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MULTIRESPONSE ROBUST ENGINEERING: CASE WITH ERRORS IN FACTOR LEVELS

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The model-based robust approach for improving the quality of the process is successfully applied to different industrial processes. In the case of multiple correlated responses the estimation of the mean and variance models of the quality characteristics in production conditions, taking into account the correlation between the multiple responses, together with the heteroscedasticity of the observations due to errors in the factor levels is considered at multivariate regression fit, robust engineering modeling and the optimization stages. The application of the proposed method gives the possibility to use raw industrial data for mean and variance models estimation and leads to reduction of the predicted variance of the responses in production conditions. The proposed approach is applied for electron beam melting and refining experiments.

1. Introduction

The Robust Parameter Design (RPD) is an issue of numerous papers in the literature since 1990 [1, 2], but there are much less of them in the area of application of RPD [3, 4] for multiple responses. Some of these articles consider the multiresponse case, when replicated observations are available [5], while others are focused on formulation of appropriate optimization criteria. Examples for such

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criteria are: (i) a criterion, representing an appropriate compromise between both the process economics and the correlation structure among responses [6], (ii) a new loss function, incorporating small bias, high robustness and high quality of predictions [7].

The model-based robust approach for improving the quality of the process [4, 8] can be successfully applied to different industrial processes. For each of the quality performance characteristics, using their regression models, two other models are estimated – for their mean values and their variances. The quality improvement is performed using some overall criterion or simply by the performance characteristic variance minimization, while keeping the mean values close to their target values. The model of the mean value of the performance characteristic, which is a function of process parameters that are subject to errors during the industrial production process, is [4]:

$$\tilde{y}(\mathbf{p}) = E[y(\mathbf{z})] = \eta(\mathbf{p}) + \hat{\theta}' E(\mathbf{g}) \tag{1}$$

where $\eta(\mathbf{p})$ is a model of the quality performance characteristic, for example a polynomial regression model, obtained by the response surface methodology. The second term takes into account the bias caused by the errors transmitted from the process parameters $\mathbf{p}$ to the performance characteristic $\tilde{y}(\mathbf{p})$, where $\hat{\theta}'$ is the vector of the estimates of the regression coefficients in the model $\eta(\mathbf{p})$. $E(\mathbf{g})$ stands for the mathematical expectation of $\mathbf{g} = \mathbf{h} - \mathbf{f}$, $\mathbf{h}$ is a vector of the regressors $\mathbf{z}$ in the regression model, considered as containing errors $\mathbf{e}$ (for any process parameter – $z_i = p_i + e_i$) and $\mathbf{f}$ is the regressors vector of the process parameters $\mathbf{p}$.

The model for the variance of the quality performance characteristic that is due to errors in factor levels, if the bias that comes from the precision of the estimation of the regression model (negligible in many cases) is taken into account (by the second term), is [4]:

$$\hat{s}^2 = \tilde{s}^2 - tr[\mathbf{\Psi}\ \mathbf{V}(\hat{\theta})] = \hat{\theta}'\mathbf{\Psi}\hat{\theta} + s_\varepsilon^2 \left(1 - \sum_{i=1}^{k} \psi_{ii} c_{ii} - 2\sum_{i=1}^{k-1}\sum_{j=i+1}^{k} \psi_{ij} c_{ij}\right) \tag{2}$$

where $\boldsymbol{\psi} = \mathbf{g} - E(\mathbf{g})$, is defined on the basis of the variances for each process parameters $\mathbf{p}$, which can be calculated using the tolerance limits of the process parameters or on the base of replicated observations, $\mathbf{\Psi} = E(\boldsymbol{\psi}\boldsymbol{\psi}')$ depends on the structure of the regression model and the experimental design, s_ε^2 is the estimate of the random error of the performance characteristic; ψ_{ii} and ψ_{ij} are correspondingly the diagonal and non-diagonal elements of $\mathbf{\Psi}$, c_{ii} and c_{ij} are the diagonal and non-diagonal elements of the variance-covariance matrix, which become smaller with the growth of the number N of the experiments (observations), and k is the number of terms in the regression model. With $\tilde{s}^2$ is denoted the variance of the quality performance characteristic, which is due to the errors in factor levels $(\hat{\boldsymbol{\theta}}' \mathbf{\Psi} \hat{\boldsymbol{\theta}})$ and the random error s_ε^2 . For a big number of observations or small values of s_ε^2 the bias is negligible.

This paper considers estimation of the models of the means and the variances in the typical for an industrial process case of multiple correlated responses, when heteroscedasticity of the observations and errors in the factors levels are present. The parameter estimation, when there are correlations between the multiple responses [9, 10] and errors in the factors levels in the production stage (there is heteroscedasticity [4, 8] by applying of a new combined method [11, 12] is considered. Both the correlation and the heteroscedasticity should be taken into account in order to improve the accuracy of the estimated models. A big advantage of the proposed method is the possibility to use raw industrial experimental data, instead of the necessary very precise parameter estimation of the regression models without errors in the factor levels, done for example in laboratory conditions.

2. Combined method for regression parameter estimation

The multiresponse approach [9] gives as a result estimates of the regression coefficients that take into consideration the correlation between the responses, which is usually the case. They can be estimated through a two-stage Aitken estimator [13]. The heteroscedasticity of observations can be considered through the application of the weighted least square estimates [4] The two approaches are combined and a new combined method for regression parameter estimation is applied here [11, 12]. Using this method, the parameter estimates are calculated iteratively in several stages [11]:

Step 1. The ordinary least squares estimates (OLSE) $\mathbf{b}_0$ are found for each of the responses:

$$\mathbf{b}_{0,i} = (\mathbf{X}_i' \ \mathbf{X}_i)^{-1} \mathbf{X}_i' \mathbf{Y}_i,$$

where $\mathbf{X}_i$ are the matrices of known functions $\mathbf{f}$ (regressor vectors) of the process parameters $\mathbf{p}$, defined by the regression models and the performed experiments for each of the responses $\mathbf{Y}_i$, $i = 1, 2, \ldots, r$.

Step 2. An estimate of the random error can be found by:

$$s^2_{\varepsilon,i} = \frac{1}{N-k_i}\sum_{u=1}^{N}(y_{u,i}-\hat{y}_{u,i})^2.$$

Step 3. The models for the mean eq.(1) and the variance eq.(2) are estimated for each of the performance characteristics.

Step 4. The matrix $\tilde{\mathbf{\Sigma}}_{\rm h,i}$ is estimated:

$$\tilde{\mathbf{\Sigma}}_{\rm h,i} = \begin{bmatrix} \tilde{\sigma}_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \tilde{\sigma}_N^2 \end{bmatrix} \tag{3}$$

by calculation of the estimates of the variances $\tilde{\sigma}^2_{i,u}$ at each experimental run $u = 1, \ldots, N$ for each of the $i = 1, \ldots, r$ responses, using eq. (2). The matrices $\tilde{\mathbf{\Sigma}}_{\rm h,i}$ estimates the heteroscedasticity of the observations.

Step 5. The variance-covariance matrix $\tilde{\mathbf{\Sigma}}_m$ of the random error of all performance characteristics takes into account also their correlation. If it is unknown, its elements $(\hat{\sigma}_{ij})$ can be estimated by [9]:

$$\tilde{\mathbf{\Sigma}}_m = (\hat{\sigma}_{ij}),$$

$$\hat{\sigma}_{ij} = \mathbf{Y}'_i[\mathbf{I}_N - \mathbf{X}_i(\mathbf{X}'_i\mathbf{X}_i)^{-1}\mathbf{X}'_i][\mathbf{I}_N - \mathbf{X}_j(\mathbf{X}'_j\mathbf{X}_j)^{-1}\mathbf{X}'_j]\ \mathbf{Y}_j/N,$$

for $i, j = 1, 2, \ldots, r$.

Step 6. The combined method variance-covariance matrix is:

$$\tilde{\mathbf{\Delta}} = \begin{bmatrix} \tilde{\hat{\sigma}}_{11,1} & \cdots & 0 & & \tilde{\hat{\sigma}}_{1r,1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \tilde{\hat{\sigma}}_{11,N} & & 0 & \cdots & \tilde{\hat{\sigma}}_{1r,N} \\ & \cdots & & \ddots & & \cdots & \\ \tilde{\hat{\sigma}}_{r1,1} & \cdots & 0 & & \tilde{\hat{\sigma}}_{rr,1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \tilde{\hat{\sigma}}_{r1,N} & & 0 & \cdots & \tilde{\hat{\sigma}}_{rr,N} \end{bmatrix} \tag{4}$$

where $\tilde{\mathbf{\Delta}}$ is calculated with elements:

$$\begin{cases} \tilde{\hat{\sigma}}_{ii,u} = \hat{\sigma}_{ii}\tilde{\sigma}^2_{i,u} \\ \tilde{\hat{\sigma}}_{ij,u} = \hat{\sigma}_{ij}\tilde{\sigma}_{i,u}\tilde{\sigma}_{j,u} \end{cases}$$

where $\tilde{\sigma}^2_{i,u}$ and $\hat{\sigma}_{ij}$ are elements of the variance-covariance matrices $\tilde{\mathbf{\Sigma}}_{h,i}$ and $\tilde{\mathbf{\Sigma}}_m$ correspondingly. One ($\tilde{\mathbf{\Sigma}}_{h,i}$) takes into account the heteroscedasticity of observations (the difference in variances at each experimental run) and the other ($\tilde{\mathbf{\Sigma}}_m$) takes into account the correlation between the responses.

Step 7. A combined method parameter estimates are calculated by:

$$\tilde{\mathbf{b}} = (\mathbf{Z}'\tilde{\mathbf{\Delta}}^{-1}\mathbf{Z})^{-1}\mathbf{Z}'\tilde{\Delta}^{-1}\mathbf{Y}, \tag{5}$$

where $\mathbf{Z}$=diag($\mathbf{X}_1$,...,$\mathbf{X}_r$) is a block-diagonal matrix with diagonal elements – the matrices $\mathbf{X}_i$; and $\mathbf{Y}=[\mathbf{Y}'_1,\ldots,\mathbf{Y}'_r]'$ is a vector, consisting of the observations for each of the r responses.

Step 8. The criterion Cr_j is calculated by:

$$Cr_j = \sum_{i=1}^{k} \frac{\left(\tilde{\theta}_{j,i} - \tilde{\theta}_{j-1,i}\right)^2}{\tilde{\theta}^2_{j,i}}, \tag{6}$$

where $k = k_1 + k_2 + \cdots + k_r$ is the sum of the regression coefficients in the regression models for each of the r responses. The criterion Cr_j is calculated for j-th iteration, using the coefficients from j^{th} and $(j-1)^{th}$ iterations.

Step 9. The procedure is iterative and continues from *Step 2*, until $Cr_j \leq \delta$, where δ is a small positive number. For initiation of the procedure initial estimates of the regression coefficients are needed. For that purpose the ordinary least squares estimates (OLSE) $\mathbf{b}_0$ are found for each of the responses.

The proposed procedure for regression parameter estimation takes into account both the heteroscedasticity of the observations and the correlation between the multiple responses. This is an iteration procedure, the convergence of which depends on the accuracy of the initial regression OLSE parameter estimates, nonlinearity of the estimated model, as well as the magnitude of the errors in factors variances, transmitted to the performance characteristics. The proposed method can be applied with row industrial data (when there are errors in factor levels) for the regression parameter estimation needed for the model-based robust engineering approach. The usual approach includes obtaining of experimental data without errors in factor levels (for example in laboratory conditions) for the regression parameter estimation.

3. Models of the mean and the variance in the case of multiple responses and errors in the factors levels

The regression model in the multiresponse case can be presented as [10]:

$$\mathbf{Y}(\mathbf{z}) = \mathbf{Z}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where:

$$\mathbf{Z} = \begin{bmatrix} \mathbf{f}_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathbf{f}_r \end{bmatrix} \text{ and } \boldsymbol{\beta} = \begin{bmatrix} \boldsymbol{\beta}_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \boldsymbol{\beta}_r \end{bmatrix}.$$

$\mathbf{Z}$ is a $r \times k$ vector-diagonal matrix of the regressors $\mathbf{f}_i$, which are known functions of the factors $\mathbf{p}$ and $\boldsymbol{\beta}$ is a $r \times k$ vector-diagonal matrix of the regression parameters for each of the responses $i = 1, \ldots, r$.

If there are errors in the factor levels $\mathbf{z} = \mathbf{p} + \mathbf{e}$, then [4]:

$$\mathbf{Y}(\mathbf{z}) = \mathbf{Z}\boldsymbol{\beta} + \mathbf{G}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where the matrix $\mathbf{G}$ is:

$$\mathbf{G} = \begin{bmatrix} \mathbf{g}_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathbf{g}_r \end{bmatrix} = \begin{bmatrix} \mathbf{h_1}(\mathbf{p}+\mathbf{e}) - \mathbf{f}_1(\mathbf{p}) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathbf{h}_r(\mathbf{p}+\mathbf{e}) - \mathbf{f}_r(\mathbf{p}) \end{bmatrix},$$

where the vectors $\mathbf{g}_i = \mathbf{h}_i - \mathbf{f}_i$, $\mathbf{h}_i$ are vectors of the regressors $\mathbf{z}$ in the regression models, considered as containing errors $\mathbf{e}$ (for any process parameter) and $\mathbf{f}_i$ are the regressors vectors of the process parameters $\mathbf{p}$, for each of the responses $i = 1, \ldots, r$.

Then the model for the mean value of the performance quality characteristics in the correlated multiple responses case when there are errors in factor levels, after substitution of the parameters $\boldsymbol{\beta}_i$ with their estimates (for example the combined method estimates $\tilde{\mathbf{b}}$), is:

$$\tilde{\mathbf{Y}}(\mathbf{p}) = \tilde{E}[\mathbf{Y}(\mathbf{z})] = \mathbf{Z}\tilde{\mathbf{b}} + E(\mathbf{G})\tilde{\mathbf{b}}. \tag{7}$$

This equation is an analogue of eq. (1) for multiple correlated responses. Let us accept the following notations: $\boldsymbol{\phi} = \mathbf{G} - E(\mathbf{G})$ is a $r \times k$ matrix of errors and $\boldsymbol{\Phi} = E[\boldsymbol{\phi}'\boldsymbol{\phi}]$ is a $k \times k$ matrix.

The variance model of the performance quality characteristics, in the multiresponse case when there are errors in the factor levels, taking into account both the variances of the responses and their correlations, and assuming that the errors $\mathbf{e}$ and $\boldsymbol{\varepsilon}$ are non-correlated: $cov(\mathbf{e},\boldsymbol{\varepsilon}) = 0$ and $cov(\mathbf{G}\boldsymbol{\beta},\boldsymbol{\varepsilon}) = 0$, is:

$$(8)\quad \tilde{\mathbf{s}}^2 = v\tilde{a}r[\mathbf{Y}(\mathbf{z})] = \sigma^2(\mathbf{Z}\boldsymbol{\beta}) + \sigma^2(\mathbf{G}\boldsymbol{\beta}) + \sigma^2(\boldsymbol{\varepsilon}) = \tilde{\mathbf{b}}'E[\boldsymbol{\phi}'\boldsymbol{\phi}]\tilde{\mathbf{b}} + \boldsymbol{\Sigma}_\varepsilon = \tilde{\mathbf{b}}'\boldsymbol{\Phi}\tilde{\mathbf{b}} + \boldsymbol{\Sigma}_\varepsilon,$$

where $\boldsymbol{\Sigma}_\varepsilon$is of the variance-covariance matrix of the random errors of all performance characteristics. The matrix $\tilde{\boldsymbol{\Sigma}}_m$ can be used as an estimate of $\boldsymbol{\Sigma}_\varepsilon$. If the bias due to the inaccuracy of estimation of the regression model is taken into account, then the variance model is:

$$(9)\qquad \tilde{\mathbf{s}}^2 = v\tilde{a}r[\mathbf{Y}(\mathbf{z})] = \tilde{\mathbf{b}}'\boldsymbol{\Phi}\tilde{\mathbf{b}} + (1 - tr(\boldsymbol{\Phi}\ \mathbf{V}(\tilde{\mathbf{b}}))\boldsymbol{\Sigma}_\varepsilon,$$

where $\mathbf{V}(\tilde{\mathbf{b}}) = var(\tilde{\mathbf{b}}) = (\mathbf{Z}'\tilde{\boldsymbol{\Delta}}^{-1}\mathbf{Z})^{-1}$ is the variance-covariance matrix of the parameter estimates $\tilde{\mathbf{b}}$.

The optimization task can be formulated generally as:

$$\min f(v\tilde{a}r(\mathbf{Y})),$$

under the restriction condition:

$$\mathbf{l} \leq \tilde{E}(\mathbf{Y}) \leq \mathbf{u},$$

where $\mathbf{l}$ and $\mathbf{u}$ are $k \times 1$ vectors, of the lower and the upper limit requirements for all the responses. The optimization criterion $f(\cdot)$ should be formulated depending on the level the correlation should be taken into account. It could be one of the following: trace($v\tilde{a}r(\mathbf{Y})$); the determinant $|(v\tilde{a}r(\mathbf{Y}))|$; trace($v\tilde{a}r(\mathbf{Y})^2$); the difference between the eigenvalues $\lambda_{\max} - \lambda_{\min}$, etc. If the determinant is used as a criterion, the covariance between the multiple responses is taken into account, while the trace considers the change mainly of the individual variances.

4. Experimental application

The proposed approach for multiple robust engineering is applied to an industrial experiment. Electron beam melting and refining (EBMR) of highly oxidized Ti wastes [14] was performed using 60 kW equipment with horizontal feeder and the drip molten metal crystallized in a water-cooled copper crucible with diameter 60 mm. The vacuum pressure in the melting chamber was in the range $5 - 8 \times 10^{-3}$ Pa.

The surface temperature in the crucible was measured by an optical pyrometer. As a feeding material waste rods with diameter 45 mm were used. The values of the process parameters changed during the experiments are: the electron beam power P, the surface temperature of the molten metal in the crucible T, the casting velocity v_C and the refining time τ. The initial and the final impurities concentrations were determined by a chemical analysis. In Table 1 are presented the process parameter conditions of the performed experiments. Quality performance characteristics that are considered are the concentrations of the impurities (O, Al, Fe, Si, Ni and Cr) after EBMR of Ti.

The obtained experiments are taken directly from production. In order to optimize the quality of the produced Ti ingots the minimization of the residual oxygen concentration, together with the variances of all the impurity concentrations at production conditions is performed. This means that the produced ingots will have fewer variations in their characteristics, which corresponds to better quality production without any investments.

In order to fulfil this, first regression models need to be estimated. The combined method is applied for this purpose. Initial ordinary least squares parameter estimates are found and given in Table 2. They are used for applying the combined method for parameter estimation.

Table 1: Experimental process parameter conditions.

Factors	Dimensions	Coded factors	Min	Max	$\tilde{p}_{io}$	ω_i	Tolerance limits
P-$\tilde{p}_1$	kW	p_1	11.25	18.75	15	3.75	$P \pm 2\%$
$v_c - \tilde{p}_2$	mm/s	p_2	0.05	0.15	0.1	0.05	$v_c \pm 3\%$
$\tau - \tilde{p}_3$	min	p_3	2.78	11.85	7.315	4.535	$\tau \pm 4\%$

Table 2: Ordinary least squares parameter estimation

$\ln(C_O) =$	$6.65 + 0.157x_1 + 0.253x_3 - 0.256x_1^2 - 0.330x_2^2 + 0.959x_1^2x_2 + 1.05x_1^2x_3$
$\ln(C_{\mathrm{Al}}) =$	$5.85 - 0.0738x_1 - 0.0260x_3 + 0.0996x_1x_3 + 0.0788x_1^2 + 0.345x_3^2$ $+0.133x_1^2x_3 + 0.359x_1x_3^2$
$\ln(C_{\mathrm{Fe}}) =$	$6.74 - 0.0522x_1 - 0.307x_2 - 0.287x_3 + 0.0792x_1x_2 + 0.0588x_1x_3$ $-0.0864x_2x_3 + 0.176x_1^2$
$\ln(C_{\mathrm{Si}}) =$	$5.30 - 0.347x_1 - 0.173x_1x_2 - 0.231x_1^2 - 0.173x_1^2x_2 + 0.173x_1x_2^2$
$\ln(C_{\mathrm{Ni}}) =$	$5.52 - 0.0400x_1 + 0.0435x_2 - 0.0320x_1x_2 - 0.0767x_2^2 - 0.0532x_1^2x_2$ $+0.0720x_1x_2^2$
$\ln(C_{\mathrm{Cr}}) =$	$4.95 - 0.0943x_1 + 0.556x_2 + 0.567x_3 - 0.130x_1^2 - 0.498x_1^2x_2 - 0.651x_1^2x_3$

The variance-covariance matrix $\tilde{\mathbf{\Sigma}}_m$ of the random error of all performance characteristics that takes into account their correlation in this case is:

$$\tilde{\mathbf{\Sigma}}_m = 10^{-4}\begin{bmatrix} 0.3798 & -0.0089 & -0.0017 & -0.0204 & -0.0014 & -0.0381 \\ -0.0089 & 0.0122 & -0.0149 & 0.5498 & 0.0245 & -0.2349 \\ -0.0017 & -0.0149 & 0.0368 & -0.6848 & -0.0461 & 0.5199 \\ -0.0204 & 0.5498 & -0.6848 & 44.4868 & 0.9822 & -5.2927 \\ -0.0014 & 0.0245 & -0.0461 & 0.9822 & 0.1694 & -1.5363 \\ -0.0381 & -0.2349 & 0.5199 & -5.2927 & -1.5363 & 15.5429 \end{bmatrix}$$

The matrices $\tilde{\mathbf{\Sigma}}_{h,i}$ for each of the $i = 1, \ldots, r$ responses, which estimate the heteroscedasticity of the observations, have the elements, presented in Table 3. They are estimated using eq.(2) on the base of the ordinary least squares parameter estimates. Then the combined method iterative procedure is applied and 14 iterations are performed for obtaining the combined method parameter estimates (see Table 4). The convergence of the combined method is illustrated on Fig. 1, using the criterion Cr (eq.(6)). It can be seen that after 5–6 iterations it has already a sufficiently small value.

Table 3: Variances of concentrations at each experimental run (heteroscedasticity) – initial values.

$\tilde{\mathbf{\Sigma}}_{h,i}$	$10^4\tilde{\sigma}_1^2$	$10^4\tilde{\sigma}_2^2$	$10^4\tilde{\sigma}_3^2$	$10^4\tilde{\sigma}_4^2$	$10^4\tilde{\sigma}_5^2$	$10^4\tilde{\sigma}_6^2$	$10^4\tilde{\sigma}_7^2$	$10^4\tilde{\sigma}_8^2$	$10^4\tilde{\sigma}_9^2$
$\tilde{\mathbf{\Sigma}}_{h(O)} = \text{diag}(\tilde{\sigma}_u^2)$	25.90	18.27	6.22	2.93	2.01	5.83	31.00	38.96	5.09
$\tilde{\mathbf{\Sigma}}_{h,Al} = \text{diag}(\tilde{\sigma}_u^2)$	0.12	0.17	0.12	2.23	0.47	0.70	11.32	0.89	1.15
$\tilde{\mathbf{\Sigma}}_{h,Fe} = \text{diag}(\tilde{\sigma}_u^2)$	1.59	1.11	1.54	0.29	0.03	0.26	0.63	0.534	1.13
$\tilde{\mathbf{\Sigma}}_{h,Si} = \text{diag}(\tilde{\sigma}_u^2)$	133.4	133.4	134.8	133.5	134.3	134.3	133.6	140.9	147.4
$\tilde{\mathbf{\Sigma}}_{h,Ni} = \text{diag}(\tilde{\sigma}_u^2)$	0.87	0.77	1.48	0.83	0.78	0.87	1.08	0.79	0.90
$\tilde{\mathbf{\Sigma}}_{h,Cr} = \text{diag}(\tilde{\sigma}_u^2)$	3.59	4.43	3.37	6.33	4.87	6.34	3.85	8.67	3.11

On Fig. 2 are presented the contour lines of the mean value (solid lines) and the variance (dashed lines) of the oxygen concentration, using the estimated individual response approach and the combined method parameter estimates. It can be seen a big region of minimum variance values $\hat{s}^2(\mathbf{p})$ (below 0.0005, eq. (2)), which coincide with the highest oxygen concentration mean values after EBMR. The obtained results are similar to that, obtained by the application of the individual response approach using the ordinary least squares for parameter estimation estimated in laboratory conditions. This confirms that the combined method can be used for parameter estimation with raw industrial experimental data.

Table 4: Combined method parameter estimation

$\ln(C_O) =$	$6.6515 + 0.1689x_1 + 0.2553x_3 - 0.2501x_1^2 - 0.3375x_2^2 + 0.9812x_1^2x_2$ $+1.0757x_1^2x_3$
$\ln(C_{Al}) =$	$5.8467 - 0.0722x_1 - 0.0245x_3 + 0.0989x_1x_3 + 0.0747x_1^2 + 0.3452x_3^2$ $+0.1260x_1^2x_3 + 0.3502x_1x_3^2$
$\ln(C_{Fe}) =$	$6.7371 - 0.0509x_1 - 0.3017x_2 - 0.2792x_3 + 0.0781x_1x_2 + 0.0571x_1x_3$ $-0.0861x_2x_3 + 0.1766x_1^2$
$\ln(C_{Si}) =$	$5.9582 - 0.3861x_1 - 0.1419x_1x_2 - 1.2400x_1^2 - 0.19410.173x_1^2x_2$ $+0.1615x_1x_2^2$
$\ln(C_{Ni}) =$	$5.5232 - 0.0417x_1 + 0.0431x_2 - 0.0308x_1x_2 - 0.0802x_2^2 - 0.0525x_1^2x_2$ $+0.0738x_1x_2^2$
$\ln(C_{Cr}) =$	$4.7514 - 0.0015x_1 + 0.2750x_2 + 0.2185x_3 - 0.1787x_1^2 - 0.1024x_1^2x_2$ $-0.1496x_1^2x_3$

Then the models of the mean and the variance in the case of multiple responses and errors in the factors levels described by eq. (7) and eq. (9) are estimated. The variance-covariance matrices $\tilde{\mathbf{\Sigma}}_{h,i}$ and $\tilde{\mathbf{\Sigma}}_m$ and the combined method parameter estimates, obtained after 14 iterations, are used for that purpose. The matrix of the mathematical expectations $E(\mathbf{G})$ has the following matrix-diagonal elements $E(\mathbf{g}_i)$:

$$E(\mathbf{g}_1) = [0,0,0,\sigma_1^2,\sigma_2^2,p_2\sigma_1^2,p_3\sigma_1^2]; \quad E(\mathbf{g}_2) = [0,0,0,0,\ \sigma_1^2,\sigma_3^2,p_3\sigma_1^2,p_1\sigma_3^2];$$

$$E(\mathbf{g}_3) = [0,0,0,0,0,0,0,\sigma_1^2]; \quad E(\mathbf{g}_4) = [0,0,0,\sigma_1^2,p_2\sigma_1^2,p_1\sigma_2^2];$$

$$E(\mathbf{g}_5) = [0,0,0,0,\ \sigma_2^2,p_2\sigma_1^2,p_1\sigma_2^2]; \quad E(\mathbf{g}_6) = [0,0,0,0,\sigma_1^2,p_2\sigma_1^2,p_3\sigma_1^2].$$

The variances of the factors are estimated on the base of the tolerance limits and are given in Table 5.

Table 5: Coded variances of the factors, calculated using the tolerance limits

Factors	Variances	Coded variances σ_i^2
p_1	σ_1^2	$0.0007111 + 0.00035556\ p_1 + 0.00004444\ p_1^2$
p_2	σ_2^2	$0.0004 + 0.0004\mathrm{p}_2 + 0.0001\ p_2^2$
p_3	σ_3^2	$0.000462542 + 0.000573515\mathrm{p}_2 + 0.0001778p_2^2$

The oxygen concentration in the Ti ingots is critical for most applications; therefore, the optimization task here is formulated to search a compromise (Pareto

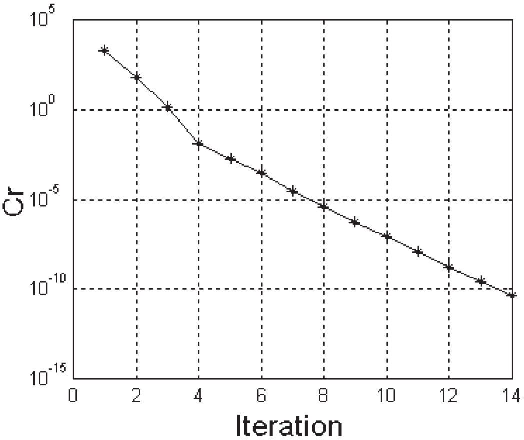

Figure 1: Convergence of the combined method

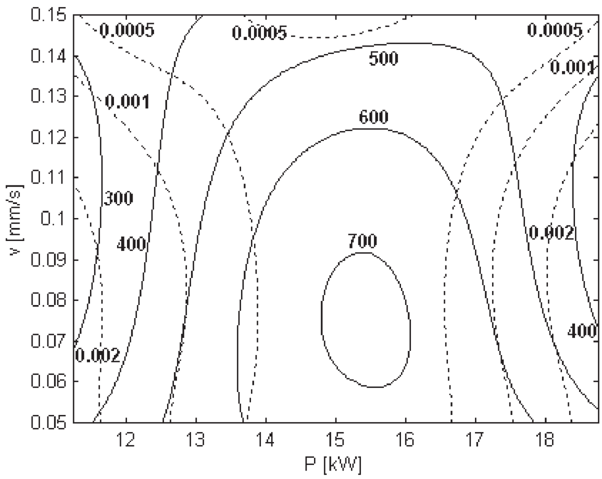

Figure 2: Contour lines of the mean value (solid lines) and the variance (dashed lines) of the oxygen concentration by individual response approach and the combined method parameter estimates

optimal) solution, which minimizes both the variance of the responses and the oxygen concentration. The final concentrations of the other impurities can be used as additional constraints, depending on the specific material application requirements. In order to perform such optimization the multiple responses robust engineering approach is applied and the models for the means and the variances are estimated.

The chosen criterion for the variance minimization is the determinant $|(v\tilde{a}r(\mathbf{Y}))|$. The obtained optimal solution for the mean values of the responses is:

$$\tilde{\mathbf{Y}}(\mathbf{p}) = diag(5.5229, 5.9905, 7.1368, 5.1007, 5.5656, 4.7446),$$

which after inverse transformation presents the following impurities concentrations: $C_O = 250.4$ ppm; $C_{Al} = 399.6$ ppm; $C_{Fe} = 1257.4$ ppm; $C_{Si} = 164.1$ ppm; $C_{Ni} = 261.3$ ppm; $C_{Cr} = 115.0$ ppm. The variance matrix is (eq.(9)):

$$\tilde{\mathbf{s}}^2(\mathbf{p}) = 10^{-4} \begin{bmatrix} 20.1087 & -0.0089 & -0.0017 & -0.0204 & -0.0014 & -0.0381 \\ -0.0089 & 0.0129 & -0.0149 & 0.5498 & 0.0245 & -0.2349 \\ -0.0017 & -0.0149 & 1.3941 & -0.6848 & -0.0461 & 0.5199 \\ -0.0204 & 0.5498 & -0.6848 & 62.3455 & 0.9822 & -5.2927 \\ -0.0014 & 0.0246 & -0.0461 & 0.9822 & 0.1745 & -1.5363 \\ -0.0381 & -0.2392 & 0.5199 & -5.2927 & -1.5363 & 16.0856 \end{bmatrix}.$$

The obtained minimal values of the determinant and the oxygen concentration are: $|(v\tilde{a}r(\mathbf{Y}))| = 3.665 * 10^{-24}$ and $C_O = 250.4$ ppm, obtained at $p_1 = -1$; $p_2 = 0.08$; $p_3 = -0.59$ or in natural units the values of the process parameters are: $P = 11.25$ kW; $v = 0.104$ mm/s; $\tau = 4.64$ min.

5. Conclusions

This article presents a new combined method for parameter estimation, which gives the possibility to consider the correlation between the multiple responses, together with the heteroscedasticity of observations. A big advantage of the method is the possibility to use raw industrial experimental data, instead of the necessary very precise parameter estimation of the regression models without errors in the factor levels, done for example in laboratory conditions. This new method is applicable in both cases: when there are replicated observations at each experimental run and when there are no such replications. If there are no replicated observations the variance estimation for each experimental run can be done through the tolerance intervals of the factors in the industrial (or laboratory) production process.

Models for the mean and the variance for the case of multiple responses and errors in factor levels are presented. The proposed methodology together with the combined method for parameter estimation is applied successfully for the refining of Ti wastes by electron beam melting. Optimal conditions are found, that minimize the response variances and the oxygen concentration.

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