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Model Development to Study Uncertainties in Electric Arc Furnace Plants to Improve Their Economic and Environmental Performance

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Abstract: A statistical model is developed in order to simulate the melt composition in electric arc furnaces (EAFs) with respect to uncertainties in (1) scrap composition, (2) scrap weighing and (3) element distribution factors. The tramp element Cu and alloying element Cr are taken into account. The model enables simulations of a charge program as well as backwards estimations of the element concentrations and their variance in scrap. In the backwards calculation, the maximum likelihood method is solved by considering three cases corresponding to the involved uncertainties. It is shown that the model can estimate standard deviations for elements so that the real values lie within the estimated 95% confidence interval. Moreover, the results of the model application in each target product show that the estimated scrap composition results in a melt composition, which is in good agreement with the measured one. The model can be applied to increase our understanding of scrap chemical composition and lower the charged material cost and carbon footprint of the products.

Keywords: scrap; tramp element; uncertainty; standard deviation; maximum likelihood; EAF



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1. Introduction

Mixing raw materials is critical in scrap-based plants, such as electric arc furnaces (EAFs), where meeting chemical composition targets and a cost-efficient mix of raw materials should be simultaneously taken into account. Mathematical models developed to study the mixing of raw materials can be classified into the following groups: (i) mass–energy balance, (ii) optimization and (iii) statistical models. The mass and energy balance models are divided into static and dynamic models and used to calculate energy consumption, melt chemical composition and tapping time [1–4]. In the calculations, the scrap composition is assumed to be known, and uncertainties are not taken into account.

The raw material optimization models can be classified into deterministic and stochastic models [5–7]. In a linear deterministic optimization model developed by Lahdelma et al. [5], safety margins are considered to account for uncertainties in the scrap composition. The element concentration and its variance were estimated by applying the ordinary and recursive least squares and maximum likelihood methods. Additionally, several stochastic models have been developed to include uncertainties in scrap materials by using chance constraint (CC) programming. In chance constraint optimization, the constraint fulfillment under uncertainties is expressed by probability estimations. Gaustad et al. [6] developed a chance constraint model in which the production cost is minimized subject to probability constraints for lower and upper limits of a target product. It is assumed that element considerations are normally distributed in each scrap material. The constraints are written for the normally distributed element concentration, and the variance of the chemical composition of the different types of scrap is known. The variances can be estimated by methods such as

the random sampling analysis (RSA), which is followed by optical emission spectroscopy determinations [8].

Some statistical models use process data to predict scrap properties [9,10]. Birat et al. [9] developed a model to estimate the average concentration of tramp elements in scrap by solving linear regression equations. The scrap compositions were related to the melt compositions through the raw material recipe data and yields of the heats. The partial least squares-based method was applied in a model developed by Sandberg et al. [10], in which the scrap properties were estimated by using EAF process data. A scrap chemical composition was calculated for a “pure heat”, which corresponds to a heat charged by 100% of that scrap type. The Cu content in different types of scrap was estimated by a 95% confidence interval. The reliability of the results was studied by checking if the scrap portion in the mix is close to one in a pure heat simulation of a specific scrap type. The results showed that the method is applicable when there is a correlation between a scrap and other scrap types and the target product chemical composition.

Uncertainties are not limited to scrap composition as described above, but they involve all measurements from loading scrap to tapping the liquid steel. In this study, the aim is to develop a statistical model as a calculation tool that can mainly be used in an EAF plant to deal with the uncertainties in steel scrap analysis. Furthermore, it should deal with lack of scrap analysis and facilitate production planning of a heat to meet the target composition. In doing this, the tramp element copper in scrap is taken into account. This element is difficult to remove from steel, and exceeding the maximum allowed concentration can result in detrimental effects on final products, such as reducing ductility and causing hot cracks [11]. Thus, it is important to evaluate the copper concentration and its dispersion in different types of charged scrap. This importance is described by Gyllenram et al. [12] by obtaining a relationship between the quality cost, confidence interval and percent of low-quality scrap with high Cu content (with an average of 0.3 and standard deviation of 0.03), which can be used to determine the risk percent lying outside the target product limits. Moreover, identifying the Cu content can lead to a lower charging of high-purity raw materials. This is clearly demonstrated by charge optimizations conducted for two hypothetical scenarios by using the web-based software RAWMATMIX® (Kobolde & Partners AB, Stockholm, Sweden) [13,14]. The main input data for these are listed in the Appendix A. The real copper content in a scrap type is considered to be 0.1%, and the content considered by a hypothetical steel plant is 0.3%. Therefore, in the optimizations, the copper content is assumed to be 0.1% and 0.3% in the first and second scenario, respectively. The results show that pig iron is added to dilute the melt in order to not exceed the maximum concentration of copper in the target product, as shown in Table 1. This results in an increase in material cost and scope 3 carbon footprint by 74 USD/tm and 638 kgCO₂eq/tm, respectively.

Table 1. Cost and scope 3 carbon footprint results for two scenarios of copper content assumptions in a scrap type.

Scenario	Actual Cu in Scrap (%)	Assumed Cu in Scrap (%)	Scrap Amount (kg)	Pig Iron Amount (kg)	Material Cost (USD/tm)	Carbon Footprint Scope 3 (kgCO ₂ eq/tm)
1	0.1	0.1	102,301	0	238	9
2	0.1	0.3	68,027	34,561	300	647

Moreover, the uncertainties with respect to the alloying element chromium are also investigated. Determining the content of alloying elements in scraps contributes to a planned material recipe that makes use of such elements. This leads to a lower usage of primary alloys, with high upstream carbon footprint values, which consequently reduces the costs and the carbon footprint of products.

The developed statistical model simulates the melt composition by taking into account different uncertainties involved in the EAF process. The model uses the maximum likelihood method to estimate variances in scrap chemical composition. This method was briefly mentioned by Lahdelma et al. [5], while it is described here in detail. Addition-

ally, the uncertainties involved in weighing of scrap and in element distribution factors are included.

2. Model Description

The model is divided into two parts, namely (1) a simulation of a charge program containing several heats and (2) a backward estimation of scrap composition. The model is developed as a Java web application.

2.1. Simulation of a Charge Program

The melt chemical composition in an EAF is estimated for each heat in two following process stages:

2.1.1. Scrap Simulation

The scrap composition is considered to be normally distributed. The concentration of element i in scrap j is written as follows:

$$C_{i,j} = \bar{C}_{i,j} + z \sigma_{i,j} \quad (1)$$

where $\bar{C}_{i,j}$ is the average concentration of element i ; $\sigma_{i,j}$ is the standard deviation for element i in material j ; and z is a Gaussian random number, $N(0,1)$.

2.1.2. Charge Program Simulation

The scrap simulation is conducted for each heat in a charge program. Then, the melt chemical composition, $C_{i,k}$, for each heat k is calculated as follows by using the loading/weighing accuracy of scrap and the distribution factor accuracy (σ_{d_i}):

$$C_{i,k} = 0.01 \frac{M_{i,m}}{M_{tot}} \quad (2)$$

where $M_{i,m}$ is the mass of element i in the melt and M_{tot} is the total mass of the melt, which can be expressed as follows:

$$M_{i,m} = M_i d_i \quad (3)$$

$$M_{tot} = \sum_i M_{i,m} \quad (4)$$

where d_i is the distribution factor of element i between the melt and slag, and M_i is the total element mass in scrap, which can be estimated by the average distribution factor for element i , \bar{d}_i , as follows:

$$d_i = \bar{d}_i + z \sigma_{d_i} \quad , \quad 0 \leq \bar{d}_i \leq 1 \quad (5)$$

$$M_i = \sum_j 0.01 M_j \sum_i C_{i,j} \quad (6)$$

where

$$M_j = M_{j,crane} + z \sigma_w \quad (7)$$

$$M_{j,crane} = M_{j,recipe} + z \sigma_l \quad (8)$$

where σ_w and σ_l are the weighing and loading accuracies (kg), respectively. Moreover, $M_{j,crane}$ and $M_{j,recipe}$ are the amount of material j weighted by crane and according to recipe of a specific steel grade, respectively.

2.2. Backward Estimation of Scrap Composition

First, the Lawson and Hanson non-negative least squares (NNLS) method [15] is used to estimate the scrap composition, which is an optimal solution, C , such that the following relationship is valid [15]:

$$\min \|XC - Y\|_2^2, \quad C \geq 0 \quad (9)$$

where X is a $k \times j$ matrix and contains amounts of scrap in a charge program with k heats and j scrap types, and Y is a column vector ($k \times 1$) containing a mass of the element in the melt in each charge. $y_{i,k}$ is obtained by multiplying the melt weight by the concentration of element i in the melt in charge k . The results, vector C , are the absolute estimated concentrations of elements in scrap excluding uncertainties.

$$X = \begin{bmatrix} x_{1,1} & \cdots & x_{1,j} \\ \vdots & \ddots & \vdots \\ x_{k,1} & \cdots & x_{k,j} \end{bmatrix}, \quad Y = \begin{bmatrix} y_{1,1} \\ \vdots \\ y_{i,k} \end{bmatrix}, \quad C = \begin{bmatrix} \bar{C}_{i,1} \\ \vdots \\ C_{i,j} \end{bmatrix} \quad (10)$$

In the next method, in addition to the average concentration of element, the standard deviations for the concentration of each element in scrap are included as unknown parameters. It is assumed that element concentrations in scrap are normally distributed. In doing this, the three cases described below are taken into account. The loading accuracy is set to zero for all cases.

2.2.1. Uncertainties in Scrap Chemical Composition

The distribution factor for element i is considered to be constant, $\sigma_{d_i} = 0$, and uncertainty in the raw material weighing is zero so that $M_j = M_{j, \text{recipe}}$. The following equation is solved for each element, in which $\sigma_{i,j} = \sigma_j$, $y_{i,k} = y_k$ and $\bar{C}_{i,j} = \bar{C}_j$:

$$d_i \begin{bmatrix} x_{1,1} & \cdots & x_{1,j} \\ \vdots & \ddots & \vdots \\ x_{k,1} & \cdots & x_{k,j} \end{bmatrix} \begin{bmatrix} \bar{C}_1 \\ \vdots \\ \bar{C}_j \end{bmatrix} + d_i \begin{bmatrix} x_{1,1} z_{1,1} \sigma_1 + \cdots + x_{1,j} z_{1,j} \sigma_j \\ \vdots \\ x_{k,1} z_{k,1} \sigma_1 + \cdots + x_{k,j} z_{k,j} \sigma_j \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_k \end{bmatrix} \quad (11)$$

This equation is rewritten as follows:

$$\begin{bmatrix} x_{1,1} & \cdots & x_{1,j} \\ \vdots & \ddots & \vdots \\ x_{k,1} & \cdots & x_{k,j} \end{bmatrix} \begin{bmatrix} \bar{C}_1 \\ \vdots \\ \bar{C}_j \end{bmatrix} + \varepsilon = \frac{1}{d_i} \begin{bmatrix} y_1 \\ \vdots \\ y_k \end{bmatrix} \quad (12)$$

where $\text{Var}(\varepsilon) = \text{diag}\{x_{1,1}^2 \sigma_1^2 + x_{1,2}^2 \sigma_2^2 + \cdots + x_{1,j}^2 \sigma_j^2, \dots, x_{k,1}^2 \sigma_1^2 + x_{k,2}^2 \sigma_2^2 + \cdots + x_{k,j}^2 \sigma_j^2\}$ since $\text{cov}(x_{1,m} z_{1,m} \sigma_1, x_{k,j} z_{k,j} \sigma_j) = 0 \quad \forall l \neq k \text{ \& } m \neq j$.

2.2.2. Uncertainties in Scrap Chemical Composition and Weighing

Besides variances in the scrap chemical composition, uncertainty in scrap weighing is taken into account, $\sigma_w \neq 0$, which is assumed to be a constant value. Thus, $\text{Var}(\varepsilon)$ is written as $\text{Var}(\varepsilon) = \text{diag}\{x_{1,1}^2 \sigma_1^2 + \cdots + x_{1,j}^2 \sigma_j^2 + \bar{C}_1^2 \sigma_w^2 + \cdots + \bar{C}_j^2 \sigma_w^2 + \sigma_1^2 \sigma_w^2 + \cdots + \sigma_j^2 \sigma_w^2, \dots, x_{k,1}^2 \sigma_1^2 + \cdots + x_{k,j}^2 \sigma_j^2 + \bar{C}_1^2 \sigma_w^2 + \cdots + \bar{C}_j^2 \sigma_w^2 + \sigma_1^2 \sigma_w^2 + \cdots + \sigma_j^2 \sigma_w^2\}$

2.2.3. Uncertainties in Scrap Chemical Composition and Element Distribution Factors

In this scenario, variances in the element distribution factors are included, $\sigma_{d_i} \neq 0$, while $\sigma_w = 0$. Therefore, the following equation is solved:

$$(\bar{d}_i + z_k \sigma_{d_i}) \begin{bmatrix} x_{1,1} & \cdots & x_{1,j} \\ \vdots & \ddots & \vdots \\ x_{k,1} & \cdots & x_{k,j} \end{bmatrix} \begin{bmatrix} \bar{C}_1 \\ \vdots \\ \bar{C}_j \end{bmatrix} + (\bar{d}_i + z_k \sigma_{d_i}) \begin{bmatrix} x_{1,1} z_{1,1} \sigma_1 + \cdots + x_{1,j} z_{1,j} \sigma_j \\ \vdots \\ x_{k,1} z_{k,1} \sigma_1 + \cdots + x_{k,j} z_{k,j} \sigma_j \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_k \end{bmatrix} \quad (13)$$

$$\text{where } \text{Var}(\varepsilon) = \text{diag}\left\{(\bar{d}_i x_{1,1})^2 \sigma_1^2 + \dots + (\bar{d}_i x_{1,j})^2 \sigma_j^2 + (\sigma_{d_i} x_{1,1})^2 \sigma_1^2 \dots + (\sigma_{d_i} x_{1,j})^2 \sigma_j^2 + (\bar{C}_1 \sigma_{d_i} x_{1,1} + \dots + \bar{C}_j \sigma_{d_i} x_{1,j})^2, \dots, (\bar{d}_i x_{k,1})^2 \sigma_1^2 + \dots + (\bar{d}_i x_{k,j})^2 \sigma_j^2 + (\sigma_{d_i} x_{k,1})^2 \sigma_1^2 + \dots + (\sigma_{d_i} x_{k,j})^2 \sigma_j^2 + (\bar{C}_1 \sigma_{d_i} x_{k,1} + \dots + \bar{C}_j \sigma_{d_i} x_{k,j})^2\right\}$$

Due to the normally distributed concentrations, the parameters C and σ can be estimated by using the maximum likelihood method [16]. In fact, the parameters of probability function that maximize the log-likelihood function are estimated. The log-likelihood function is written in the matrix form by taking the logarithm over the probability density function and ignoring constant terms [16]:

$$\log l = -\frac{1}{2} \log(|\text{Var}(\varepsilon)|) - \frac{1}{2} (Y - XC)^T (\text{Var}(\varepsilon))^{-1} (Y - XC) \quad (14)$$

Then, a bound constraint quasi-Newton method in R software environment v 3.6.2 (R Foundation for Statistical Computing, Vienna, Austria) [17], which is a variant of the L-BFGS-B (limited memory Broyden–Fletcher–Goldfarb–Shanno Bound constrained) method [18], is used to estimate the values for different parameters of this function, at which the objective function, $-\log l$, reaches its minimum values.

3. Model Validation and Application

The model is first validated by using hypothetical data. Two variations of standard deviations are applied to Cu concentration for six different types of scrap. The distribution factor for Cu is 1, so the distribution accuracy for Cu is not taken into account, $\sigma_{d_i} = 0$. Tables 2 and 3 show the average concentrations and standard deviations for Cu in different scrap types, respectively. In cases 1 and 2, $\sigma_w = 0$; $\sigma_w = 10$ kg in case 3; and $\sigma_w = 50$ kg in case 4.

Table 2. Average concentration of Cu and Cr in scrap, $C_{Cu,j}$ and $C_{Cr,j}$ in six scrap types (x_j).

j	1	2	3	4	5	6
$C_{Cu,j}$ (%)	0.05	0.05	0.14	0.3	0.2	0.05
$C_{Cr,j}$ (%)	0.15	0.2	1.43	0.2	0.1	1

Table 3. Standard deviations for Cu and Cr in each scrap type, standard deviations for weighing and standard deviation for Cr distribution factor.

Case	$\sigma_{Cu,1}$	$\sigma_{Cu,2}$	$\sigma_{Cu,3}$	$\sigma_{Cu,4}$	$\sigma_{Cu,5}$	$\sigma_{Cu,6}$	σ_w (kg)	σ_{dCu} (%)
1	0.02	0.02	0.02	0.02	0.02	0.02	0	0
2	0.02	0.015	0.04	0.01	0.03	0.025	0	0
3	0.02	0.015	0.04	0.01	0.03	0.025	10	0
4	0.02	0.015	0.04	0.01	0.03	0.025	50	0
Case	$\sigma_{Cr,1}$	$\sigma_{Cr,2}$	$\sigma_{Cr,3}$	$\sigma_{Cr,4}$	$\sigma_{Cr,5}$	$\sigma_{Cr,6}$	σ_w (kg)	σ_{dCr} (%)
5	0.01	0.04	0.03	0.04	0.02	0.3	0	0
6	0.01	0.04	0.03	0.04	0.02	0.3	0	0.05

For Cr, two cases (5 and 6) are considered. In case 5, only variances in scrap composition are applied, and in case 6, the standard deviation in Cr distribution factor is included, so that $\sigma_{dCr} = 0.05$, while $\sigma_w = 0$ in both cases. The average concentration of Cr and its standard deviation in six scrap types are shown in Tables 2 and 3, respectively.

For each case, charge program simulation is performed for 7000 heats. Then, in backward estimation of scrap composition, the bootstrap resampling method is used to generate several datasets from the heats.

In the next step, the model is used to investigate the accuracy of scrap composition used by a real plant and to estimate uncertainties in element concentrations in scrap and

uncertainties in distribution factors of elements in each target product. The flowchart in Figure 1 demonstrates the steps involved in the model application. First, the aforementioned model is used to simulate a charge program by using heat data from an EAF, including approximately 700 heats and 10 scrap types. The input data include the heat recipe as well as scrap and melt chemical compositions. The melt analysis is carried out using the optical emission spectrometry technique in the plant. Since there is no dispersion on the element concentration in scrap, the standard deviations are set to zero for all elements, $\sigma_{i,j} = 0$. The predicted results of the melt chemical compositions are compared to those of the measured melt compositions for Cu and Cr. If the difference between the average concentration and standard deviation of each element in the melt in the calculated and measured results is considerable ($|C_{i,calc} - C_{i,m}| > 0.01$ and $|\sigma_{i,calc} - \sigma_{i,m}| > 0.009$) in a target product, the backwards calculations (NNLS and ML methods) are applied to estimate the element concentration and its uncertainty in each scrap type. Thereafter, these results are used as scrap composition inputs in the model to calculate a new melt composition. Three target products (A, B and C) are taken into account.

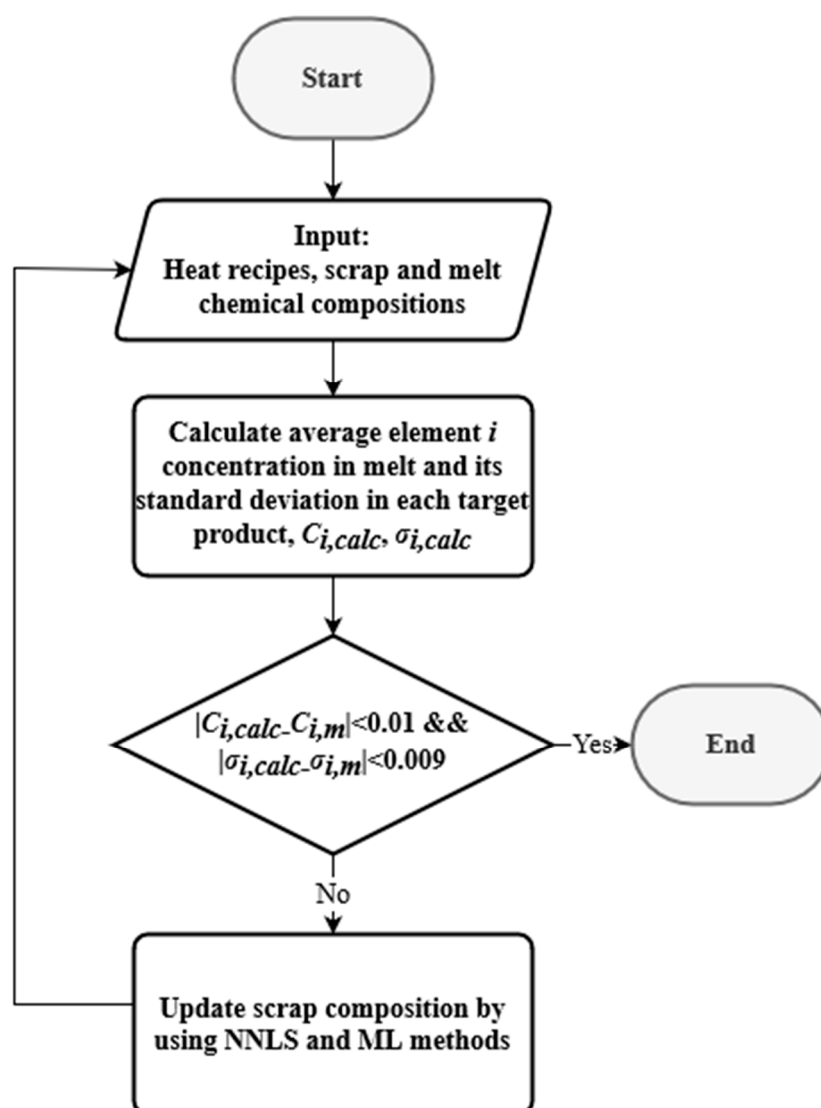


Figure 1. A flowchart of the procedure to estimate the accuracy of the scrap chemical composition.

4. Results and Discussion

The results include the model validation and its application. In the first part, the results of the backwards estimation of the Cu and Cr concentrations and standard deviation in

scrap are compared to the real input values. Afterwards, the model is used to investigate the accuracy of Cu and Cr concentrations in the reported scrap compositions in an EAF plant.

4.1. Model Validations Results

The results of the backward calculations of the Cu concentration and the standard deviations for the six cases are shown in Tables 4 and 5 using the NNLS and maximum likelihood methods (ML), respectively. The difference between the average concentration of Cu in scrap estimated by these two methods is low, namely between 0 and 0.003. Furthermore, the difference between the real concentrations and calculated ones is between 0 and 0.014, obtained by using the results in Tables 4 and 5 and inputs from Table 2. The differences between the calculated (by the ML method) and real values for the standard deviations are between 0 and 0.009, which can be obtained by using the results in Table 5 and inputs in Table 3. It can be concluded that the ML method can be used to estimate standard deviations for Cu, meaning that the maximum difference between the calculated and real values is around 0.01.

Table 4. Calculated average concentration of Cu in scrap, $C_{Cu,j}$, in six scrap types (x_j) using the NNLS method.

Cases	x1	x2	x3	x4	x5	x6
1	0.049	0.051	0.142	0.302	0.201	0.042
2	0.048	0.048	0.145	0.303	0.202	0.055
3	0.049	0.049	0.142	0.301	0.204	0.046
4	0.049	0.049	0.140	0.302	0.199	0.065
5	0.151	0.195	1.427	0.196	0.104	0.993
6	0.147	0.204	1.435	0.209	0.104	0.943

Table 5. Calculated mean concentration of Cu in scrap, \bar{C}_{Cu} , and its standard deviation, $\bar{\sigma}_{Cu}$, in six scrap types (x_j) using the maximum likelihood method for nine cases.

Cases	Variable	x1	x2	x3	x4	x5	x6
1	\bar{C}_{Cu}	0.05	0.051	0.139	0.303	0.201	0.043
	$\bar{\sigma}_{Cu}$	0.02	0.023	0.017	0.017	0.021	0.019
2	\bar{C}_{Cu}	0.048	0.048	0.145	0.303	0.201	0.055
	$\bar{\sigma}_{Cu}$	0.021	0.011	0.035	0.010	0.029	0.027
3	\bar{C}_{Cu}	0.049	0.052	0.143	0.302	0.204	0.046
	$\bar{\sigma}_{Cu}$	0.021	0.018	0.036	0.002	0.027	0.021
4	\bar{C}_{Cu}	0.050	0.048	0.141	0.301	0.197	0.064
	$\bar{\sigma}_{Cu}$	0.019	0.008	0.041	0.013	0.028	0.016
5	\bar{C}_{Cu}	0.151	0.195	1.426	0.196	0.103	1.011
	$\bar{\sigma}_{Cu}$	0.01	0.04	0.031	0.038	0.018	0.299
6	\bar{C}_{Cu}	0.150	0.202	1.429	0.204	0.097	0.994
	$\bar{\sigma}_{Cu}$	0.010	0.041	0.011	0.018	0.012	0.297

For Cr, the differences between the mean concentration of Cr estimated by the ML and NNLS methods vary mainly between 0 and 0.01. However, for case 6 and material 6, the difference is higher, around 0.05, when it is calculated using the results in Tables 4 and 5. The comparison of these results with the real values in Table 2 shows that the estimated average value obtained using the ML method is close to the real values, with a difference of only 0.006. The estimated standard deviations differ from the real values when there is standard deviation on the Cr distribution factor. Specifically, the maximum difference is around 0.02, calculated by using data from Tables 3 and 5.

Figures 2 and 3 show the comparison between the measured values for Cu and Cr concentrations and their estimated mean values by considering a 95% confidence interval. It can be seen that the real values lie in the confidence interval for all cases.

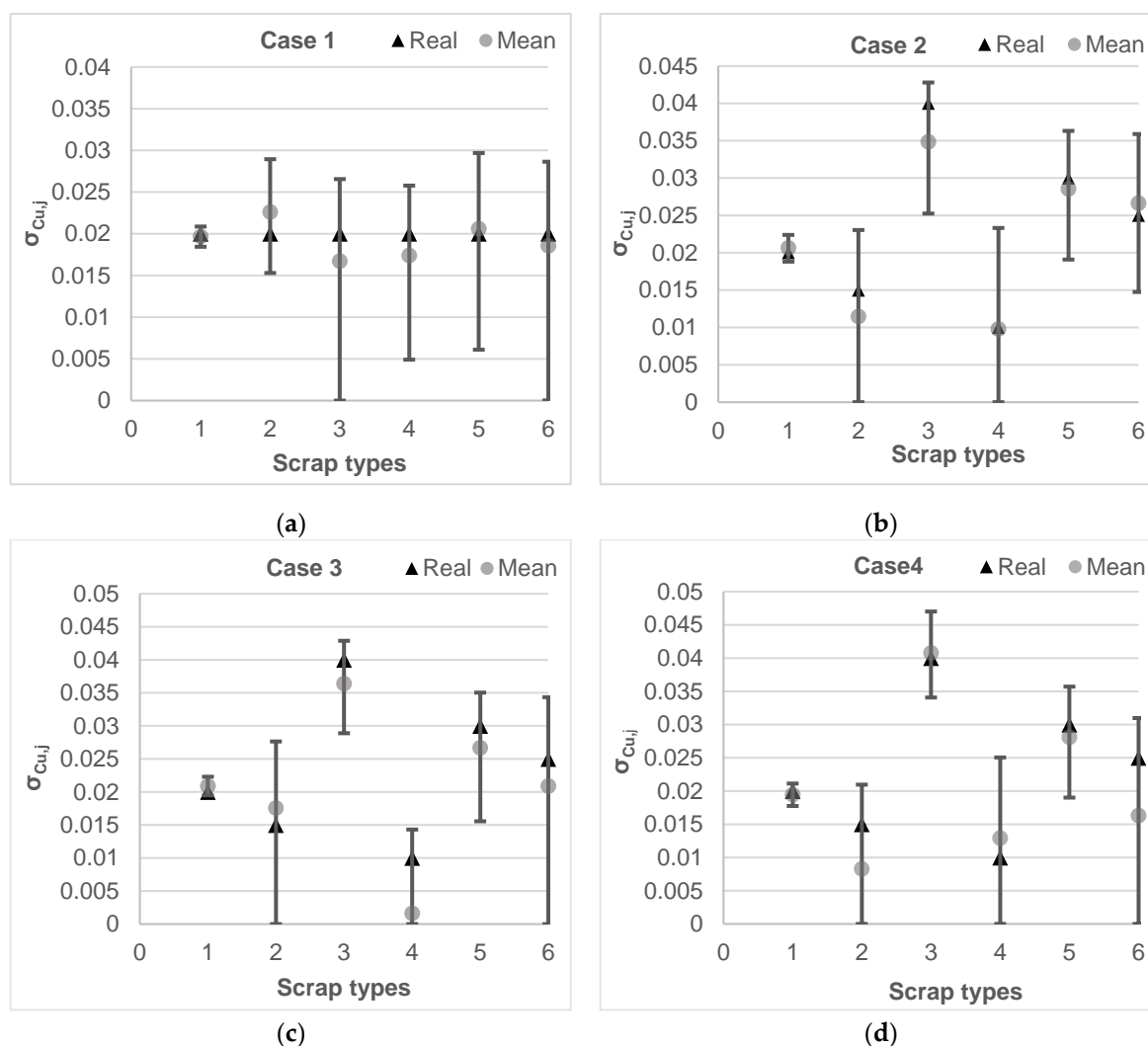


Figure 2. Estimated mean standard deviations for concentration of Cu (σ_{Cu}) with a 95% confidence interval in scrap types, x1–x6 for cases 1–4, (a–d).

4.2. Model Application Results

The density plot of the Cu concentration for the target product A, including 103 heats, is shown in Figure 4. The melt chemical composition is almost normally distributed and has an estimated skewness of ≈ 0.17 and a kurtosis of ≈ 2.86 .

As described in Figure 1, first, a charge program simulation is conducted using the reported scrap composition for target product A. This resulted in an average concentration of Cu in the melt equal to 0.1, which is around 0.015 higher than the measured value. This indicates the inaccuracy in the Cu concentration in the charged scrap. This also shows that the reported scrap composition is not the average value, but it is considered at a confidence interval. Since $|C_{Cu,calc} - C_{Cu,m}| > 0.01$, the next step is to estimate the Cu concentration in scrap by using the NNLS method, as suggested in Figure 1. The melt weight is estimated by summing of charged materials and assuming a metallic yield of 0.96. The comparison between the reported Cu concentrations and the estimated values is shown in Figure 5 for 10 scrap types. The new scrap analysis is applied in the charge program simulation, which results in a better predicted concentration of Cu for target product A, so that $|C_{Cu,calc} - C_{Cu,m}| \approx 0.0019$. This can be seen in Figure 6a, which illustrates the normal distribution plots for Cu concentrations in the melt. R denotes the primary results obtained by the reported scrap chemical composition. Then, the Cu concentration in scrap is estimated using the ML method. The estimated average values and standard deviations

(shown as $\pm\sigma$) are presented in Figure 5. The estimated standard deviation is high in some scrap types, especially in x2, x4 and x9. It can be seen that the reported Cu content is much higher than the estimated value in scrap x4, around 0.1%. The overestimation of Cu content can lead to a material recipe that effects the cost and carbon footprint, as described in Table 1. These values are used in the charge program simulation to estimate the melt composition as depicted by the green lines in Figure 6.

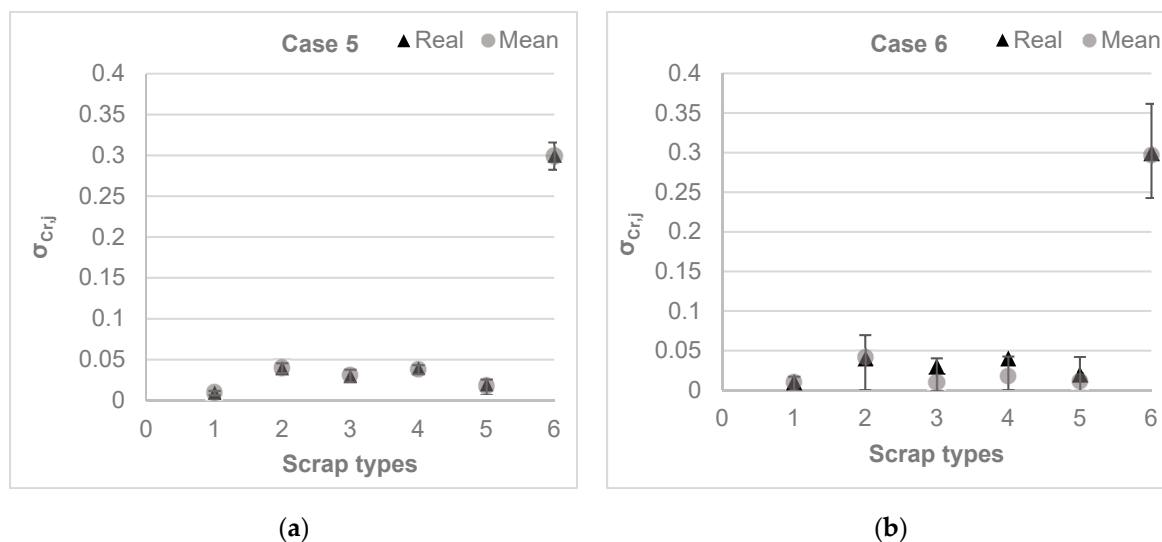


Figure 3. Estimated mean standard deviations for concentration of Cr (σ_{Cr}) with a 95% confidence interval in six scrap types, x1–x6 for cases 5 and 6, (a,b).

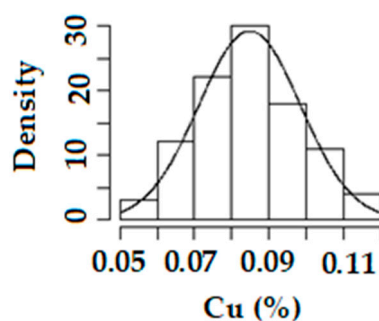


Figure 4. Density plot of Cu concentration in target product A.

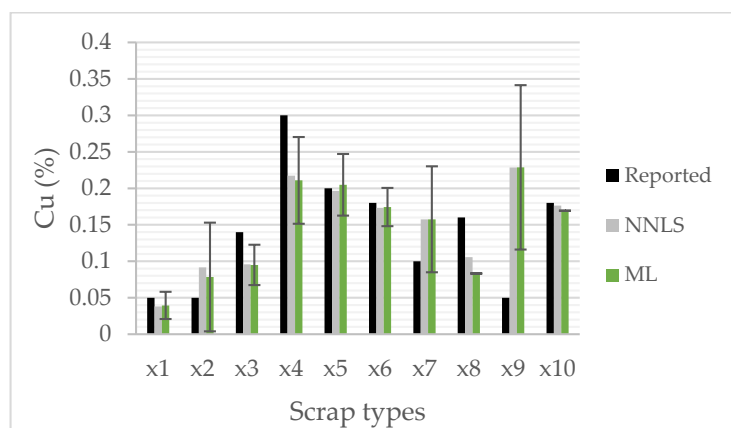


Figure 5. Comparison between the reported Cu concentration and calculated values in scrap (x1–x10).

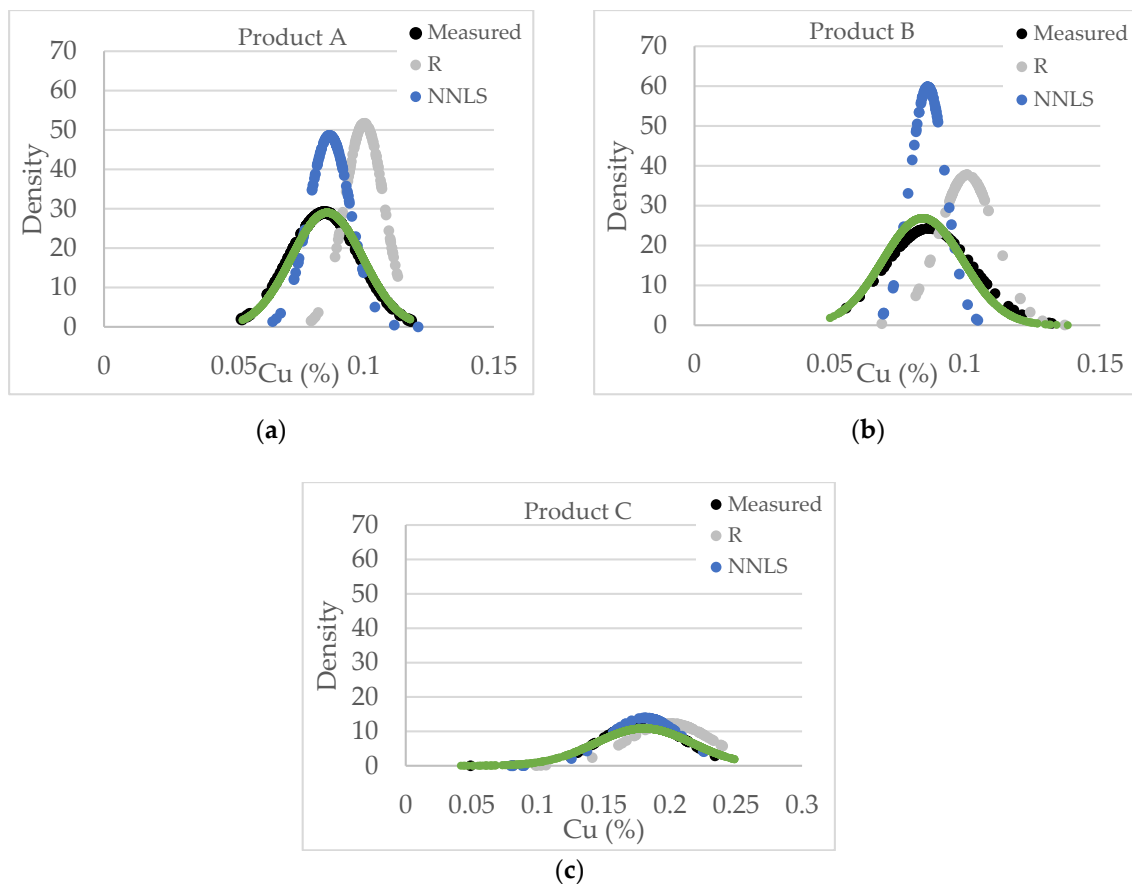


Figure 6. Comparison between the concentrations of Cu calculated using the reported scrap compositions (R) and the calculated scrap compositions using the NNLS and ML methods. Data are presented for three target products: A, B and C, (a–c).

The results of the Cu dispersion in the melt, $\sigma_{Cu,m} \approx 0.015$, are in very good agreement with the measured data. More specifically, $\sigma_{Cu,calc} \approx 0.014$, so that $|\sigma_{Cu,calc} - \sigma_{Cu,m}| \approx 0.001$, as depicted in Figure 6a. The same procedure is applied to target products A and B, as seen in Figure 6b,c.

The results of the estimated Cr concentrations using NNLS and ML (shown with $\pm\sigma$) in 10 scrap types are compared to those reported in Figure 7. When the reported Cr concentration in scrap is used in a simulation, the average concentrations of Cr in the melt are close to the measured concentrations. This can be seen in the normal distribution plots for the Cr concentration for all target products, as shown in Figure 8, (Measured and R). However, the differences among the standard deviations of Cr concentrations in the melt are 0.03, 0.04 and 0.01 for products A, B and C, respectively. Therefore, the Cr concentration is estimated using the NNLS and ML methods. In the ML method, σ_{d_i} is assigned to 0.1 for target products A and B and 0.08 for target product C. This means that the third approach in the backward calculation of the scrap composition is applied. The results of the melt composition using the scrap composition estimated by the NNLS method results in higher differences in standard deviations of Cr concentrations in the melt, as depicted in the blue line in Figure 8. By using the inputs from ML methods, the differences decrease to 0.003, 0.008 and 0.004 for products A, B and C, respectively, as shown in Figure 8a–c.

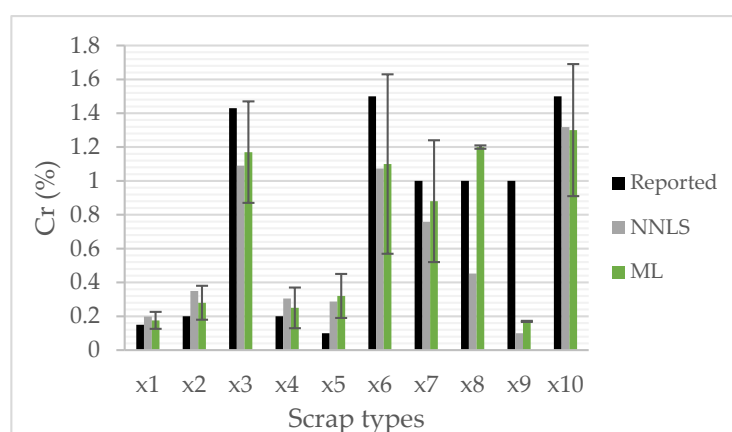


Figure 7. Comparison between the reported Cr concentration and calculated ones in scrap (x1–x10).

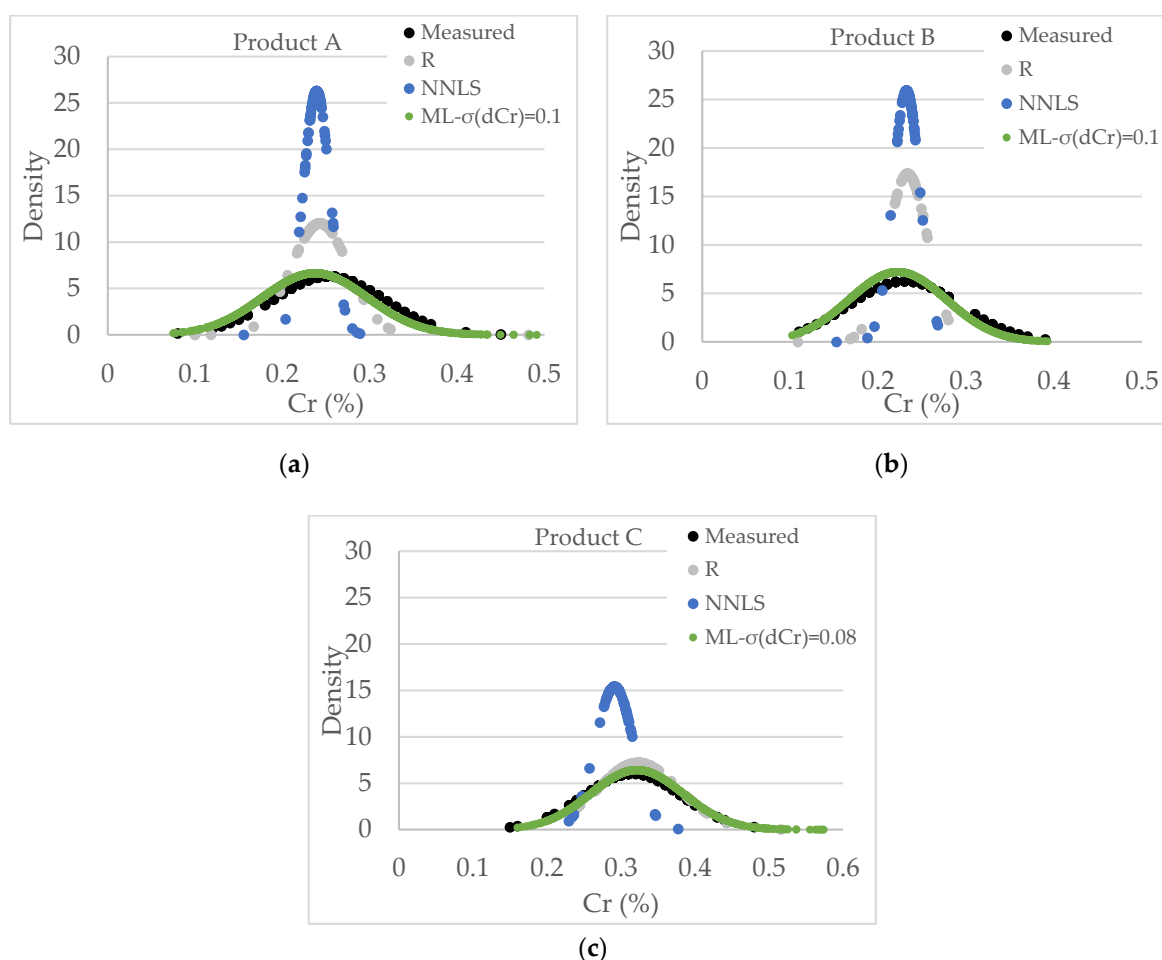


Figure 8. Comparison between the concentration of Cr calculated using the reported scrap composition (R) and the calculated scrap composition using the NNLS and ML methods. Data are given for three target products: A, B and C, (a–c).

4.3. Use of the Model

Today's pursuit of continuous improvement in terms of cost, quality and environmental performance requires the application of powerful calculation tools. The model described here can be applied to increase our knowledge about the uncertainties in raw material analysis and other measurements. This knowledge contributes to designing raw material

recipes that result in lower material costs and CO₂ emissions (as outlined in Table 1), and it forms a basis for determining the optimal risk level.

5. Conclusions

A model was developed with the aim to investigate uncertainties involved in scrap melting plants, including (i) scrap composition, (ii) weighing and (iii) distribution factors. The maximum likelihood method was applied to predict these uncertainties by assuming that they are normally distributed. The results of the model validation showed that the real values for the average and standard deviation for the concentration of each element in scrap lie within a nominal confidence interval, and the model can be used to determine variances in scrap composition.

The model was then applied to real heat data of an EAF in order to examine the accuracy of the reported scrap chemical compositions with a focus on the tramp element Cu and the alloying element Cr. The differences between the mean and standard deviations in Cu and Cr concentrations in three target products and the simulated values suggested that uncertainties in the scrap composition and Cr distribution factor exist. The use of the predicted new scrap concentrations and variances in the model resulted in melt chemical compositions that are in better agreement with the measured ones. It is finally suggested that the model can be used in a continuous improvement process at a plant to improve the raw material risk assessment and also lower the input raw material costs and CO₂ emissions.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. Input data used for calculations shown in Table 1.

Furnace capacity (tonne)	100
Maximum concentration of copper in target product (%)	0.2
Scrap Price (USD/kg)	0.23
Scrap upstream carbon footprint (kg CO ₂ eq/kg)	0.007
Pig iron price (USD/kg)	0.41
Pig iron upstream carbon footprint (kg CO ₂ eq/kg)	1.85

References

1. Bekker, J.; Craig, I. Modeling and Simulation of an Electric Arc Furnace. *ISIJ Int.* **1999**, *32*, 23–32. [\[CrossRef\]](#)
2. Gaustad, G.; Preston, L.; Kirchain, R. Modeling Methods for Managing Raw Material Compositional Uncertainty in Alloy Production. *Resour. Conserv. Recycl.* **2007**, *52*, 180–207. [\[CrossRef\]](#)
3. Badr, K.; Kirschen, M.; Cappel, J. Chemical Energy and Bottom Stirring Systems-Cost Effective Solutions for a Better Performing EAF. In Proceedings of the METEC InSteelCon, Düsseldorf, Germany, 27 June–1 July 2011.
4. MacRosty, R.; Swartz, C. Dynamic Modeling of an Industrial Electric Arc Furnace. *Ind. Eng. Chem. Res.* **2005**, *44*, 8067–8083. [\[CrossRef\]](#)
5. Logar, V.; Dovžan, D.; Škrjanc, I. Modeling and Validation of an Electric Arc Furnace: Part 1, Heat and Mass Transfer. *ISIJ Int.* **2012**, *52*, 402–412. [\[CrossRef\]](#)

6. Lahdelma, R.; Hakonen, H.; Ikäheimo, J. AMRO—Adaptive Metallurgical Raw Material Optimization. In Proceedings of the IFORS'99, Beijing, China, 16–20 August 1999.
7. Rong, A.; Lahdelma, R. Fuzzy Chance Constrained Linear Programming Model for Optimizing the Scrap Charge in Steel Production. *Eur. J. Oper. Res.* **2008**, *186*, 953–964. [\[CrossRef\]](#)
8. Gauffin, A.; Tilliander, A.; Jönsson, P.G. Alloy content in steel scrap by use of random sampling analysis and its impact on the Electric arc furnace. In Proceedings of the Shechtman International Symposium, Cancun, Mexico, 29 June–4 July 2014.
9. Birat, J.P.; Coq, X.L.; Russo, P. *Quality of Heavy Market Scrap: Development of New and Simple Methods for Quality Assessment and Quality Improvement*; Technical Steel Research; European Commission: Brussels, Belgium, 2002.
10. Sandberg, E.; Lennox, B.; Undvall, P. Scrap Management by Statistical Evaluation of EAF Process Data. *Control Eng. Pract.* **2007**, *15*, 1063–1075. [\[CrossRef\]](#)
11. Savov, L.; Volkova, E.; Janke, D. Copper and Tin in Steel Scrap Recycling. *Mater. Geoenviron.* **2003**, *50*, 627–640.
12. Gyllenram, R.; Westerberg, O. The impact of scrap upgrading on EAF production cost and performance. *Stahl Eisen* **2016**, *1*, 31–36.
13. RAWMATMIX[®] Manual System, Version 2.16; Kobilde & Partners AB: Stockholm, Sweden, 2020.
14. Arzpeyma, N.; Gyllenram, R.; Jönsson, P.G. Development of a Mass and Energy Balance Model and its Application for HBI Charged EAFs. *Metals* **2020**, *10*, 311. [\[CrossRef\]](#)
15. Lawson, C.L.; Hanson, R.J. *Solving Least Squares Problems*; Society for Industrial and Applied Mathematics: Philadelphia, PA, USA, 1995.
16. Rossi, R.J. *Mathematical Statistics: An Introduction to Likelihood Based Inference*; John Wiley & Sons: New York, NY, USA, 2018.
17. R. C. Team. A Language and Environment for Statistical Computing. R Foundation for Statistical Computing. Vienna, Austria. 2020. Available online: <http://www.R-project.org/> (accessed on 2020).
18. Nash, J.C. On Best Practice Optimization Methods in R. *J. Stat. Softw.* **2014**, *20*, 1–14.