

# A Multiple Response Function for Optimization of Analytical Strategies Involving Multi-elemental Determination

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**Abstract:** This paper presents a comparison between a multiple response function (MR) proposed for optimization of analytical strategies involving multi-element determinations with the desirability function D, which was proposed by Derringer and Suich in 1980. The MR function is established by the average of the sum of the normalized responses for each analyte considering the highest value of these. This comparison was performed during the optimization of an spectrometer for quantification of six elements using inductively coupled plasma optical emission spectrometry (ICP OES). Four instrumental factors were studied (auxiliary gas flow rate, plasma gas flow rate, nebulizer gas flow rate and radio frequency power). A ( $2^4$ ) two-level full factorial design and a Box Behnken matrix were developed to evaluate the performance of the two multiple response functions. The results found demonstrated great similarity in the interpretations obtained considering the effect values of the factors calculated using the two-level full factorial design employing the two multiple responses. Also a Box Behnken design was performed to compare the applicability of the two multiple response functions in quadratic models. The results achieved demonstrated high correlation (0.9998) between the regression coefficients of the two models. Also the response surfaces obtained showed great similarity in terms of formats and experimental conditions found for the studied factors. Thus, the multiple response (MR) is presented as a simple tool, easy to manipulate, efficient and very helpful for application in analytical procedures involving multi-response. An overview of applications of this function in several multivariate optimization tools as well as in various analytical techniques is presented.

**Keyword:** Multiple response function, Experimental design, Desirability function D, ICP OES.

## 1. INTRODUCTION

In recent times, the multivariate optimization techniques have been widely employed during the development of analytical methods [1, 2], considering that these strategies allow obtaining mathematical models that permit assessment of the statistical significance of the factors studied, as well as evaluate the effects of the interactions between these factors. Furthermore, these designs have as advantages the reduction in the number of experiments that need to be executed, lower reagent consumption and considerably less laboratory work [3, 4]. The chemometric tools more employed for optimization of analytical methods are: factorial design [5-8], central composite design [9], Doehlert matrix [1, 10] and Box- Behnken design [1, 11, 12].

During the multivariate optimization of analytical systems that involve many responses (dependent variables), the establishment of a multiple response is necessary. This multiple response obtained should be compatible with the goals of the optimization, prioritizing and/or minimizing individual responses according to the proposed interests. The strategy more utilized to optimize multiple responses is the desirability function D, which was proposed by Derringer and Suich [13]. The function is built considering that the quality of a product or process that has many features is completely unacceptable if one of them is beyond a "desirable" limit. According to this, the main object is to find operating conditions that ensure compliance with the criteria of all the involved responses and, at the same time, provide the best value of compromise in the desirable joint response. Thus, the multiple responses are converted into a single one by combining the individual responses into a composite function followed by its optimization. The function is established in view of the experimental conditions which allow reaching simultaneously the optimal value for all the evaluated variables. This concept includes the researcher's priorities during

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the optimization procedure. Consequently, an individual desirability function ( $d_i$ ) is created for each response using the fitted models and establishing the optimization criteria. The new function is built in such a way that it should take values between 0 (undesirable response) and 1 (a completely desirable value or ideal response). Intermediate values of ( $d_i$ ) indicate more or less desirable responses. Finally, once the  $n$  responses are transformed in desirability functions, they are combined in a unique function named Global Desirability (D), computed as the product among the different individual desirability's ( $d_i$ ), to find out the best joint responses [13].

Other approaches with greater sophistication [14, 15], requiring a user with background knowledge in mathematics, statistics and computer science have been also proposed, such as: compromise programming [16], goal programming [17], inspection of contour plots [18], physical programming [19], a Bayesian approach with unrelated regression models [20], multi-response optimization using multiple regression-based weighted signal-to-noise ratio [21], neural networks [22] and vectorial optimization [23]. Obviously, all of these tools have their great merits and also possible disadvantages.

Despite this variety of alternatives (more complexes) for obtaining multiple responses, other attempts have also been proposed requiring the user's less sophistication in data processing. So, during the optimization step of an on-line pre-concentration system for the determination of copper by flame atomic absorption spectrometry a response was established by normalization of the analytical signal (absorbance) in function of pre-concentration time. This parameter named as "sensitivity efficiency" was used as a response for evaluation of the results of an experiment using Doehlert matrix [24]. Another method was developed for selective extraction and determination of catechol in water samples using differ-

ential pulse voltammetry (DPV). The optimization step was performed using factorial design and Doehlert matrix having as response also the "sensitivity efficiency". In this case, it was determined considering the electrochemical signal and the pre-concentration time on the electrode [25]. In a method proposed for simultaneous determination of the methylxanthines: caffeine, theobromine and theophylline by high performance liquid chromatography (HPLC) the optimization step was performed using full three-level factorial design, being that a response was established considering the resolution among the peaks of the theobromine and theophylline and the analysis time [26].

A Brazilian research group proposed a multiple response function (MR) that has been often used during the optimization of analytical strategies developed for multi-element determinations [27]. In it, a pre-concentration procedure for simultaneous determination of lead and cadmium in potable water using flame atomic absorption spectrometry (FAAS) was performed, the multiple response (MR) was calculated as being:

$$MR = (abs_{Cd}/abs_{max Cd}) + (abs_{Pb}/abs_{max Pb}),$$

where ( $abs_{Cd}$ ) and ( $abs_{Pb}$ ) are the analytical signals for each metal ion in the several experiments, and ( $abs_{max Cd}$ ) and ( $abs_{max Pb}$ ) are the maximum values of the absorbance's achieved for cadmium and lead, respectively, during all the multivariate designs that were performed [27].

The multiple response function (MR) has been utilized indiscriminately by several researcher using the followings multivariate optimization tools: full three-level factorial design [28], Box Behnken design [29-32], centroid simplex mixture design [32], two level factorial design [27, 33], Doehlert matrix [34-37] composite central [38, 39] and fractional factorial design [40]. The Table 1 shows parameters of

**Table 1. Analytical methods optimized using the response multiple function (MR).**

Analytes	Samples	Chemometric tools	Objective	Analytical technique	Ref.
Pb and Cd	Potable water	Doehlert matrix	Pre-concentration procedure	FAAS	[27]
14 chemical elements	Dog and cat foods	Three-level factorial design	Sample preparation	ICP OES	[28]
Cu and Zn	Foods	Box Behnken design	Pre-concentration system	FAAS	[29]
BTEX	Water	Box Behnken design	Extraction step	GC-FID	[30]
Cd, Cu and Pb	Water	Box Behnken design	Pre-concentration system CPE	TS-FF-AAS	[31]
Nine elements	Bean	Box Behnken design	Sample preparation	ICP OES	[32]
Nine elements	Bean	Centroid simplex mixture	Sample preparation	ICP OES	[32]
12 Persistent organic pollutants	Caiman yacare eggs	Two-level Factorial design	SPE step	GC	[33]
Trace and major elements	Marine invertebrates	Doehlert matrix	Sample preparation	ICP OES	[34]
Nine elements	Coconut milk	Doehlert matrix	Sample preparation	ICP OES	[35]
Several elements	Mineral fertilizers	Doehlert matrix	Sample preparation	ICP OES	[36]
Five elements	Petroleum produced formation waters	Doehlert matrix	Pre-concentration procedure	ICP-MS	[7]
BTEX	Wastewater	Central composite	Extraction step	GC-FID	[38]
Eight elements	Organic fertilizers	Central composite	Sample preparation	FF AAS	[39]
Several substances	Environmental	Fractional factorial design	Extraction step	CG	[40]

BTEX - Benzene, Toluene, Ethylbenzene, and Xylene; CPE - Cloud Point Extraction; FAAS - Flame Atomic Absorption Spectrometry; GC-FID - Gas Chromatography with Flame Ionization Detection; ICP-MS - inductively coupled plasma mass spectrometry; SPE - Solid Phase Extraction; TS-FF-AAS - Thermospray Flame Furnace Atomic Absorption Spectrometry.

analytical methods that were optimized using the response multiple function (MR).

In this paper, the optimization of the instrumental conditions of a ICP OES spectrometer proposed for determination of six chemical elements (B, Cd, Cr, Fe, Mn and Zn) was performed using two-level full factorial design and after Box Behnken matrix. All the results obtained were modeled using the multiple response (MR) [27] and also the response established by Global Desirability (D) [13] in order to establish the comparison.

## 2. EXPERIMENTAL

### 2.1. Instrumentation

All measurements were performed employing an ICP OES (Spectro CIRUS, Kleve, Germany) with axial view. A Scott type double pass spray chamber and a cross-flow nebulizer were used throughout the experiments. Table 2 summarizes the detailed description of the spectrometer and operational parameters used during the tests.

**Table 2. Operation parameters of ICP OES.**

Parameter	Conditions
Radio Frequency Power (W)	1200 – 1400
Generator Frequency (MHz)	27.15
Plasma gas flow rate (l min <sup>-1</sup> )	11.0 – 14.0
Auxiliary gas flow rate (l min <sup>-1</sup> )	0.5 – 1.0
Nebulizer gas flow rate (l min <sup>-1</sup> )	0.5 – 1.0
Sample flow rate (ml min <sup>-1</sup> )	1.4
Nebulizer	Cross Flow
Spray chamber	Double Pass (Scott)
View configuration	Axial
Detector	Charge Coupled Device (CCD)
Emission lines (nm)	B I (249.773); Cd II (214.438); Cr II (283.563); Fe II (238.204); Mn II (257.611); Zn I (213.856)

### 2.2. Reagents

Ultrapure water (with a specific resistivity of 18 MΩ cm<sup>-1</sup>) prepared with a Milli-Q water purification system (Millipore, Bedford, MA, USA) was used to prepare all the solutions. The reagents utilized were of analytical reagent grade. All the glassware was kept in a 10 % (v/v) nitric acid (Merck, Darmstadt, Germany) solution for 12 h, followed by washing with deionized water and finally with ultrapure water. Working standard solutions of 1.0 μg ml<sup>-1</sup> (B, Cd, Cr, Fe, Mn and Zn) diluted in 5 % nitric acid were obtained by stepwise dilution of multi-element standard solution 1000 μg ml<sup>-1</sup> (Merck). Nitric acid solution was prepared by direct dilution from the concentrated solutions (Merck).

### 2.3. Factorial Design

Initially a 2<sup>4</sup> two-level full factorial design was performed to assess the behavior of variables related to argon gas (auxiliary gas flow rate – AF, plasma gas flow rate – PF, and nebulizer gas flow rate – NF). The radio frequency (RF) power was also chosen because this variable is directly related to the energy of the plasma. Triplicate of the central point was performed in order to determine the experimental error. The assays were carried out at random and the experimental data were processed by using the STATISTICA program [41].

### 2.4. Box Behnken Design

After the preliminary evaluation that it was done by two level factorial design a Box Behnken matrix was also performed involving the variables (RF power – P, plasma gas flow rate – PF, and nebulizer gas flow rate – NF). All the experiments were also performed randomly.

### 2.5 Multiple Responses

The desirability function (D) and the multiple response (MR) were applied in the data obtained (for the six elements) during the experiments developed using factorial design and Box Behnken matrix. The desirability function (D) was calculated combining the individual desirability values by applying the geometric mean:  $D = (d_B \times d_{Cd} \times d_{Cr} \times d_{Fe} \times d_{Mn} \times d_{Zn})^{1/6}$ . Values obtained from each response were transformed to a dimension less scale. The scale of individual desirability ranges between  $d = 0$  and  $d = 1$ . The overall desirability function D is defined as the weighted geometric average of the individual desirability. The MR function was calculated as  $MR = (I_B/I_{max,B}) + (I_{Cd}/I_{max,Cd}) + (I_{Cr}/I_{max,Cr}) + (I_{Fe}/I_{max,Fe}) + (I_{Mn}/I_{max,Mn}) + (I_{Zn}/I_{max,Zn})$ , being that, I is the intensity of the analytical signal to an element in a particular experiment and  $I_{max}$  is the larger signal obtained in the set of experiments.

## 3. RESULTS AND DISCUSSIONS

### 3.1. Full Two-level Factorial Design

Firstly, a 2<sup>4</sup> full two-level factorial design was performed involving four factors. The experimental dominions as coded and real values for the factors and the six responses (emission intensities) obtained for each element are shown in Table 3. The multiple responses (D) and (MR) were calculated as their expressions and results achieved and are also shown in Table 3.

The factorial design was evaluated and the effects of the principal factors and its interactions were calculated [1, 4], considering the multiple responses (D) and (MR), as presented in Table 3. Table 4 shows the values of these effects.

An evaluation of the effect values (Table 4) obtained using the multiple response (D) indicates that:

- All the four principal factors studied and their interactions are statistically significant, except the (RF power - P) X (auxiliary gas flow rate - AF) interaction.

**Table 3.** Design matrix and results of the 2<sup>4</sup> full factorial design.

Run	Variables			Emission intensities							Multiple responses	
	P (W)	AF (l min <sup>-1</sup> )	PF (l min <sup>-1</sup> )	NF (l min <sup>-1</sup> )	B 249.773	Cd 214.438	Cr 283.563	Fe 238.204	Mn 257.611	Zn 213.856	D	MR
1	(-1) 1200	(-1) 0.70	(-1) 12.0	(-1) 0.50	93158800	136496000	183196000	88521900	210747000	151330000	0.534	3.414
2	(-1) 1200	(-1) 0.70	(-1) 12.0	(+1) 1.00	14029200	11322400	23252500	11094700	56191300	17230400	0.011	0.492
3	(-1) 1200	(-1) 0.70	(+1) 14.0	(-1) 0.50	73780900	112316000	148981000	69386400	147462000	130107000	0.405	2.719
4	(-1) 1200	(-1) 0.70	(+1) 14.0	(+1) 1.00	11982900	10038400	20959900	9832490	51471100	15111100	0.002	0.437
5	(-1) 1200	(+1) 1.00	(-1) 12.0	(-1) 0.50	84861300	146667000	196372000	94784100	248582000	161708000	0.572	3.619
6	(-1) 1200	(+1) 1.00	(-1) 12.0	(+1) 1.00	13118700	11077200	22561700	10726800	54445600	16673500	0.008	0.473
7	(-1) 1200	(+1) 1.00	(+1) 14.0	(-1) 0.50	76895200	126983000	166115000	79075700	185006000	143646000	0.470	3.062
8	(-1) 1200	(+1) 1.00	(+1) 14.0	(+1) 1.00	11770100	9857580	20381900	9650140	48520000	14671100	0.000	0.423
9	(+1) 1400	(-1) 0.70	(-1) 12.0	(-1) 0.50	147477000	230599000	331080000	155330000	337558000	233456000	0.938	5.660
10	(+1) 1400	(-1) 0.70	(-1) 12.0	(+1) 1.00	44820300	59244300	105365000	52473000	250240000	91515600	0.300	2.193
11	(+1) 1400	(-1) 0.70	(+1) 14.0	(-1) 0.50	137185000	200519000	288847000	133499000	254550000	208824000	0.795	4.896
12	(+1) 1400	(-1) 0.70	(+1) 14.0	(+1) 1.00	43337600	56264000	102420000	51046400	242187000	87482800	0.287	2.116
13	(+1) 1400	(+1) 1.00	(-1) 12.0	(-1) 0.50	151173000	243363000	345562000	165198000	381362000	244738000	1.000	6.000
14	(+1) 1400	(+1) 1.00	(-1) 12.0	(+1) 1.00	44047400	55947400	100367000	50339400	235170000	86784700	0.283	2.088
15	(+1) 1400	(+1) 1.00	(+1) 14.0	(-1) 0.50	140130000	217234000	307986000	144594000	302947000	224227000	0.871	5.297
16	(+1) 1400	(+1) 1.00	(+1) 14.0	(+1) 1.00	42041200	53003000	96328000	47983900	228282000	83819700	0.269	2.006
17 (CP)	(0) 1300	(0) 0.85	(0) 13.0	(0) 0.75	63126100	112830000	168098000	87802600	375139000	147642000	0.525	3.486
18 (CP)	(0) 1300	(0) 0.85	(0) 13.0	(0) 0.75	62700400	113860000	168932000	88407300	376522000	148265000	0.527	3.500
19 (CP)	(0) 1300	(0) 0.85	(0) 13.0	(0) 0.75	62809100	113613000	168577000	88823700	376849000	147845000	0.528	3.500

P - RF power; AF - Auxiliary gas flow rate; PF - Plasma gas flow rate; NF - Nebulizer gas flow rate; D - Desirability function; MR - Multiple Response; CP - Central point.

**Table 4.** Effects of factors and its interactions using the two response functions.

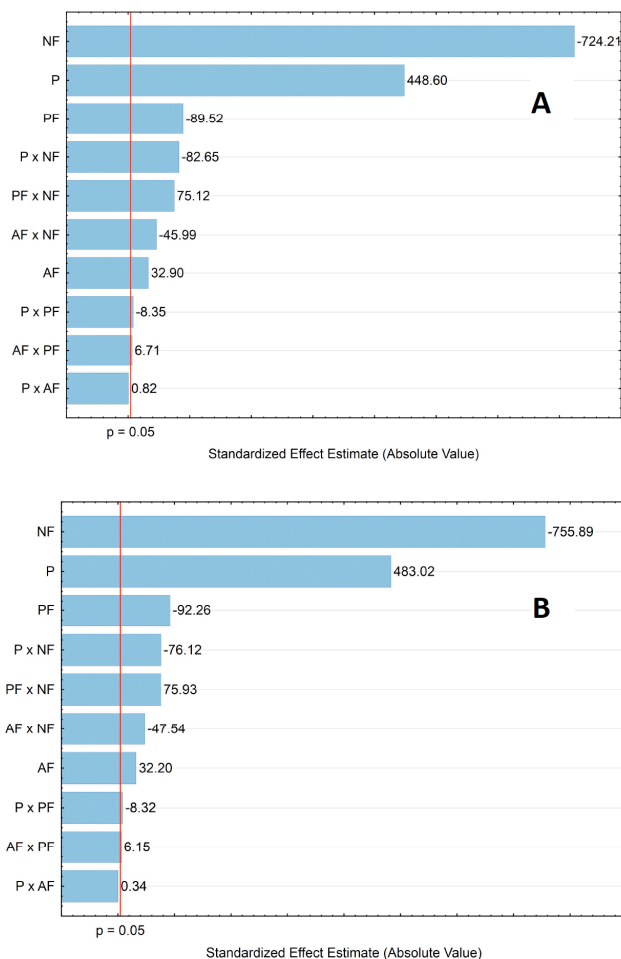
Factor	Effect Desirability function	Effect Multiple Response
Mean	0.438194	2.91476
P	0.342440	1.95209
AF	0.025116	0.13006
PF	-0.068604	-0.37279
NF	-0.553076	-3.05492
P x AF	0.000727	0.00134
P x PF	-0.006361	-0.03370
P x NF	-0.063181	-0.30785
AF x PF	0.005111	0.02479
AF x NF	-0.035074	-0.19181
PF x NF	0.057105	0.30707

P - radio frequency power; AF - auxiliary gas flow rate;  
PF - plasma gas flow rate; NF - nebulizer gas flow rate.

- The principal factor is the nebulizer gas flow rate (NF), which has a negative effect (-0.5531). This suggests that the increase of this factor decreases the aerosol production and the transport efficiency, consequently decreased the emission intensities of the elements.
- The second more important factor is the RF power with positive effect (0.3424). It suggests that increasing RF power provides an increase in the analytical signals. This increase is due to obtaining a hotter plasma when using higher powers resulting in higher amounts of ionized atoms or ions, increasing the emission signal from the elements.
- The (RF power - P) x (nebulizer gas flow rate - NF) interaction has a higher influence on the plasma than the (auxiliary gas flow rate - AF) factor. The negative effect for this interaction indicates that the best conditions for a good performance of the spectrometer found when RF power is adjusted for the higher level (+1, 1400) and nebulizer gas flow rate at lower level (-1, 0.50). For analyte species that require more energy for excitation and ionization, a higher power would provide greater sensitivity. The nebulizer argon flow rate is a critical parameter because it determines directly the residence time of the analyte on the center of the plasma discharge. This way, the nebulizer gas flow rate can influence the atomization, excitation and ionization of the species. For an element that emits strong ionic lines and also has a high ionization potential, a lower nebulizer argon flow rate is required in order to get a long residence time of the species on the optimal region of the plasma.
- The plasma gas flow rate had a negative effect (-0.0686), it suggesting that the higher emission intensities for the elements occurs when this factor is in a lower level (-1, 12.0). This can be observed in the experiments 9 and 13 of the Table 3.
- The auxiliary gas flow rate factor has a positive effect (0.0251), which could suggest that the best condition for this factor will be at higher level (+1, 1.0). However, although statistically significant the effect magnitude is low and this factor has a low influence on the performance of the instrument in the studied conditions.
- The effects of the factors and their interactions were also calculated using the multiple response (MR) as chemometric response. The effect values are also shown in Table 4. An assessment of this Table reveals a complete coherency between the effect values of the principal factors and their interactions found by the response functions (D) and (MR). Also the numeric values and signs presented a good similarity. This way, all the conclusions about the influence of these factors and their interactions found using the response

function (D) can be perfectly applied in the results obtained by response function (MR).

- A linear regression was established using the values of the effects of the significant factors. A correlation coefficient of 0.9998 was obtained, it also indicates a strong correlation between the effect values calculated using the two response functions (D) and (MR). The Pareto charts (Fig. 1A and B) also show the similarity between the results achieved.



**Fig. (1).** Pareto Chart for the full factorial design  $2^4$  using (A) desirability and (B) multiple response.

### 3.2- Box Behnken Design

Box Behnken design was also performed to compare the applicability of the two functions during the generation of a quadratic model. In this step, the auxiliary gas flow rate (AF) was fixed. Table 5 shows the experimental conditions of the three factors as coded and real values, the emission intensities for the six elements studied and also the responses (D) and (MR), which were calculated using the emission intensities of the six elements.

The data obtained employing (D) and (MR) as responses generated two quadratic models (both without lack of fit). The regression coefficients found for these models are shown in Table 6. A regression linear was applied on the

**Table 5.** Design matrix and results of the Box-Behnken design.

Run	Variables			Emission intensities						Multiple responses	
	P (W)	PF (l min <sup>-1</sup> )	NF (l min <sup>-1</sup> )	B 249.773	Cd 214.438	Cr 283.563	Fe 238.204	Mn 257.611	Zn 213.856	D	MR
1	(-1) 1300	(-1) 11.0	(0) 0.65	113956000	270436000	305975000	144674000	636907000	193141000	0.555	4.324
2	(+1) 1400	(-1) 11.0	(0) 0.65	140576000	346527000	368725000	178073000	734912000	229870000	0.801	5.242
3	(-1) 1300	(+1) 13.0	(0) 0.65	96975600	207673000	249185000	122730000	513997000	153086000	0.340	3.516
4	(+1) 1400	(+1) 13.0	(0) 0.65	121789000	300030000	335636000	158549000	668070000	205103000	0.646	4.663
5	(-1) 1300	(0) 12.0	(-1) 0.50	128443000	321956000	355682000	166891000	583515000	202495000	0.654	4.713
6	(+1) 1400	(0) 12.0	(-1) 0.50	167862000	415078000	453175000	213300000	724709000	249594000	0.995	5.986
7	(-1) 1300	(0) 12.0	(+1) 0.80	64083700	98167600	164527000	73926100	358089000	105145000	0.000	2.236
8	(+1) 1400	(0) 12.0	(+1) 0.80	97708900	164827000	236958000	106889000	508070000	151436000	0.283	3.301
9	(0) 1350	(-1) 11.0	(-1) 0.50	159488000	398480000	429401000	203626000	701650000	241920000	0.929	5.736
10	(0) 1350	(+1) 13.0	(-1) 0.50	141712000	352620000	389531000	182627000	631837000	218292000	0.770	5.144
11	(0) 1350	(-1) 11.0	(+1) 0.80	87539700	137854000	206902000	92802000	445513000	133004000	0.171	2.884
12	(0) 1350	(+1) 13.0	(+1) 0.80	79049300	124588000	200726000	84138200	438354000	128533000	0.125	2.720
13 (CP)	(0) 1350	(0) 12.0	(0) 0.65	130654000	311030000	344111000	165528000	709497000	215459000	0.708	4.892
14 (CP)	(0) 1350	(0) 12.0	(0) 0.65	123642000	286686000	320523000	153579000	647482000	197870000	0.611	4.528
15 (CP)	(0) 1350	(0) 12.0	(0) 0.65	127332000	309875000	341808000	164437000	702851000	214016000	0.694	4.844

P – RF power; PF – Plasma gas flow rate; NF – Nebulizer gas flow rate; D – Desirability function; MR – Multiple Response; CP – Central point.

**Table 6.** Effects and Regression Coefficients of factors and its interactions obtained for Box–Behnken design using the two response functions.

Factor	Mean	P(L)	P(Q)	PF(L)	PF(Q)	NF(L)	NF(Q)	P(L) by PF(L)	P(L) by NF(L)	PF(L) by NF(L)
Effect (D)	0.670906*	0.294102*	-0.101045	-0.14391	-0.069869	-0.692040*	-0.274627*	0.030143	-0.029295	0.056512
Effect (MR)	4.75471*	1.10052*	-0.38021	-0.53597	-0.25661	-2.60943*	-1.01062*	0.11481	-0.10395	0.21401
Regression Coefficients (D)	-40.7381	0.0552	-0.0000	0.2371	-0.0349	6.0030	-6.1028*	0.0003	-0.0020	0.1884
Regression Coefficients (MR)	-149.703	0.207	-0.000	0.798	-0.128	21.292	-22.458*	0.001	-0.007	0.713

P – RF power; PF – Plasma gas flow rate; NF – Nebulizer gas flow rate; D – Desirability function; MR – Multiple Response; \*Significant.

data of the regression coefficients of the two models obtained. The correlation coefficient obtained was 0.9997, indicating a good correlation between these two models.

These two quadratic models obtained established response surfaces with a great similarity in terms of the experimental conditions of the factors and also of formats, as can be seen in (Fig. 2A and B). The critical values found for the three factors using the two multiple responses are also very similar as shown in Table 7.

## CONCLUSION

Multivariate optimization of methods developed for determination of species by multi-elemental techniques requires compromises between the studied factors to obtain experimental conditions that allow the quantification of all species with a same efficiency. In this context, the multiple response functions are always necessary.

The effect values of the factors calculated by the application of two-level factorial design using the desirability

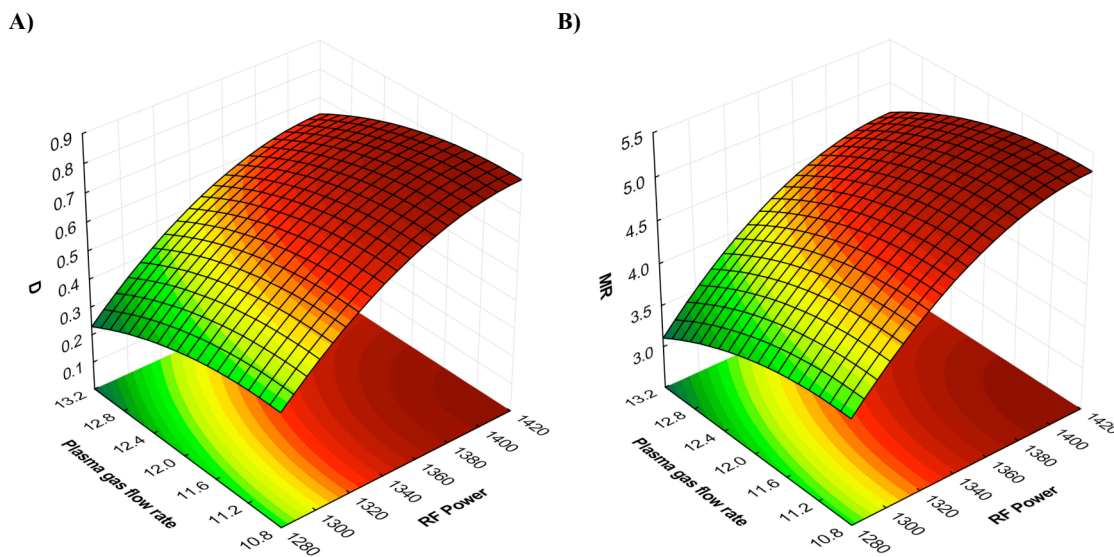


Fig. (2). ?????????????????????????????????.

Table 7. Critical values obtained for Box–Behnken design using individual intensity and multiple responses.

Variable	Experimental domain	Emission intensities						Multiple response	
		B 249.773	Cd 214.438	Cr 283.563	Fe 238.204	Mn 257.611	Zn 213.856	D	MR
P	1300 – 1400	1442.7	1444.3	1448.0	1464.4	1397.6	1403.3	1423.7	1422.5
PF	11.0 – 13.0	9.60	10.43	10.05	10.57	11.24	10.74	10.69	10.65
NF	0.50 – 0.80	0.20	0.38	0.17	0.35	0.57	0.47	0.43	0.42

P – RF power; PF – Plasma gas flow rate; NF – Nebulizer gas flow rate; D – Desirability function; MR – Multiple Response.

function (D) and the function (MR) are similar in terms of sign and magnitude. This way, the interpretation done by data obtained using the desirability function (D) can be perfectly applied for the data achieved by response function (MR).

The regression coefficients found by two quadratic models showed high correlation and the response surfaces obtained have high similarity in terms of formats, confirming the efficiency of the multiple response function (MR) during optimization of analytical strategies involving multi-elemental determinations.

The MR function is very simple and does not require great knowledge in mathematics and computer science and it has been applied in various chemometric tools during optimization of analytical systems involving several multi-elemental determination techniques.

Although the multiple function (MR) has been used by many researchers employing different optimization techniques, this is the first study that reports the comparison of results obtained using the multiple function (MR) and the desirability function (D).

#### CONFLICT OF INTEREST

The authors confirm that this article content has no conflict of interest.

#### ACKNOWLEDGEMENTS

The authors are grateful to Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for providing grants and fellowships as well as financial support for this work.

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