PROGRAM FOR NON-LINEAR MODELLING OF A PROCESS

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Abstract: *On every process there are many factors that intervene. Every factor has a greater or lesser influence on the process. In order to optimize a process it is necessary to know the influences and the interactions of these factors on the process, respectively to know the mathematical model of the process. One of the most used models is a non-linear second order model. If this model is unknown, it is possible to obtain it through modelling with rotatable experiments. The aim of this paper is to present the theoretical bases and a program for experimenting and modelling processes with rotatable experiments.*

Key words: *rotatable experiments, process modelling.*

1. Introduction

The optimization of a process is possible when its mathematical model is known. These models could be linear or nonlinear.

When the mathematical model is unknown it's possible to determine it by using different experimental and modelling methods.

2. Objectives

The objectives of this paper are to present an experimental and modelling method for second order mathematical models and to conceive a program for experimenting and modelling.

3. Complete Factorial Experiments

The optimization of a process can be done in two stages [3].

In the first stage linear models are used in order to find the optimal domain, like the following linear model:

$$y = b_0 + b_i x_i + b_{ij} x_i x_j. \tag{1}$$

In the second stage, a detailed analysis of the response surface of the dependent factor must be done. This analysis is not possible with a linear model. Only a higher order model can be used to find the optimal point. The most used non-linear model is a second order polynomial $y = f(z_1, z_2, ..., z_n)$:

$$y = \beta_0 + \sum_{i=1}^{N} \beta_i x_i + \sum_{\substack{i,j=1, \\ i \neq j}}^{N} \beta_{ij} x_i x_j + \sum_{i=1}^{N} \beta_{ii} x_i^2 + ... \tag{2}$$

where: β_0, β_i, β_{ij}, β_{ii} - real coefficients of the equation; x_i, x_j, …, x_k - codified values of the factors.

When replacing the codified values of the factors with the calculated values it results:

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$$y = b_0 + \sum_{i=1}^{N} b_i x_i + \sum_{\substack{i,j=1, \\ i \neq j}}^{N} b_{ij} x_i x_j$$
$$+ \sum_{i=1}^{N} b_{ii} x_i^2 + ... \tag{3}$$

The mathematical model (2) can be obtained with special programs, the most important programs are named Central Composed Programs (C.C.E.). These programs are based on C.F.E. 3^n (Complete Factorial Experiments for n factors on three levels) programs where a factor is modified at three levels as in Table 1.

Between the codified and the real values of the factors the following dependence exists:

$$x_i = \frac{z_i \pm z_{i_0}}{\Delta z_i}, \tag{4}$$

where: x_i - codified values; z_i - real (natural) values; z_{i_0} - real (natural) values in the center of the experiment; Δz_i - variation interval.

The C.F.E. 3^n (Table 2) programs became uneconomical for three or more factors. Box and Wilson studied this problem in 1951 and found that the number of experiments could be reduced if a C.F.E. 2^n experiment (*n* factors on 2 levels) would be completed with some points of the factorial space ((−2, 0), (+2, 0), (0, −2) and

(0, +2)). These new points are equally spaced from the center point (0, 0) with the distance α.

In Figure 1 and Table 1 an example of the codified and the real values of a C.F.E. 2^2 and a C.F.E. 3^2 experiment (the cutting power of beech milling in function of the feed speed and the cutting height) is presented.
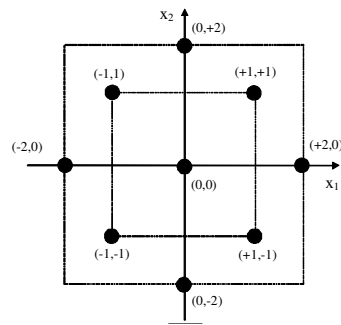

Fig. 1. *Points in the factorial space*

Thus the number of experiments *N* is:

$$N = n_0 + n_c + n_\alpha, \tag{5}$$

where: *N* - number of experiments; n_0 - number of experiments in the center of the experiment; n_c - number of experiments of a C.F.E. 2^n program; n_α - number of experiments in the extreme points; α - distance from the center point.

C.F.E. 2^2 *and C.F.E.* 3^2 *experiment*   Table 1

Nr.	Type of experiment		Codified values			Real (natural) values		
			x_1	x_2	Y	u, [m/min]	h, [mm]	P, [kW]
1	C.F.E. 3^2	C.F.E. 2^2	−1	−1		5	10	
2			+1	−1		25	10	
3			−1	+1		5	50	
4			+1	+1		25	50	
5			−1	−1		5	10	
6			+1	−1		25	10	
7			−1	+1		5	50	
8			+1	+1		25	50	
9			0	0		15	30	

The values of the number n, n_0, n_c, n_∞ and α are presented in Table 3.

Table 2
Comparison between a C.F.E. 3^n and a BW program [3]

Number of factors	2	3	4	5
C.F.E. 3^2 program	9	27	81	243
BW program	9	15	25	43

In practice two types of C.C.E. programs, orthogonal and rotatable programs are used, but the most used programs are rotatable programs [3].

4. Rotatable Programs of Second Order

In order to obtain the second order mathematical model with rotatable programs of second order (RP2) the following steps must be performed [3]:

Step 1. The levels of the natural factors z_i are established. Firstly the minimum $z_i^{\min}$ and maximum value $z_i^{\max}$ of the factor is established. Apart from these two values, the value in the center of the experiment z_i^0 (6) and the variation interval Δz_i (7) are calculated:

$$z_i^0 = \frac{z_i^{\max} - z_i^{\min}}{2} \; ; \; \Delta z_i = \frac{z_i^{\max} - z_i^0}{\alpha}. \quad (6)$$

The correspondence between the codified and real values is presented in Table 4.

Step 2. With the help of the information presented at step 1, the programming matrix from Table 5 is created (the cutting power for beech milling according to the cutting speed v and the feed speed u).

Step 3. Using the real values from Table 5 experiments are conducted and the measured values are written in the adequate column of Table 5.

Step 4. After conducting the experiment the coefficients b_0, b_i, b_{ij} and b_{ii} of the mathematical model (3) are calculated with [3]:

$$b_0 = D\sum_{u=1}^{N} y_u + E\sum_{i=1}^{N}\sum_{u=1}^{N} x_{iu}^2 y_u, \quad (7)$$

$$b_i = \frac{\sum_{u=1}^{N} x_{iu} y_u}{e}, \quad (8)$$

$$b_{ij} = \frac{\sum_{u=1}^{N} x_{iu} x_{ju} y_u}{N_c}, \quad (9)$$

$$b_{ii_1} = (F-G)\sum_{u=1}^{N} x_{iu}^2 y_u + G\sum_{i=1}^{n}\sum_{u=1}^{N} x_{iu}^2 y_u, \quad (10)$$

Table 3
Number of experiments for the C.C.E. program [3]

Number of factors	n	n_c	n_α	n_0	α
2	13	4	4	5	1.414
3	20	8	6	6	1.682
4	31	16	8	7	2
5	52	32	10	10	2.378

Correspondence between the codified and real values of a RP2 program Table 4

Codified values x_i	$-\alpha$ or -2	-1	0	$+1$	$+\alpha$ or $+2$
Real values z_i	$z_i^{\min}$	$z_i^0 - \Delta z_i$	z_i^0	$z_i^0 + \Delta z_i$	$z_i^{\max}$

Codified and real programming matrix for a PR2 program Table 5

Nr. exp.	Codified values		Dependent factor	Real values		Dependent factor
	x_1	x_2	y	v, [m/s]	u,[m/min]	P, [kW]
1	+1	+1		60	20	
2	−1	+1		40	20	
3	+1	−1		60	10	
4	−1	−1		40	10	
5	0	+α (+1.41)		50	≈22	
6	0	−α (−1.41)		50	≈8	
7	+α (+1.41)	0		≈64	15	
8	−α (−1.41)	0		≈36	15	
9	0	0		50	15	
10	0	0		50	15	
11	0	0		50	15	
12	0	0		50	15	
13	0	0		50	15	

$$b_{ii_2} = E\sum_{u=1}^{N} y_u , \qquad (11)$$

$$b_{ii} = b_{ii_1} + b_{ii_2} , \qquad (12)$$

$$e = n_c + 2\alpha^2 , \qquad (13)$$

$$f = n_c + 2\alpha^4 , \qquad (14)$$

$$D = 2\alpha^4 H^{-1}\left[f + (n-1)n_c\right], \qquad (15)$$

$$E = -2H^{-1}e\alpha^4 , \qquad (16)$$

$$F = H^{-1}\left[Nf + (n-2)Nn_c - (n-1)e^2\right], \quad (17)$$

$$G = H^{-1}(e^2 - Nn_c) , \qquad (18)$$

$$H = 2\alpha^4\left[Nf + (n-1)Nn_c - ne^2\right], \qquad (19)$$

$$N = n_c + 2n + n_0 , \qquad (20)$$

where: N - number of all experiments; n - number of factors; n_c - number of experiments of a C.F.E. 2^n program; n_0 - number of experiments in the center. The values of n, n_0, α, D, E, F and G are presented in Table 6.

Step 5. The reproductibility dispersion (experimental error) s_0^2 is calculated with:

$$s_0^2 = \frac{S_0}{v_0} = \frac{1}{N_0 - 1}\sum_{k=1}^{N_0}(y_{0k} - \bar{y}_0)^2 , \qquad (21)$$

where: v_0 - number of degrees of freedom for the experiments in the center; N_0 - number of experiments in the center; y_{ok} - measured values of the dependent factor in the center of the experiment; $\bar{y}_0$ - main value of the y_{ok} values.

Values of n, n_0, α, D, E, F and G [3] Table 6

n	N	n_0	α	D	E	F	G
2	13	5	1.414	0.200	−0.1000	0.1437	0.0187
3	20	6	1.682	0.1663	−0.0568	0.0694	0.0069
4	31	7	2.000	0.1428	−0.0357	0.0350	0.0037
5	52	10	2.378	0.0988	−0.0191	0.0180	0.0015

Step 6. The dispersions $s_{b_0}^2$, $s_{b_i}^2$, $s_{b_{ii}}^2$, $s_{b_{ij}}^2$ of the regression coefficients are calculated with:

$$s_{b_0}^2 = Ds_0^2 \, , \; s_{b_i}^2 = \frac{s_0^2}{e} \, , \quad (22)$$

$$s_{b_{ij}}^2 = \frac{s_0^2}{n_c} \, , \; s_{b_{ii}}^2 = Fs_0^2 \, . \quad (23)$$

Step 7. The significance of the coefficients is tested with the Student test:

$$t_{b_i} = \frac{|b_i|}{s_{b_i}} \, ; \; t_{b_{ij}} = \frac{|b_{ij}|}{s_{b_{ij}}} \, ; \; t_{b_{ii}} = \frac{|b_{ii}|}{s_{b_{ii}}} \, , \quad (24)$$

$$i := 1, l; \; t_{tab} = t_{0.05(v_0)}; \; v_0 = n_0 - 1 \, , \quad (25)$$

where: t_{b_i}, $t_{b_{ij}}$, t_{ii} - calculated values of the Student test; t_{tab} - tabular value of the Student test; v_0 - number of degrees of freedom; n_0 - number of experiments in the center.

If t_{b_i}, $t_{b_{ij}}$, $t_{ii} > t_{tab}$ then the coefficient, respectively the factor is significant and can be kept in the mathematical model.

The residual dispersion s_r^2 is calculated with:

$$s_r^2 = \frac{s_r}{v_r} = \frac{\sum_{u=1}^{N}(y_u - \tilde{y}_u)^2}{N - l} \, , \quad (26)$$

where: l - the number of terms of the regression equation; N - the number of experiments; y_u - the measured values of the dependent factor; $\tilde{y}_u$ - the values estimated with the mathematical model.

Step 8. The concordance of the model with the experimental data is tested with the Fisher test. In this order the concordance dispersion s_{con}^2 and the Fischer criteria F_c is

calculated with:

$$s_{con}^2 = \frac{\sum_{u=1}^{N}(y_u - \tilde{y}_u)^2 - \sum_{k=1}^{n_0}(y_{0k} - \bar{y}_0)^2}{v_{con}} \, , \quad (27)$$

$$v_{con} = v_r - v_0 \, , \quad (28)$$

$$F_c = \frac{s_{con}^2}{s_0^2} \, , \quad (29)$$

where: v_{con} - number of freedom for the concordance dispersion; s_0^2 - reproductibility dispersion (22); F_c - calculated value of the Fischer criteria.

The calculated value F_c is compared with the tabular value $F_{tab} = F_{0.05(v_{con}; v_0)}$ of the Fischer criteria [3].

If $F_c \leq F_{tab}$ then the mathematical model is adequate and can be used in the optimization process [3]. If the Fischer test is not performed then the variation interval must be decreased and all steps repeated.

5. Presentation of the Program

Based on the information presented above and in [1] and [2] a program which allows the following operations was conceived:
- generating the programming matrix with the codified values for PR2 programs for $2 \div 5$ factors;
- generating the programming matrix with the real values for PR2 programs for $2 \div 5$ factors;
- allowing creation of the data base with the measured values;
- calculating the coefficients of the non-linear model;
- realizing a statistical analysis of the mathematical model;
- displaying the non-linear mathematical model and the results of the statistical analysis.

In Figure 2 the main menu of the program is presented. In the left panel the codified and the real programming matrixes are displayed. In the left bottom window the mathematical models and the results of the statistical analysis appear. In the right side information for maximum five factors could be entered or displayed: information about the experiment, the name and the measuring units of the factor, the real value in the centre of the experiment the variation interval, the number of factors, the number of experiments and the number of parallel experiments in the centre.

The main menu also allows choosing the type of experiment (orthogonal OP or rotatable RP programs) and the type of mathematical model (linear or non-linear models).

With the buttons placed on the bottom of the right panel the following operations are performed:

- displaying the codified (Figure 3) and the real programming matrixes without (Figure 4) and with measured values (Figure 5);

- loading or saving the real programming matrixes without or with the measured values;

- calculating and displaying (Figures 6 and 7) the mathematical model with or without the significant factors and the result of the concordance test of the mathematical model.
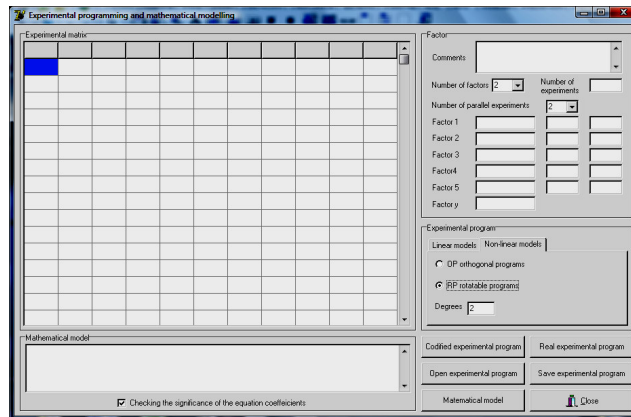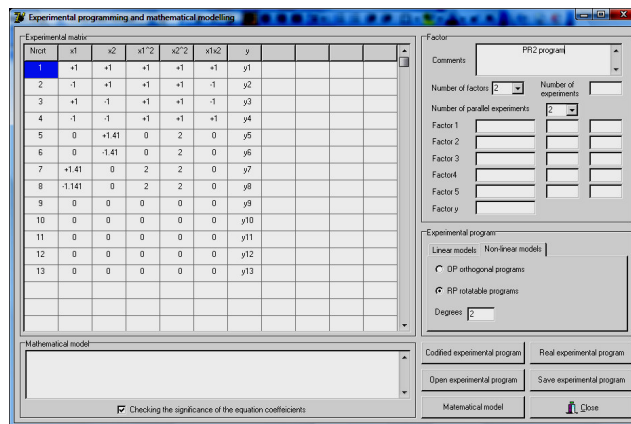

Fig. 2. *Main menu of the PR2 program*

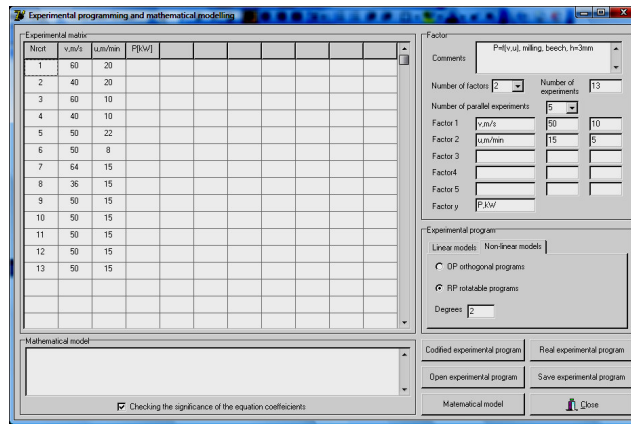Fig. 3. *Codified programming matrix*
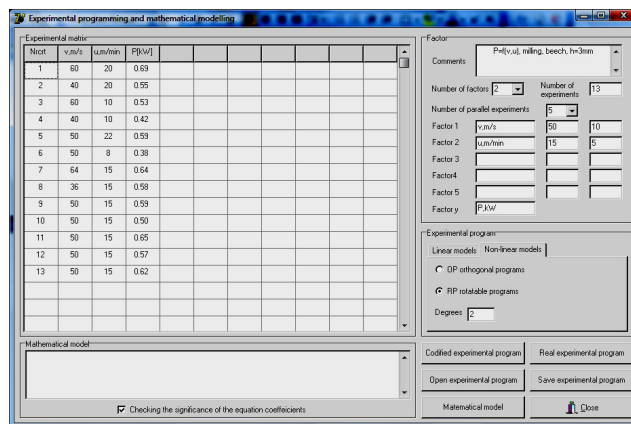
Fig. 4. *Real programming matrix*

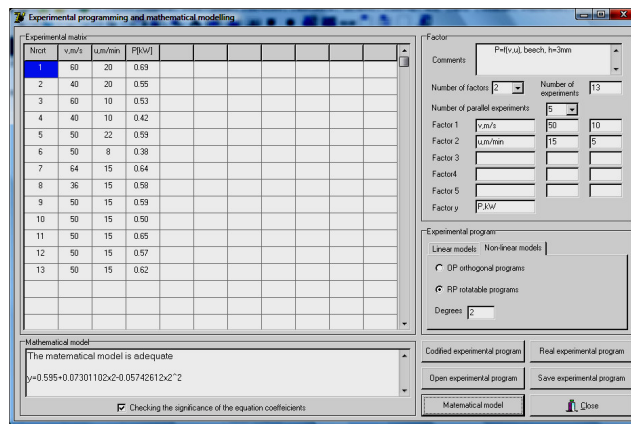

Fig. 5. *Real programming matrix with measured values*

Fig. 6. *Mathematical model for two factors with all significant coefficients*
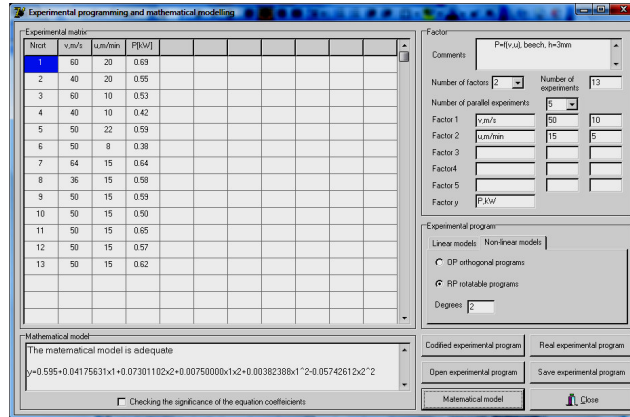
Fig. 7. *Mathematical model for two factors with all coefficients*

6. Conclusions

The experimenting and modelling method presented in this paper is very useful in process optimizing. Using rotatable experimental programs the number of experiments could be reduced without significant precision losses. Also the method allows obtaining mathematical models of second order which can be used in the optimizing process. The program which is based on this method is very easy to use and constitutes a real help in different experimental and modelling research.

References

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