeyeye and Oyawale [6] extended the work of Kanjilal et al. [7] beyond prediction by performing optimisation with the models for single criterion cases. Later, the approach was further extended to address real-world multiple criteria welding flux design situations [10, 11, 13]. The multi-response flux formulation situations are encountered more often in practice; hence, it has received a lot of attention [3, 23, 24, 26-32]. Since regression equations for attributes are needed for prediction and optimisation, researchers need to look for more models to cater for edge effects and other situations where the models currently in use are inadequate.

2.0 METHODOLOGY

The procedure for fitting mixture models to data starts from a simple model and progresses through models with increasing complexity such as planar, overall curvature, third order curvature and asymmetric third order curvature and the inverse terms is presented in this section. The commonly used mixture model proposed by Scheffe [33, 34] and model fitting procedure suggested by Adeyeye and Oyawale [5] and Draper and John [25] are adopted in this study.

Step 1: Start with a simple model and increase the complexity of the model until acceptable model adequacy is achieved. Start the model fitting with Scheffe's First Order Polynomial (SFOP) to see if the response/quality attribute surface is a plane (equation 1).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i \tag{1}$$

where,
$f_n(x_i)$: The response variable representing weld-metal quality attribute
x_i: Predictor variable representing the proportion of the i^{th} flux ingredient in the flux mixture,
β_i: Coefficient representing the individual effect of the i^{th} flux ingredient

Check for the adequacy of the model. If the model is adequate go to step 9, otherwise, go to the next step.

Step 2: Fit SFOP with Inverse Terms (SFOPIT) to check if there is a planar surface with edge effects as in equation 2 below.

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{i=1}^{I} \beta_{-i} x_i^{-1} \tag{2}$$

where,
β_{-i}: Coefficient of the inverse term of flux ingredient i

If the model is adequate go to step 9, otherwise, go to the next step.

Step 3: Fit Scheffe's Quadratic Canonical Polynomial (SQCP) to check the overall curvature of the surface (equation 3).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{1\le i<j\le I} \beta_{ij} x_i x_j \tag{3}$$

where,
x_j: The proportion of the j^{th} flux ingredient in the flux mixture
β_{ij}: Coefficient representing the binary effect of flux ingredients $i \text{ and } j$

If the model is adequate, go to step 9, otherwise, go to the next step.

Step 4: Fit SQCP with Inverse Terms (SQCPIT) to the experimental data to check for the overall curvature of the surface and edge effect (equation 4).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{1\le i<j\le I} \beta_{ij} x_i x_j + \sum_{i=1}^{I} \beta_{-i} x_i^{-1} \tag{4}$$

Check for model adequacy. If adequate, go to step 9, otherwise, go to the next step.

Step 5: Fit Scheffe's Special Cubic Canonical Polynomial (SSCCP) to the experimental data to check for third-order curvature of the model (equation 5).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{1\le i<j\le I} \beta_{ij} x_i x_j + \sum_{1\le i<j<k\le I} \beta_{ijk} x_i x_j x_k \tag{5}$$

where,
x_k: The proportion of the k^{th} flux ingredient in the flux mixture
β_{ijk}: Coefficient representing the ternary effects of flux ingredients $i, j \text{ and } k$

If the model is adequate go to step 9 otherwise, go to the next step.

Step 6: Fit SSCCP with Inverse Terms (SSCCPIT) to the experimental data to check for third-order curvature and edge effects (equation 6).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{1\le i<j\le I} \beta_{ij} x_i x_j + \sum_{1\le i<j<k\le I} \beta_{ijk} x_i x_j x_k + \sum_{i=1}^{I} \beta_{-i} x_i^{-1} \quad (6)$$

If the model is adequate go to step 9 otherwise, go to the next step.

Step 7: Fit Scheffe's Full Cubic Canonical Polynomial (SFCCP) to the experimental data to check for asymmetric third-order curvature (equation 7).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{1\le i<j\le I} \beta_{ij} x_i x_j + \sum_{1\le i<j\le I} \gamma_{ij} x_i x_j (x_i - x_j) + \sum_{1\le i<j<k\le I} \beta_{ijk} x_i x_j x_k \quad (7)$$

where,
x_j: The proportion of the j^{th} flux ingredient in the flux mixture
γ_{ij}: Cubic coefficient representing the binary effect of flux ingredients $i \ and \ j$

If the model is adequate go to step 9 otherwise, go to the next step.

Step 8: Fit SFCCP with Inverse Terms (SFCCPIT) to the experimental data to check for asymmetric third-order curvature and edge effects (equation 8).

$$f_n(x_i) = \sum_{i=1}^{I} \beta_i x_i + \sum_{1\le i<j\le I} \beta_{ij} x_i x_j + \sum_{1\le i<j\le I} \gamma_{ij} x_i x_j (x_i - x_j) + \sum_{1\le i<j<k\le I} \beta_{ijk} x_i x_j x_k + \sum_{i=1}^{I} \beta_{-i} x_i^{-1} \quad (8)$$

If the model is adequate go to step 9 otherwise, this procedure can not fit the data.

Step 9: Conduct a confirmatory test.

Step 10: Accept the model for prediction and optimisation.

Note: Carry out this procedure for each of the welding flux quality attributes (for $\forall\, n$). If necessary, after obtaining an adequate model, the modeller may explore the remaining models to gain more insight into the interactions among ingredients and their relationships to the various response.

3.0 NUMERICAL EXAMPLES

The problem for illustration in this example is taken from Kanjilal et al. [7] in which SQCP was fitted to flux experiment data for the prediction of weld-metal chemical composition. The lower and upper limits of flux ingredients and the extreme vertices design matrix with the corresponding experimental data are presented in Tables 1 and 2, respectively. The proportions of CaO, MgO, CaF_2 and Al_2O_3 were varied as per mixture design and the experiments were conducted in four replicates. The remaining ingredients were made up of silica (10%), ferromanganese (4%), ferrosilicon (3%), nickel (1%) and bentonite (2%). The SQCP model used by Kanjilal et al. [7] was not able to adequately predict carbon, phosphorus and nitrogen contents in the weld-metal. The constant proportion ingredients were excluded from the models. The efficacy and usefulness of mixture models with inverse terms (SFOPIT, SQCPIT, SSCCPIT and SFCCPIT) are tested by fitting them to Kanjilal et al. [7] data for carbon, phosphorus and nitrogen. The stepwise model reduction approach is adopted to fit the models using Minitab®17 software.

Table 1: Limits of welding Flux Ingredients. Kanjilal et al, [7]

Flux Ingredient	Lower Limit	Upper Limit
CaO (wt %)	15.00	35.00
MgO (wt %)	15.00	32.40
CaF_2 (wt %)	10.00	40.00
Al_2O_3 (wt %)	8.00	40.00

4.0 RESULT

The summary of the ANOVA of the models are presented in Table 3 below. None of the models could provide a good fit for carbon and nitrogen content in the weld-metal. The values of R^2_{Adj} and $R^2_{(Pred)}$ are low ($<$ 50%). The highest values of R^2_{Adj} and $R^2_{(Pred)}$ for Carbon are 48.73 and 45.51 while that of nitrogen are 44.86 and 43.32% respectively (see Table 3). However, all the models (SFOPIT, SQCPIT, SSCCPIT and SFCCPIT) showed some promise for modelling phosphorus content in the weld-metal with R^2_{Adj} and $R^2_{(Pred)}$ values $> 50\%$. The R^2_{Adj} obtained by fitting SFOPIT, SQCPIT, SSCCPIT and SFCCPIT for phosphorus in the current study are $55 < R^2_{Adj} <$ 81.57%. The performance of the models in terms of describing the variations in the phosphorus content in weld deposit and predictive ability in ascending order

Table 2: Flux Formulations Determined by Mixture Design. Kanjilal et al, [7]

Case No.	Mixture Variables/Flux composition (wt %)				Oxygen (ppm)				Phosphorus (wt%)				Nitrogen (ppm)			
	CaO	MgO	CaF_2	Al_2O_3	Replicates				Replicates				Replicates			
					1	2	3	4	1	2	3	4	1	2	3	4
C1	15.00	15.00	10.00	40.00	0.07	0.068	0.069	0.067	0.025	0.024	0.026	0.024	92	93	90	90
C2	15.00	15.00	40.00	10.00	0.07	0.071	0.068	0.068	0.028	0.026	0.026	0.03	95	96	98	98
C3	15.00	32.40	10.00	22.60	0.07	0.07	0.071	0.073	0.025	0.025	0.027	0.026	103	102	100	100
C4	15.00	17.00	40.00	8.00	0.06	0.061	0.062	0.059	0.023	0.026	0.025	0.027	86	88	88	90
C5	15.00	32.40	24.60	8.00	0.068	0.067	0.07	0.065	0.024	0.027	0.026	0.025	86	87	86	92
C6	35.00	15.00	10.00	20.00	0.098	0.096	0.095	0.093	0.021	0.022	0.022	0.02	65	66	68	63
C7	17.00	15.00	40.00	8.00	0.072	0.076	0.072	0.07	0.026	0.027	0.025	0.028	68	68	66	66
C8	35.00	15.00	22.00	8.00	0.07	0.069	0.078	0.072	0.022	0.024	0.022	0.024	62	66	61	65
C9	29.60	32.40	10.00	8.00	0.068	0.07	0.069	0.07	0.023	0.025	0.025	0.025	61	63	63	64
C10	35.00	27.00	10.00	8.00	0.063	0.067	0.066	0.06	0.022	0.026	0.024	0.02	70	69	70	62
C11	24.43	23.14	24.43	8.00	0.073	0.072	0.074	0.075	0.046	0.045	0.045	0.042	62	64	64	68
C12	15.67	15.67	40.00	8.66	0.095	0.092	0.091	0.091	0.04	0.044	0.044	0.038	73	73	71	63
C13	25.92	24.36	10.00	19.72	0.084	0.08	0.082	0.085	0.032	0.03	0.033	0.032	70	73	72	75
C14	23.40	15.00	24.40	17.20	0.089	0.085	0.087	0.091	0.047	0.043	0.043	0.042	66	64	67	67
C15	19.87	32.40	14.86	12.87	0.094	0.095	0.093	0.092	0.046	0.042	0.042	0.044	68	66	66	63
C16	15.00	22.36	24.92	17.72	0.061	0.062	0.059	0.057	0.025	0.026	0.024	0.03	76	75	75	75
C17	35.00	19.00	14.00	12.00	0.082	0.082	0.082	0.078	0.045	0.041	0.043	0.041	75	74	78	77
C18	22.67	21.63	21.63	14.07	0.058	0.057	0.055	0.06	0.044	0.043	0.042	0.043	101	100	100	100

is SFOPIT $< SQCPIT < SSCCPIT < SFCCPIT$. The response functions are presented in eqautions (9 – 12).

Scheffe' First Order Polynomial with Inverse Terms

$$P_{SFOPIT} = 0.01963\text{CaO} + 0.15897\text{MgO} + 0.19672\text{Ca}F_2 + 0.20857Al_2O_3 - \frac{0.01702}{\text{CaO}} - \frac{0.00480}{\text{MgO}} - \frac{0.00269}{\text{Ca}F_2} - \frac{0.00103}{Al_2O_3} \quad (9)$$

Scheffe's Quadratic Canonical Polynomial with Inverse Terms

$$P_{SQCPIT} = 0.068\text{CaO} + 0.011\text{MgO} + 0.211\text{Ca}F_2 + 0.277Al_2O_3 + 1.180\text{CaO.MgO} - 1.398\text{Ca}F_2.Al_2O_3 + \frac{0.007}{\text{MgO}} - \frac{0.013}{\text{Ca}F_2} - \frac{0.008}{Al_2O_3} \quad (10)$$

Scheffe's Special Cubic Canonical Polynomial with Inverse Terms

$$P_{SSCCPIT} = 0.623\text{CaO} + 0.705\text{MgO} + 0.831\text{Ca}F_2 + 0.695Al_2O_3 - 0.875\text{CaO.MgO} - 0.731\text{CaO.Ca}F_2 - 0.977\text{MgO.Ca}F_2 - 4.807\text{CaO.MgO.}Al_2O_3 - 6.594\text{MgO.Ca}F_2.Al_2O_3 - \frac{0.024}{\text{CaO}} - \frac{0.039}{\text{MgO}} - \frac{0.011}{\text{Ca}F_2} - \frac{0.009}{Al_2O_3} \quad (11)$$

Scheffe's Full Cubic Canonical Polynomial with Inverse Terms

$$P_{SFCCPIT} = 0.373\text{CaO} + 0.719\text{MgO} - 0.653\text{Ca}F_2 + 0.709Al_2O_3 - 6.027\text{MgO.Ca}F_2.Al_2O_3 + 0.734\text{CaO.MgO}(\text{CaO} - \text{MgO}) - 2.078\text{CaO.Ca}F_2(\text{CaO} - \text{Ca}F_2) - 2.545\text{MgO.Ca}F_2(\text{MgO} - \text{Ca}F_2) + 3.188\text{Ca}F_2.Al_2O_3(\text{Ca}F_2 - Al_2O_3) - \frac{0.038}{\text{Ca}F_2} \quad (12)$$

This shows that it is possible to have more than one response functions that adequately describe a response. It may be necessary to explore all potential models and then pick the one that gives the best fit. To do this, more than one statistic is required. The R^2 values were not used to assess the fit of the models in the current study because it could give misleading results in situations where the models have different number of terms. For instance, if we use R^2 to select the best model, SSCCPIT with $R^2 = 84.56\%$ will be adjudged better than SFCCPIT with $R^2 = 83.91\%$ but the reverse was the case when R^2_{Adj}values were used. The R^2_{Adj} value for SFCCPIT shows it is better in explaining the variations in phosphorus content in the weld-metal than the SSCCPIT. This is so because R^2_{Adj}, takes the number of terms in the model relative to the number of observations into account.

Table 3: Summary of Major Statistic for Assessing the Various Models

Response	Model	R^2	R^2_{Adj}	$R^2_{(Pred)}$	S	$Press$
Carbon	SFOPIT	46.11	41.13	36.87	0.0090	0.00618
	SQCPIT	53.06	48.73	45.51	0.00840	0.00533
	SFCCPIT	53.06	48.73	45.51	0.00840	0.00533
	SSCCPIT	53.06	48.73	45.51	0.008405	0.00533
Phosphorus	SFOPIT	59.43	55.00	50.34	0.00591	0.00274
	SQCPIT	72.42	68.92	65.60	0.00491	0.001896
	SFCCPIT	83.91	81.57	80.48	0.00378	0.00108
	SSCCPIT	84.47	81.32	80.27	0.00381	0.00109
Nitrogen	SFOPIT	46.59	42.55	37.56	10.1839	8002.52
	SQCPIT	48.60	43.85	39.45	10.0675	7760.52
	SFCCPIT	48.74	44.86	43.32	9.977	7264.20
	SSCCPIT	48.60	43.85	39.45	10.9675	7760.52

Although the R^2_{Adj} statistic explains the variations in the flux quality attributes, it does not necessarily indicate the predictive ability of the model. From the R^2_{Pred} and $Press$ statistic values, SFCCPIT has superior predictive ability compared to SSCCPIT (see Table 3). The R^2_{Pred} and $Press$ statistic values also show that none of the models for phosphorus content is overfit. The reduced response model for SSCCPIT and SFCCPIT and the ANOVA are presented in Tables 4 and 5. The F and p values in the ANOVA Tables, show that the regression models and the terms in them (linear, quadratic, special cubic, full cubic and inverse) are significant, while terms that are not significant and do not make positive contribution to the predictive ability of the models were automatically eliminated. For instance,three quadratic/binary terms ($CaO.Al_2O_3, MgO.Al_2O_3$ and $CaF_2.Al_2O_3$) and one special cubic term ($CaO.MgO.CaF_2$) were eliminated from the SSCCPIT model (see equation (11) and Table 4). In the case of SFCCPIT, all the quadratic terms and three out of four inverse terms were among the terms that were eliminated (see eqaution (12) and Table 5).

Table 4: Analysis of Variance for SSCCPIT

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Regression	12	0.004656	0.004656	0.000388	26.75	0.000
Linear	3	0.000121	0.000713	0.000238	16.39	0.000
Quadratic	3	0.000979	0.000219	0.000073	5.03	0.004
CaO.MgO	1	0.000000	0.000066	0.000066	4.53	0.037
$CaO.CaF_2$	1	0.000899	0.000038	0.000038	2.60	0.112
$MgO.CaF_2$	1	0.000080	0.000084	0.000084	5.77	0.019
Special Cubic	2	0.001371	0.001139	0.000569	39.26	0.000
$CaO.MgO.Al_2O_3$	1	0.001356	0.000246	0.000246	16.98	0.000
$MgO.CaF_2.Al_2O_3$	1	0.000016	0.001101	0.001101	75.89	0.000
Inverse	4	0.002184	0.002184	0.000546	37.65	0.000
1/CaO	1	0.000384	0.000151	0.000151	10.44	0.002
1/MgO	1	0.000325	0.000504	0.000504	34.76	0.000
$1/CaF_2$	1	0.001331	0.000084	0.000084	5.82	0.019
$1/Al_2O_3$	1	0.000143	0.000143	0.000143	9.87	0.003
Residual Error	59	0.000856	0.000856	0.000015		
Lack-of-Fit	5	0.000690	0.000690	0.000138	45.13	0.000
Pure Error	54	0.000165	0.000165	0.000003		
Total	71	0.005512				

The S statistic also shows that the SFCCPIT describes the phosphorus content in weld-metal as a function of flux ingredient better than the SSCCPIT. The difference between the values of R^2_{Adj} and R^2_{Pred} for SSCCPIT and SFCCPIT are 0.0105 and 0.0109 respectively.

According to the literature [35], $R^2_{Adj} - R^2_{Pred} < 0.2$ for a regression model to be acceptable. Hence, SSCCPIT and SFCCPIT provide a good fit for phosphorus since their respective $R^2_{Adj} - R^2_{Pred}$ values (0.0109 and 0.0105) are less than 0.2. Also, the values obtained for R^2_{Adj}, R^2_{Pred}, $Press$ and S show that the models with inverse terms are good for prediction of phosphorus content and has promise for modelling flux quality attributes as a function of flux ingredients. Welding flux formulators may include models with inverse terms among candidate models for fitting welding flux data. Future studies need to focus on understanding the edge effects of flux ingredients and explore other models for the prediction of carbon and nitrogen since the commonly

Table 5: Analysis of Variance for SFCCPIT

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Regression	9	0.004625	0.004625	0.000514	35.92	0.000
Linear	3	0.000121	0.003541	0.001180	82.52	0.000
Special Cubic	1	0.000520	0.001062	0.001062	74.25	0.000
$MgO.CaF_2.Al_2O_3$	1	0.000520	0.001062	0.001062	74.25	0.000
Full Cubic	4	0.000636	0.003152	0.000788	55.09	0.000
CaO.MgO(CaO-MgO)	1	0.000471	0.000109	0.000109	7.62	0.008
$CaO.CaF_2.(CaO-CaF_2)$	1	0.000002	0.000880	0.000880	61.50	0.000
$MgO.CaF_2(MgO-CaF_2)$	1	0.000085	0.000923	0.000923	64.49	0.000
$CaF_2.Al_2O_3(CaF_2-Al_2O_3)$	1	0.000077	0.000772	0.000772	53.98	0.000
Inverse	1	0.003348	0.003348	0.003348	234.04	0.000
$1/CaF_2$	1	0.003348	0.003348	0.003348	234.04	0.000
Residual Error	62	0.000887	0.000887	0.000014		
Lack-of-Fit	8	0.000722	0.000722	0.000090	29.48	0.000
Pure Error	54	0.000165	0.000165	0.000003		
Total	71	0.005512				

used models are not able to provide adequate fit for the case under study.

5.0 CONCLUSION

The following conclusions are drawn from this study.

(i) All the four Scheffe's canonical polynomials (linear, quadratic, special cubic and full cubic) with inverse terms fitted the data for phosphorus well. However, special cubic and full cubic with inverse terms gave the best fit and predictive ability for phosphorus content in the weld-metal. They have promise for prediction and optimisation of phosphorus content as function of flux ingredients.

(ii) The models were not able to adequately fit the experimental data for carbon and nitrogen in the current study. Hence further studies are required for the development of models for carbon and nitrogen.

(iii) Scheffe's canonical polynomials with inverse terms have potential for application in modelling flux quality attributes.

(iv) Further studies are required to understand the phenomenon of edge effects of flux ingredients.

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