

## ARTICLE

# Optimal Batching Plan of Deoxidation Alloying based on Principal Component Analysis and Linear Programming

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### ABSTRACT

As the market competition of steel mills is severe, deoxidation alloying is an important link in the metallurgical process. To solve this problem, principal component regression analysis is adopted to reduce the dimension of influencing factors, and a reasonable and reliable prediction model of element yield is established. Based on the constraint conditions such as target cost function constraint, yield constraint and non-negative constraint, linear programming is adopted to design the lowest cost batching scheme that meets the national standards and production requirements. The research results provide a reliable optimization model for the deoxidation and alloying process of steel mills, which is of positive significance for improving the market competitiveness of steel mills, reducing waste discharge and protecting the environment.

## 1. Introduction

The deoxidation alloying in the steelmaking process is an important process in steel smelting. Deoxidation alloying means that for different steel types, different amounts and different types of alloys need to be added at the end of smelting to remove oxygen elements as much as possible to make the alloy elements contained meet the standards, and finally make the finished steel have certain physical properties to meet specific requirements.

The deoxidation alloying of molten steel mainly concerns the content of five elements of C, Mn, S, P, and Si. As basic alloying elements, C, Mn and Si play the role of solid solution strengthening, which significantly improves the strength and hardness of the steel and improves the

hardenability of the steel. Thus the content needs to be controlled. The presence of P and S in the steel will harm the safe use of the steel. The phenomenon of cold brittleness and hot brittleness will appear, reducing the plastic toughness of the steel. The content needs to be strictly controlled.

The general research direction is to establish a mathematical model for the deoxidation alloying link through historical data, online prediction and optimization of the type and quantity of the alloy input, while ensuring the quality of the molten steel and minimizing the production cost of alloy steel.

Scholars have done a lot of research on the deoxidation and alloying of molten steel. Hu Jingtao established the LF deoxidation and alloying model, studied the

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feeding amount of aluminum wire in molten steel, and established the minimum cost model by simplex method and considering the price factor [1]; Chunxia Zhang used the artificial neural network BP model to deal with the yield parameters of alloy elements, and used the multiple linear programming method to calculate the optimal ingredients of alloying operation, and obtained the engineering results A practical control model for deoxidization and alloying [2]. However, BP neural network algorithm requires a large amount of data, and will inevitably appear “zigzag phenomenon”, which makes BP algorithm inefficient. Zhe Xu used the fuzzy modeling method to study the prediction method of the recovery rate of molten steel alloy elements and the optimization of ingredients in the ladle refining process [3]; Wenle Zhang studied the particle swarm optimization algorithm and simulated annealing algorithm for the LF refining furnace alloying, and analyzed the main factors affecting the recovery rate of alloy in the ladle refining process [4], and the convergence speed of simulated annealing algorithm The performance of the algorithm is related to the initial value and parameter sensitivity. Ruonan Cheng, et al. Used Pearson correlation coefficient to get the relationship between different factors and element yield, established BP neural network model optimized by multiple linear programming to predict the yield of C and Mn, and analyzed the optimal proportioning scheme with SPSS [5]. However, Pearson correlation coefficient method does not consider the impact of the number of overlapping records on the similarity. Yu Dai, et al. Obtained the main factors that affect the rate of C and Mn by using the grey correlation model. On this basis, the multi-objective optimization model with the lowest price and the lowest element content error was established for the burden problem. So we can get the best proportioning scheme [6]. However, the subjectivity of grey model is too strong, and the optimal value of each index needs to be determined currently. According to the formula of alloy yield, Huiling Zhou, et al. Obtained the historical yield of C and Mn elements, and established the model of influencing factors of yield based on factor analysis. Then, the multiple linear regression equations of C and Mn element yield and influencing factors are established, and finally the predicted values of C and Mn element yield are obtained [7]. Fangyu Liu, et al. Calculated the yield of C and Mn based on the data, screened out the main factors influencing the yield by Pearson correlation coefficient, obtained the prediction equation of the yield of C and Mn by multiple linear regression analysis, and then verified and improved the prediction model by BP neural network, finally realized the optimization of the cost of deoxidization and alloying of molten steel [8]. Pengmai

Liu, et al established the BP neural network model for the prediction of the recovery rate of C and Mn elements, and further improved the model and algorithm to improve the prediction accuracy of the recovery rate of elements [9]. Combined with the research of scholars, based on the idea of mathematical model, a reliable prediction model and optimization model are designed for the recovery rate of elements and the proportioning scheme, so as to improve the utilization rate of raw materials in the deoxidization and alloying process and reduce the production cost.

## 2. Factors Affecting Yield

The yield of alloying elements is an important indicator to be concerned during the deoxidation alloying process. The element yield reflects the utilization rate of important alloying elements in the alloying batching scheme and reflects the feasibility of the scheme. Too low an element yield will cause waste of raw materials, reduce production efficiency, and cause environmental pollution. Studying the yield of alloying elements has a positive effect on establishing the deoxidation alloying batching scheme.

### 2.1 Principal Component Analysis

In production, there are many factors that affect the yield of the alloy, such as the end temperature of the converter, the net weight of the molten steel, and the addition of raw materials. For multi-factor high-dimensional problems, a mathematical model based on the principal component analysis method is established. Subsequent problems are solved by evaluating the contribution of the principal component and reducing the dimension.

Principal component analysis uses  $p$ -dimensional vectors  $\vec{x} = (x_1, x_2, \dots, x_p)$  false. Standardize the original indicator data  $\vec{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T, i = 1, 2, \dots, n$ . Then construct the sample matrix.

$$M_{sample} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix} \quad (1)$$

Standardized transformation of sample array elements.

$$Z_{ij} = \frac{x_{ij} - \bar{x}_j}{S_j}, i = 1, 2, \dots, n; j = 1, 2, \dots, p \quad (2)$$

Through the above changes, a standardized matrix  $Z$  is

obtained. Then find the correlation coefficient matrix for the standardized matrix.

$$R = [r_{ij}]_p \quad xp = \frac{Z^T Z}{n-1}, \quad r_{ij} = \frac{\sum z_{ki} \cdot z_{kj}}{n-1}, \quad i, j = 1, 2, \dots, p \quad (3)$$

Solve the characteristic equation of the sample correlation matrix.

$$\sum_{j=1}^m \lambda_j / \sum_{j=1}^p \lambda_j \geq 0.85 \quad (4)$$

Determining the value of m can satisfy the information utilization rate of more than 85%. For each  $\lambda_j (j=1,2,\dots,m)$ , Solve equations  $R\vec{b} = \lambda_{jb}$ , can get the unit feature vector  $\vec{b}_j^o$ . Convert standardized index variables to main components  $U_{ij} = Z_i^T \vec{b}_j^o, j = 1, 2, \dots, m$ . Among them,  $U_1$  is called the first principal component,  $U_2$  is called the second principal component, and  $U_p$  is called the p-th principal component. Finally, comprehensive analysis and weighted sum of the m principal components are obtained to obtain the final evaluation value, and the weight is the variance contribution rate of each principal component. The principal component analysis of the factors affecting the yield of C and Mn alloys can be achieved.

### 2.2 Regression Analysis

Based on principal component analysis, a prediction model of alloy yield can be established. However, the accuracy of Principal component analysis prediction model is not high, and its accuracy is about 50%. In order to improve the accuracy of prediction, the principal component analysis model was optimized by means of multiple regression analysis<sup>[10]</sup>.

In principal component analysis, the principal components, expressions and variables that satisfy the information contribution rate of more than 85% have been obtained.

$$U = W\vec{x} \quad (5)$$

At the same time, the alloy historical yield is transformed into a column vector and combined with the sample matrix into a new sample matrix. The principal component analysis is carried out on the new sample matrix, and the new characteristic roots and eigenvectors are obtained. The linear coefficients of each principal component can be obtained by multiple regression analysis of

the corresponding eigenvectors and principal component matrices.

The yield of the alloy can be predicted according to the coefficient matrix when the independent variables (influencing factors) are given.

### 3. Optimize the Batching Plan

Based on the actual production requirements of cost and elements, new constraints can be added to the prediction model, and the method of linear programming can be adopted to make it more in line with the reality, and the mathematical model of cost optimization can be established.

#### 3.1 Objective Function

The objective function is set to cost. The constraint conditions are set as yield constraint, element content constraint and non-negative quality constraint.

$$\omega = \sum_{a=1}^{16} (m_a \cdot s_a) \quad (6)$$

At the same time, Set the addition amount of various alloys. The cost of the alloy batching scheme is the product of the amount of raw materials added to the alloy and the unit price. The cost constraint is the requirement that the cost be as small as possible.

#### 3.2 Yield Constraint

According to formula 4 and decision variable  $m_a$ , the yield prediction formula is

$$\chi = B\vec{x} = B(x_1, x_2, \dots, x_9, m_1, m_2, \dots, m_{16})^T$$

Where B represents the coefficient matrix. It should be pointed out,  $x_1, x_2, \dots, x_9$  indicate the nature of molten steel itself, which is set as a constant in the cost optimization model.  $m_1, m_2, \dots, m_{16}$  decision variable. The yield constraint requires the alloy yield to meet the basic requirements.

$$\chi \geq [\chi] \quad (7)$$

At the same time, the yield should be no more than 1.

$$[\chi] \leq \chi \leq 1 \quad (8)$$

#### 3.3 Elemental Content Constraints

Different types of steel require that the content of each

element must conform to the national standard, so the element content constraint condition is the requirement of the target composition of molten steel.

$$Bl_j \leq \frac{\sum_{i=1}^{16} c_{a,j} \chi_j m_a + b_j P}{P + \Delta P} \leq Bu_j \quad (9)$$

In the formula,  $j$  represents the element to be alloyed,  $j = 1, 2, \dots, m$ ;  $c_{a,j}$  represents the content of  $j$  falseelement in the  $i$ -th alloy;  $\chi_j$  represents the yield of element  $j$ .  $m_a$  represents the amount of alloy added;  $b_j$  falserepresents the content of element  $j$  in the original molten steel;  $P$  is the weight of the original molten steel (kg);  $\Delta P$  represents the added weight of molten steel (kg);  $Bl_j$  represents the lower limit of the requirement of the  $j$ -th element in molten steel;  $Bu_j$  represents the upper limit of the requirement of the  $j$ -th element in molten steel [11].

### 3.4 Non-negative Constraints

The minimum alloy addition amount is 0, the addition amount below 0 has no practical significance and should not be considered here.

### 3.5 Linear Programming

In above constraints,  $\Delta P$  in the inequality of the requirement for the target component of molten steel is related to the alloy addition amount  $m_a$ , that is, the constraint condition is not a general form of linear programming problem. To use the improved simplex method, first need to use  $m_a$  to represent  $\Delta P$ , and to reduce the constraints to the general form of the linear programming problem [12]. Assuming that all the alloys are put into molten steel, the linear constraints are obtained.

$$\sum_{a=1}^n \left( c_{aj} - \frac{Bu_j}{\chi_j} \right) m_a \leq \frac{P(Bu_j - b_j)}{\chi_j} \leq \sum_{a=1}^n \left( c_{aj} - \frac{Bl_j}{\chi_j} \right) m_a \quad (10)$$

After adding relaxation variables and residual variables and combining the cost constraint and non-negative condition formula, a general mathematical model for calculating the minimum cost alloy addition in the process of deoxyalloying can be obtained. The constraints are as follows.

$$\left\{ \begin{array}{l} \sum_{a=1}^n \left( c_{a1} - \frac{Bu_{j1}}{\chi_1} \right) m_a + m_{n+1} = \frac{P(Bu_1 - b_1)}{\chi_1} \\ \sum_{a=1}^n \left( c_{a1} - \frac{Bl_1}{\chi_1} \right) m_a - m_{n+2} = \frac{P(Bl_1 - b_1)}{\chi_1} \\ \dots \\ \sum_{a=1}^n \left( c_{am} - \frac{Bu_{jm}}{\chi_m} \right) m_a + m_{2m-1} = \frac{P(Bu_m - b_m)}{\chi_m} \\ \sum_{a=1}^n \left( c_{am} - \frac{Bl_{jm}}{\chi_m} \right) m_a - m_{2m} = \frac{P(Bl_m - b_m)}{\chi_m} \\ m_a \geq 0 (a = 1, 2, \dots, n; j = 1, 2, \dots, m) \end{array} \right. \quad (11)$$

This model is suitable for the calculation of various elements in alloys. In the case that the alloy contains only one alloying element and this alloying element exists only in the alloy (such as aluminum), the addition amount of the alloy is not involved in the model calculation, and the formula can be directly applied.

$$Bl_j \leq \frac{\chi_i m_a + b_j P}{P + \Delta P} \leq Bu_j \quad (12)$$

## 4. Result Analysis

The data comes from the D question of the MathorCup Mathematical Modeling Competition 2019, including historical data of steelmaking and description of various alloy materials. In order to solve the problem, the following assumptions are proposed: it is assumed that the occurrence of abnormal data is due to the reaction of steel slag or the special effect of the deoxidizer; it is assumed that only the composition of the feed is optimized, and the influence of the addition of alloy ingredients on the furnace temperature and other factors is not considered; Assuming that the historical data of steelmaking and various alloy materials in the appendix are accurate. Through principal component regression analysis and linear analysis, the model of C and Mn alloy yield and optimization of the batching scheme can be obtained.

### 4.1 Principal Component Analysis

Using MATLAB, the main component analysis of the factors affecting the yield of C and Mn alloys was achieved. The results are shown in Table 1 and Table 2.

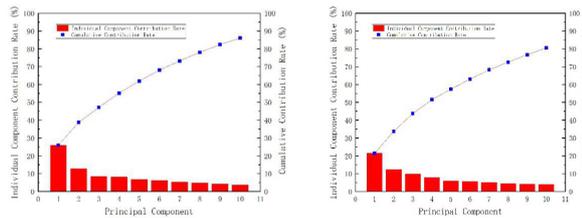
**Table 1.** The contribution of principal components to the yield of C element

No	Contribution	No	Contribution	No	Contribution
1	21.4085	7	5.175471	13	2.772642
2	12.38908	8	4.348705	14	1.887782
3	9.86408	9	4.101478	15	1.815436
4	7.824739	10	3.869279	16	1.592202
5	5.918989	11	3.355877	17	1.355792
6	5.646582	12	2.833679	18	1.254072

**Table 2.** The contribution of the main components to the yield of Mn element

No	Contribution	No	Contribution	No	Contribution
1	25.9899	6	6.124138	11	3.009176
2	12.78127	7	5.195127	12	2.801144
3	8.351011	8	4.785061	13	2.196297
4	8.048026	9	4.319319	14	1.763164
5	6.761434	10	3.676696	15	1.341023

Draw a histogram of the principal component contribution.



**Figure 1.** Cumulative contribution curve of each component to C and Mn yield

### 4.2 Multivariate Linear Analysis

Multiple regression analysis was realized, and the regression equation parameters as shown in Table 3 and Table 4 were obtained.

**Table 3.** Parameters of regression equation of C element

	Coefficients	Standard Error	t-Stat
<b>Intercept</b>	0.001047457	0.038356467	0.02730847
<b>X Variable 1</b>	0.031558432	0.017285959	1.82566858
<b>X Variable 2</b>	-0.090083783	0.022720995	-3.9647817
<b>X Variable 3</b>	-0.044355624	0.025666782	-1.7281334
<b>X Variable 4</b>	0.003899704	0.029307903	0.13305981
<b>X Variable 5</b>	-0.187262273	0.033143873	-5.6499817
<b>X Variable 6</b>	0.172774933	0.034694712	4.97986356
<b>X Variable 7</b>	0.141638615	0.035154676	4.02901213
<b>X Variable 8</b>	-0.008886455	0.038369742	-0.2316006
<b>X Variable 9</b>	0.194959025	0.039497437	4.93599184
<b>X Variable 10</b>	0.064962114	0.040714985	1.5955333

**Table 4.** Parameters of regression equation of Mn element

	Coefficients	Standard Error	t-Stat
<b>Intercept</b>	-0.000360189	0.05966	-0.00604
<b>X Variable 1</b>	-0.125833415	0.026164	-4.80947
<b>X Variable 2</b>	0.060258365	0.036076	1.670331
<b>X Variable 3</b>	-0.04655231	0.044574	-1.04438
<b>X Variable 4</b>	-0.004954195	0.046203	-0.10723
<b>X Variable 5</b>	-0.303739654	0.05332	-5.6965
<b>X Variable 6</b>	0.206682512	0.055104	3.750742
<b>X Variable 7</b>	0.037777314	0.058931	0.641044
<b>X Variable 8</b>	-0.171483094	0.061788	-2.77536
<b>X Variable 9</b>	-0.128368788	0.068568	-1.87214
<b>X Variable 10</b>	-0.052147585	0.070356	-0.74119

Knowing the regression parameters and the number of types of ingredients, a regression equation can be established to predict the yield of C and Mn elements online.

### 4.3 Linear Programming Results

For the convenience of calculation, the net weight of molten steel can be set to 70,000 kg. Establish a linear programming model and solve the cost-optimized batching plan. Related data is drawn into Table 5.

**Table 5.** Alloy batching plan (70,000kg molten steel)

Type	Inputs kg		
	HRB400	HRB500	Q345B
<b>FeV55Ni1-A</b>	5	6	
<b>Low Al ferrosilicon</b>	2	4	
<b>Vanadium Nitrogen Alloy</b>	4	2	
<b>FeV50-A</b>	40	34	
<b>FeV50-B</b>	0	0	
<b>Calcium Silicon Aluminum</b>	75	24	
<b>FeAl30Si25</b>	0	0	
<b>Silicon Aluminum Manganese Alloy Ball</b>	10	6	
<b>Silicon Manganese Slag</b>	34	36	
<b>FeSi75</b>	2	4	
<b>FeSi75-B</b>	3	0	
<b>Petroleum Coke Recarburizer</b>	85	40	
<b>FeMn64Si27</b>	1550	0	
<b>FeMn68Si18</b>	0	1360	
<b>SiC(55%)</b>	132	165	
<b>Silicon Calcium Carbon Deoxidizer</b>	24	30	

### 5. Conclusion

Based on principal component regression analysis and linear programming, optimizing the deoxidation alloying

batching plan is of great significance to actual production. The optimization model has universal significance and can be used in the production of any steel mill. When a large amount of process data is known, principal component regression analysis is used, and the main factors solved are used linear regression to obtain an optimized batching plan.

This optimization model is more directional and specific than regression analysis alone, and more general and applicable than linear programming alone. It can not only predict the yield of alloy elements online, but also obtain the optimization results of batching schemes, reduce costs, increase the yield of important elements, and improve the market competitiveness of steel mills; reduce the quality of scrap materials and play a positive role in ecological and environmental protection.

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