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How to perform a simultaneous optimization with several response variables

Como realizar uma otimização simultânea com várias variáveis de resposta

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Abstract

A problem facing the product development community is developing simultaneous solutions of response variables (to several properties) that depends on a number of independent variables or sets of responses. Harrington, among others, addressed this problem and presented a desirability function with a functional approach. Derringer and Suich altered their approach and illustrated how multiple variables can be transformed into a convenience

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function. This work redid the calculation performed by them using another software and made a comparative discussion of the results found.

Keywords: Statistical Software. Optimizer. Modeling. Desirability Function.

Resumo

Um problema enfrentado pela comunidade de desenvolvimento de produtos é o desenvolvimento de soluções simultâneas de variáveis de resposta (a várias propriedades) que dependem de um número de variáveis ou conjuntos de respostas independentes. Harrington, entre outros, abordou este problema e apresentou uma função de desejabilidade com uma abordagem funcional. Derringer e Suich alteraram sua abordagem e ilustraram como múltiplas variáveis podem ser transformadas em uma função de conveniência. Este trabalho redidiu o cálculo realizado por eles utilizando outro software e fez uma discussão comparativa dos resultados encontrados.

Palavras-chave: Software Estatístico. Otimizador. Modelagem. Função de Desejabilidade.

Introduction

A common problem in product development involves selecting a set of conditions, the X's (input variables), which will result in a product with a combination of properties, the Y's (output variables). Essentially, this becomes a problem in simultaneously optimizing the Y's, or response variables, each of which depends on a set of independent variables, X1, X2, X3, XN. As an example, from the rubber industry, consider the problem of a tire tread compound. Here there are several response variables, such as Braking Wear (Y1), Tire Elasticity (Y2), 200 Modulus (Y3) and Hardness (Y4). Each of these response variables depends on the ingredient variables, the X's, such as silica hydrate level (x1), silane coupling level (x2) and the sulfur level (x3) (Kulikov, 2020; Liu et al., 2020; Meisig et al., 2020; Yuan et al., 2020).

It was selected the levels for the X's that will maximize the Y's. Unfortunately, the levels of X that maximize Yl may not even come close to maximizing Y2. This problem was described by Derringer and Suich (1980) in the Journal of Quality Technology, and both based on the works of Harrington (1965), and Gatza and McMillan (1972), performed an optimization using a function called desirability function, the researchers made a small adjustment in the work using a pattern search method like that presented by (Hooke & Jeeves, 1961), These works were later ratified in other papers by the authors Ramalingam et al. (2013); Saha and Alam (2022); Short and Selvakumar (2020) that showed the efficiency and robustness of these methods. This paper performed the calculation again with the same data proposed by the authors using new software and came to conclusions using the desirability function.

Theoretical Referential

Determining a process improvement is typically complex due to variations in customer demand and technological advances. Generally, multiple responses must be considered to achieve an overall process improvement is important to note that an optimization process does not necessarily imply the determination of optimal operating conditions, since it is practically impossible to establish the optimal point due to the large number of variables that impact a process. Instead, what can be determined are conditions for improvement from the selection of maximum points determined within a predetermined search space (Alketbi et al., 2022; Ding et al., 2020; Laidani et al., 2020; Rathod et al., 2020).

The simultaneous optimization of multiple answers has been a priority in several industrial branches, and much of the effort has been directed to the research of alternative methods for the efficient determination of a process adjustment that achieves a given goal. Optimization problems with multiple answers usually involve conflicting objectives making it difficult to solve them, for example, the minimization of production time versus the minimization of equipment cost in manufacturing processes or the maximization of biomass production versus the minimization of substrate consumption in biotechnological processes (Muniswamaiah et al., 2020; Pesteh et al., 2019).

Currently, the most used process optimization method in scientific works is the joint employment of the Desirability agglutination method with the Generalized Reduced Gradient (GRG) mathematical search method (Bell et al., 2020; Goffe et al., 2020; Karthikeyan et al., 2020; Lebron et al., 2020). A viable explanation for this fact is that this combination is present in the Optimizer function of the Minitab® software, which would facilitate the execution of this method (Gomes, Pereira, Marins, et al., 2019).

DOE is a structured and organized method used to determine the relationship between different process input and output factors, involving the definition of the set of experiments, in which all relevant factors are systematically varied. By analyzing the results obtained, one can determine the degree of influence on the response variable of each factor used, as well as the interactions between the factors and the optimum conditions (Chen et al., 2020; Korolchenko & Minaylov, 2020; Setiawati & Yusuf, 2020; Yang et al., 2020).

In processes with multiple responses, you should model each of the responses you wish to optimize by a function that describes the so-called Response Surface, that is, that allows you to estimate the value of the response within the range of variation defined for the variables involved in the study. These functions (multiple regression equations) are usually obtained from the analysis of the results of experiments designed by the Box-Behnken, Central Composite or three-level factorial designs, and are generally second-order equations characterize these models and state that the Composite Central Design (CCD) model is the most widely used (Arifin Handoyono et al., 2020; Rajesh Ruban et al., 2020; Wang et al., 2020).

A factor ignored by many studies using Design of Experiments (DOE) for process optimization, especially those involving multiple responses, is the individual quality of the models obtained (Derringer & Suich, 1980). In many cases, one or more models end up having a low degree of fit. The success of the optimization process is closely linked to the robustness of the models (Gomes, Pereira, Silva, et al., 2019).

2.1 Desarability Method

One of the most used techniques for simultaneously optimizing multiple responses is to transform the equations that model each of these responses into individual utility functions, and then proceed to optimize an overall utility function, known as Total Desirability (D), which is described in terms of the individual utility functions. The simultaneous optimization of multiple responses thus becomes the optimization of a single function. The prime movers of this approach were Derringer and Suich (1980), and it remains a benchmark for other methods in terms of the results it provides. Furthermore, its easy interpretation and implementation motivated the method to be described and its performance reviewed in this paper.

Derringer and Suich (1980) present individual utility functions for Nominal-The-Best (NTB), Larger-The-Better (LTB), and Smaller-The-Better (STB) responses. When the target value (T) of a response (yˆ(x)) is between a maximum value (U) and a minimum value (L), as shown in Figure 1, the response is said to be of type NTB with the corresponding utility function d (yˆ(x)), which for the sake of simplification will be represented here by d and can be defined as in Figure 1.

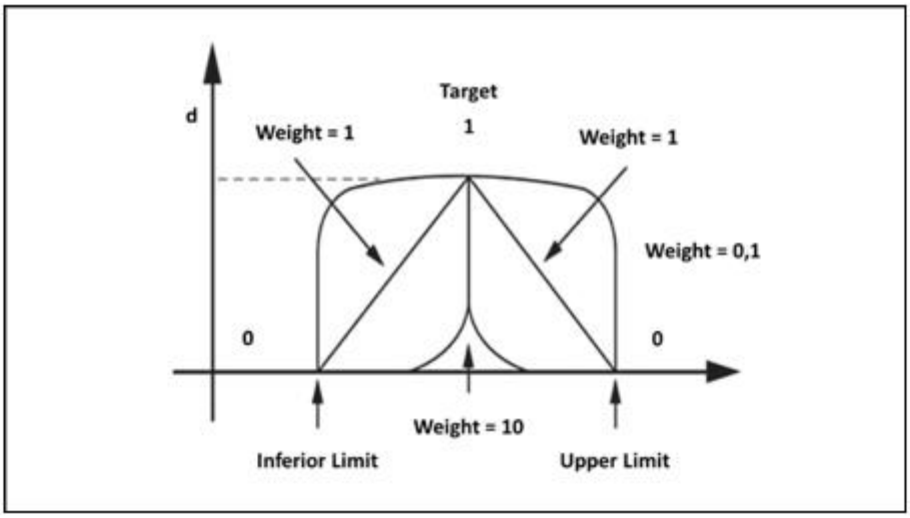

Figure 1 – Desirability Function Normalize
Source: Pimenta et al. (2015).

Where R and S are weighting factors, which can take on larger values than when you want to prioritize maximizing or minimizing the response. When the target value T must reach the maximum value of the function, the response is said to be of type LTB, as illustrated in Figure 2. When the target value must reach the minimum value of the function, as in Figure 3, the response is said to be of STB.

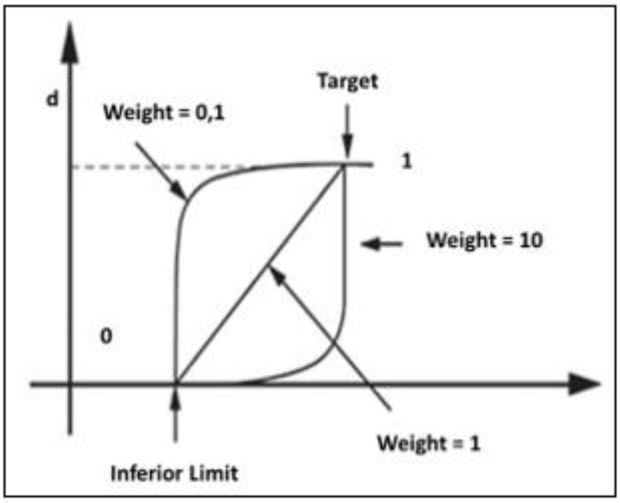

Figure 2 – Desirability maximize function
Source: Pimenta et al. (2015).

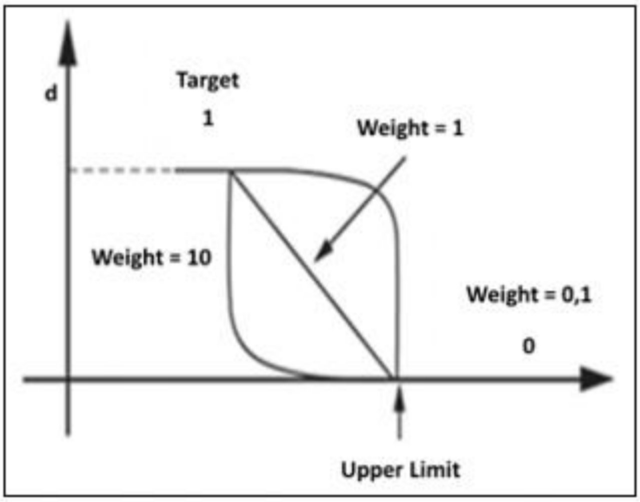

Figure 3 – Desirability minimize function
Source: Pimenta et al. (2015).

Scientific Method

Scientific research can be classified as to its nature, approach, objectives, and procedures. As for the nature, this work is characterized as applied research, because it has practical interest so that the results are applied and/or used in the solution of real problems (Araujo et al., 2021; Kothari & Garg, 2019; Reis et al., 2022; Silva et al., 2021).

As to the objectives, this research is descriptive and exploratory. Descriptive because it allows to describe the characteristics of the phenomenon observed in relation to the delimitation made in this project and exploratory because it will provide greater familiarity of the researcher with the research problem to provide her with greater in loco contact/familiarity with the elements to be studied (Kothari & Garg, 2019; Sales et al., 2022; Yin, 2017). The data were processed in March 2022 and the theoretical framework was found in the Scopus database.

Results And Discussions

The results obtained from the data contained in the work of Derringer and Suich (1980), are summarized in Table 1, and refer to the variables x1 (Hydrated Silica Level), x2 (Silane Coupling) and x3(Sulfur Level). The Response Variables are Wear to Braking (Y1), Tire Elasticity (Y2), Modulus 200 (Y3) and Hardness (Y4). The Response Variables follow the following Constraints: $120 < Y1$, $1000 < Y2$, $400<Y3<600$, $60<Y4<75$. At the time the optimization was done using FORTRAN Programming, which was the technological tool used at the time, here an analysis was performed using Minitab statistical software which is one of the most used for statistical analysis today.

A SURFACE RESPONSE experiment was created in Minitab with 20 runs, 1 block and six replicates in the central point, exactly to match the experiment of the work in question. With the Analysis of the Responsive Surface Experiment a result was obtained for each value of Y. The results for each Mathematical Model and each Pareto Graph are in Equations (1), (2), (3) and (4) and Figures 4, 5, 6 and 7.

A	B	C	Y1	Y2	Y3	Y4
-1	-1	-1	103	490	640	62,5
1	-1	-1	120	860	410	65
-1	1	-1	117	800	570	77,5
1	1	-1	139	1090	380	70
-1	-1	1	102	900	470	67,5
1	-1	1	132	1289	270	67
-1	1	1	132	1270	410	78
1	1	1	198	2294	240	74,5
-1,68179	0	0	102	770	590	76
1,681793	0	0	154	1690	260	70
0	-1,68179	0	96	700	520	63
0	1,681793	0	163	1540	380	75
0	0	-1,68179	116	2184	520	65
0	0	1,681793	153	1784	290	71
0	0	0	133	1300	380	70
0	0	0	133	1300	380	67,5
0	0	0	140	1145	430	68
0	0	0	142	1090	430	68
0	0	0	145	1260	390	69
0	0	0	142	1344	390	70

Tabela 1 – Experimental Design
Source: Adapted from Derringer and Suich (1980).

$$Y1 = 139,16 + 16,29\ A + 17,70\ B + 10,78\ C - 3,90\ A*A - 3,37\ B*B - 1,60\ C*C + 5,13\ A*B + 7,13\ A*C + 7,88\ B*C \quad (1)$$

$$Y2 = 1251 + 265,1\ A + 243,7\ B + 134,8\ C - 73,7\ A*A - 112,6\ B*B + 192,8\ C*C + 69\ A*B + 94\ A*C + 104\ B*C \quad (2)$$

$$Y3 = 400,15 - 98,48\ A - 31,15\ B - 72,99\ C + 7,88\ A*A + 16,72\ B*B + 0,81\ C*C + 8,75\ A*B + 6,25\ A*C + 1,25\ B*C \quad (3)$$

$$Y4 = 68,744 - 1,398\ A + 4,260\ B + 1,618\ C + 1,539\ A*A + 0,125\ B*B - 0,228\ C*C - 1,625\ A*B + 0,125\ A*C - 0,250\ B*C \quad (4)$$

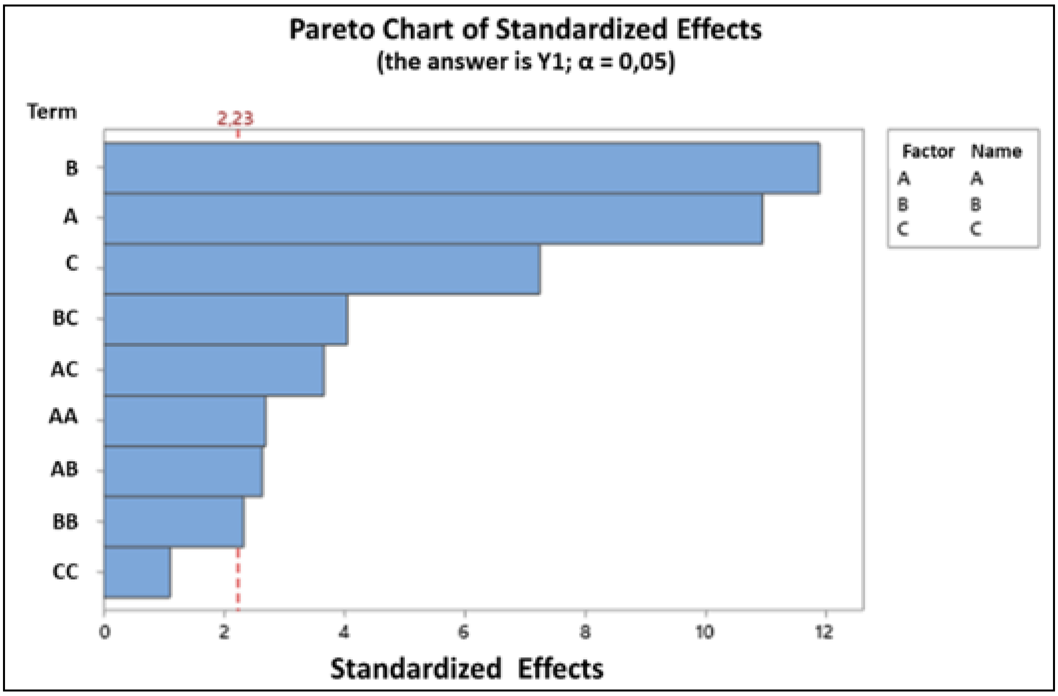

Figure 3 – Pareto chart for Response Y1

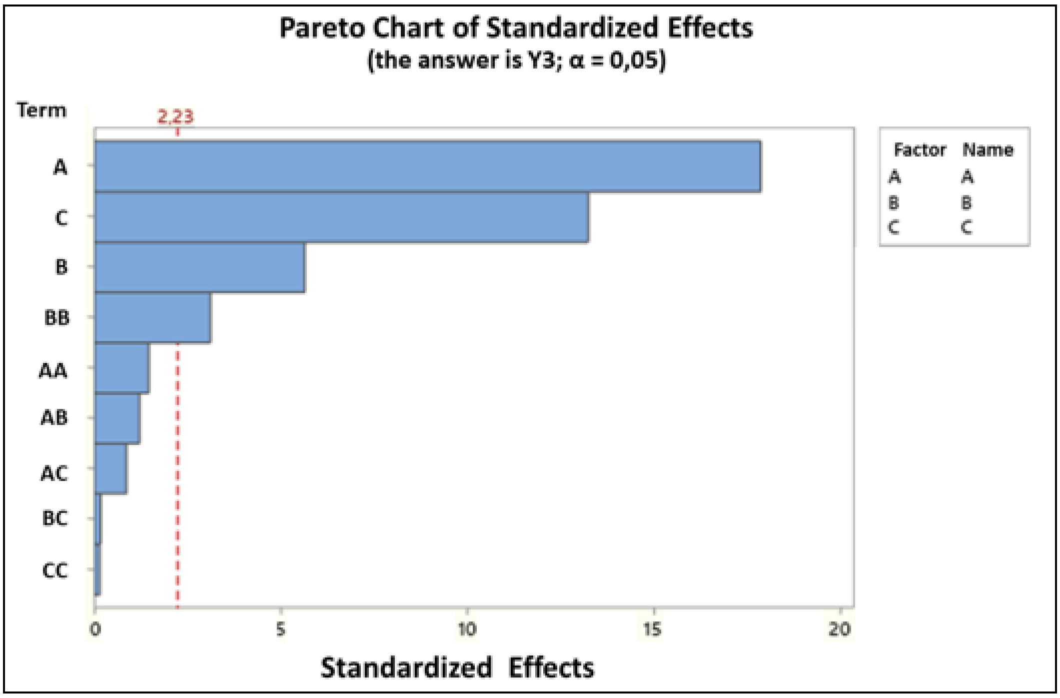

Figure 4 – Pareto chart for Response Y2

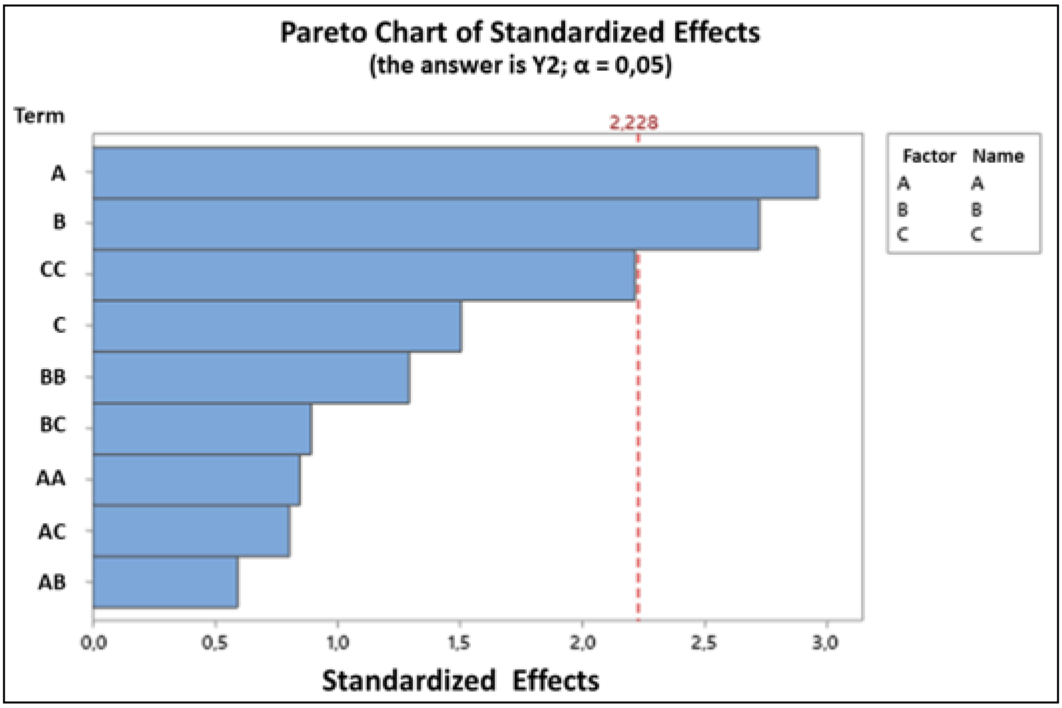

Figure 5 – Pareto chart for Response Y3

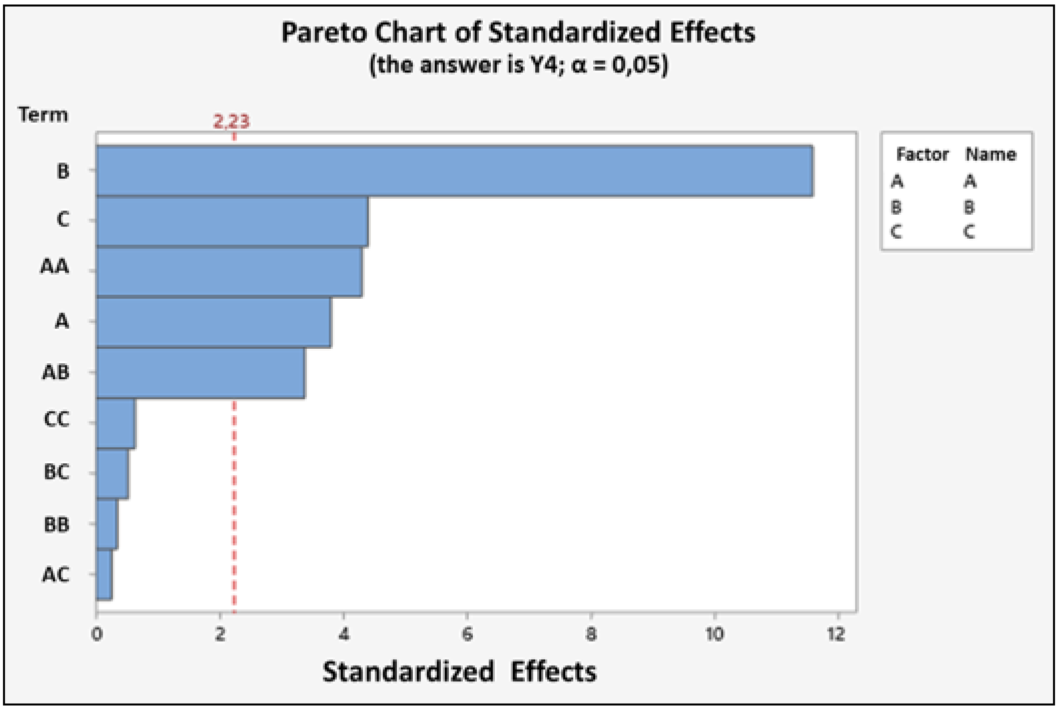

Figure 6 – Pareto chart for Response Y4

The big problem is that while a variable is Optimized to meet the conditions required by the problem, the others are outside the required optimal conditions, that is, a conflicting behavior occurs, and it is difficult to meet the proposed targets for the problem. The solution is to transform this set of four answers (Y1, Y2, Y3 and Y4) to do so we used a binding function called Desirability. In the Minitab software you use the Optimize Response function and enter the desired Targets to get the desired Optimized Response.

The result of the optimization appears in Table 2 and Figure 8. A simple analysis shows that the response variable Y1 that should get minimum value 120 and maximum value 170 found the value of 129.4208 with an individual desirability (d1=0.1884), the response variable Y2 reached the optimal value of 1300 with an individual desirability (d2=1), variable Y3 which had a target of 500 obtained a value of 465.5323 with an individual desirability (d3=0.65532) and variable Y4 whose target was 67.5 had a very good approximation of 67.9298 with an individual desirability (d4=0.94270).

Variable	**Configuration**			
A	-0,0385			
B	0,167716			
C	-0,900246			
		Adjusted		
Answer	**Adjust**	**EP**	**95% IC**	**95% IP**
Y4	67,93	0,578	(66,641;69,218)	(64,642;71,218)
Y3	465,53	8,67	(446,22;484,85)	(416,24;514,83)
Y2	1300	141	(987;1613)	(500;2100)
Y1	129,42	2,34	(124,21;134,64)	(116,11;142,73)

Tabela 2 – Multiple Response Prediction
Source: Own Authors (2022)

The fit values of the process variables coded to meet the optimal responses obtained were X1 (-0.0385), X2(0.1677) and X3(-0.9002) all within the ranges considered, it would now be enough to simply decode the variables to obtain the values that should use these variables in the process. The values obtained in this work were slightly better than those of Derringer and Suich (1980) which are respectively: Xl = -0,050; X2 = 0,145; X3= -0,868; Y1 (Peak) = 129,5 (d1 = 0,189); Y2 (Modulus) = 1300 (d2 = 1,000); Y3 (Elongation) = 465,7 (d3= 0,656); and Y4 (Hardness) = 68,0 (d4= 0,932).

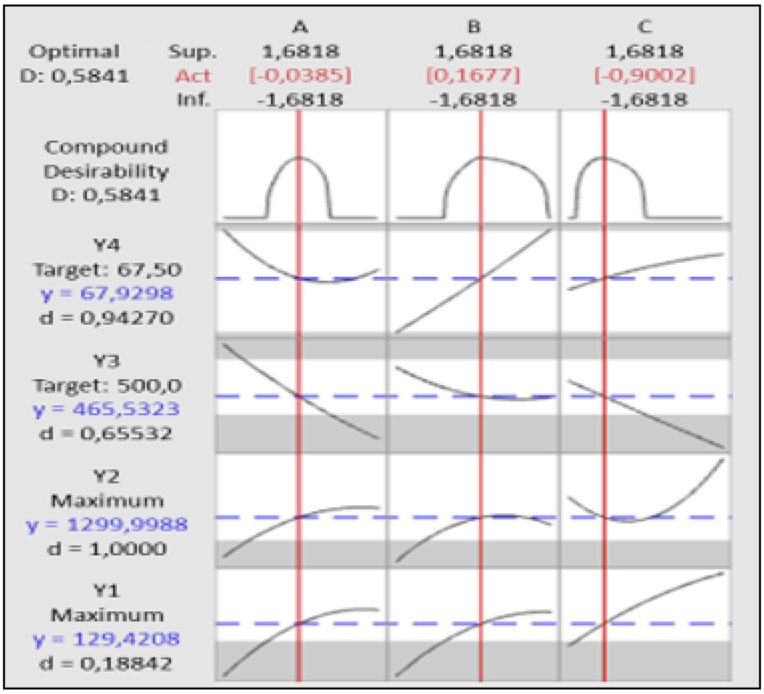

Figure 7 – Optimized Response Graphs

Conclusion

The main objective of this study was to compare the optimal results found in this work with those found in the work of Derringer and Suich, in this sense, the objective was successfully achieved. The main academic contribution of this work was to show that with the use of Minitab software, which is relatively simple and practical to work with compared to FORTRAN programming, it was found values very close to those obtained by the authors and in some cases, such as hardness, even better values, but small deviations in the value of x do not cause major changes, because as in the original work the surface is relatively flat near the optimal point.

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