Optimization using central composite design (CCD) of response surface methodology (RSM) for biosorption of hexavalent chromium from aqueous media

The objective of this research paper is to remove hexavalent chromium from aqueous media through batch technique with the use of unmodified biosorbent from Arachis hypogea husk. Design of Experiments (DoE) methodology is applied in the optimization of the independent variables influencing the adsorption process.

The factors (independent variables) examined are: X_1 = contact time (min), X_2 = pH of solution and X_3 = initial Cr(VI) concentration (mg/L). All the factors are continuous. The response (dependent variable) examined is: Y = adsorption capacity (mg/g). The applied DoE method is Circumscribed Central Composite design.

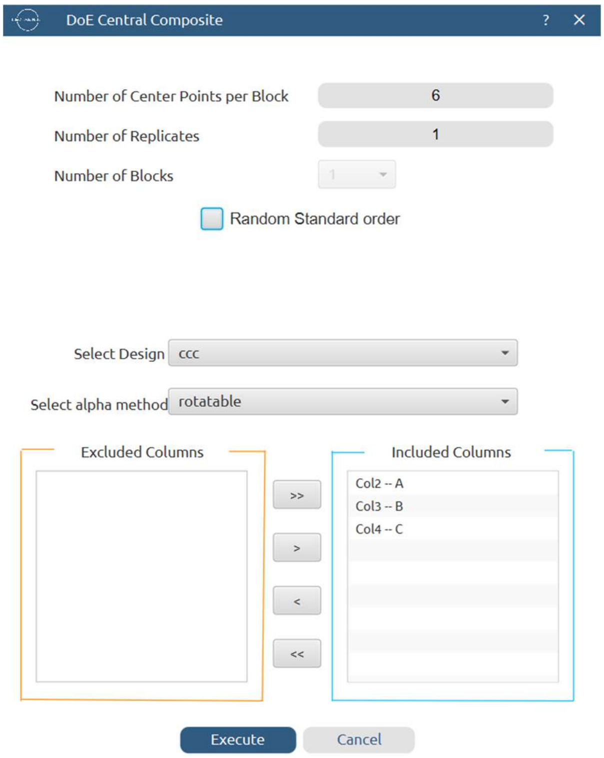
Isalos version used: 2.0.6

Scientific article: https://link.springer.com/article/10.1007/s13201-020-01213-3??utm_source=other_website&error=cookies_not_supported&code=4479f6fd-9544-4729-b4c3-7bc34671094e

Step 1: Central Composite Design

In the first tab named "Action" define the factors in the column headers and fill each column with the low and high levels of the corresponding factors. This tab can be renamed "CCC". Afterwards, apply the Circumscribed Central Composite method: *DOE → Response Surface → Central Composite*

	Col1	Col2 (I)	Col3 (I)	Col4 (I)
User Header	User Row ID	A	B	C
1		60	6	15
2		120	8	50



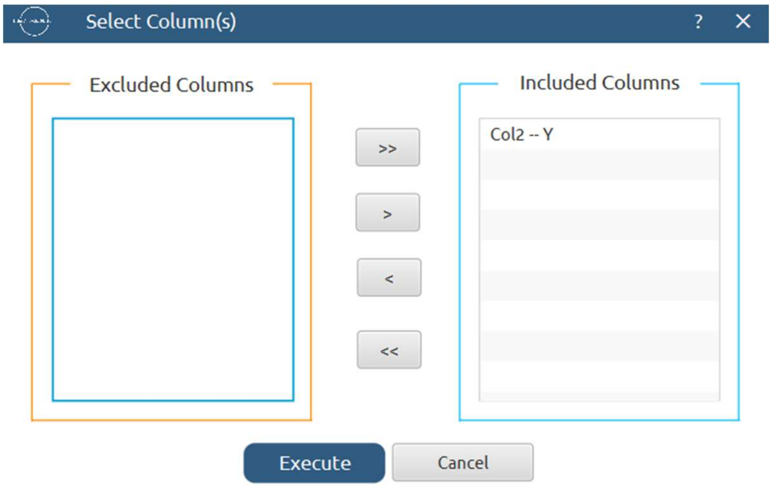
Results (right spreadsheet):

	Col1	Col2 (I)	Col3 (S)	Col4 (S)	Col5 (S)	Col6 (D)	Col7 (D)	Col8 (D)
User Header	User Row ID	Standard Order	Block Number	Replicate Number	Point Type	A	B	C
1		1	Block: 1	Replicate: 1	Design Point	60.0	6.0	15.0
2		2	Block: 1	Replicate: 1	Design Point	120.0	6.0	15.0
3		3	Block: 1	Replicate: 1	Design Point	60.0	8.0	15.0
4		4	Block: 1	Replicate: 1	Design Point	120.0	8.0	15.0
5		5	Block: 1	Replicate: 1	Design Point	60.0	6.0	50.0
6		6	Block: 1	Replicate: 1	Design Point	120.0	6.0	50.0
7		7	Block: 1	Replicate: 1	Design Point	60.0	8.0	50.0
8		8	Block: 1	Replicate: 1	Design Point	120.0	8.0	50.0
9		9	Block: 1	Replicate: 1	Design Point	39.5462151	7.0	32.5
10		10	Block: 1	Replicate: 1	Design Point	140.4537849	7.0	32.5
11		11	Block: 1	Replicate: 1	Design Point	90.0	5.3182072	32.5
12		12	Block: 1	Replicate: 1	Design Point	90.0	8.6817928	32.5
13		13	Block: 1	Replicate: 1	Design Point	90.0	7.0	3.0686255
14		14	Block: 1	Replicate: 1	Design Point	90.0	7.0	61.9313745
15		15	Block: 1	----	Center Point	90.0	7.0	32.5
16		16	Block: 1	----	Center Point	90.0	7.0	32.5
17		17	Block: 1	----	Center Point	90.0	7.0	32.5
18		18	Block: 1	----	Center Point	90.0	7.0	32.5
19		19	Block: 1	----	Center Point	90.0	7.0	32.5
20		20	Block: 1	----	Center Point	90.0	7.0	32.5

Step 2: Definition of response variables

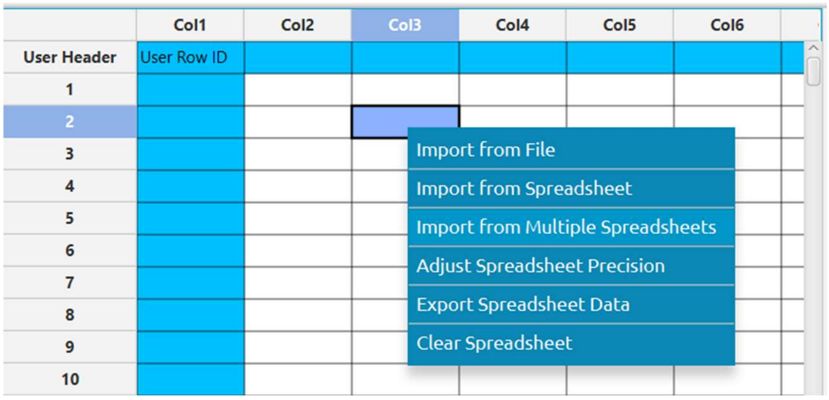
Create a new tab named "Responses" and define the response in the column headers. Fill each column with the values of the response that was observed and make sure the values follow the order of the experiments as given by the Circumscribed Central Composite method. Then, select all columns to be transferred to the right spreadsheet: *Data Transformation → Data Manipulation → Select Column(s)*

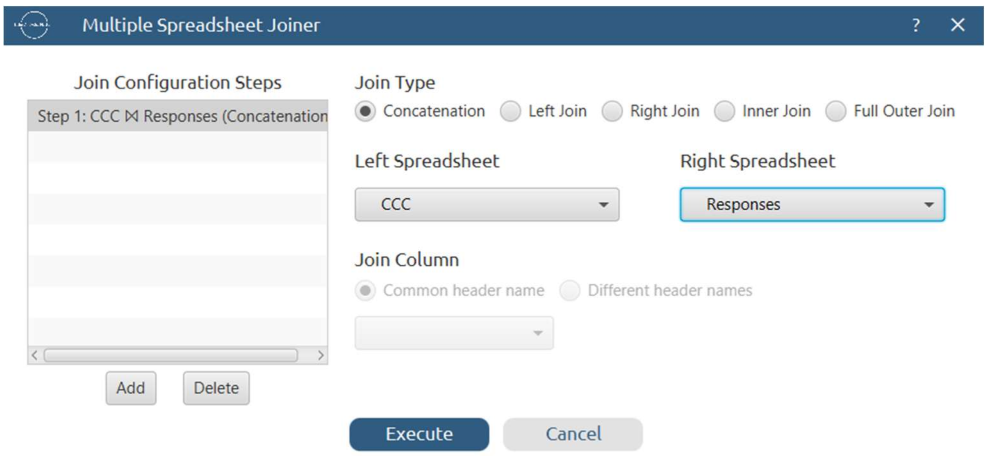
	Col1	Col2 (D)
User Header	User Row ID	Y
1		0.32
2		0.36
3		0.69
4		0.682
5		1.075
6		1.04
7		2.33
8		2.355
9		1.12
10		0.61
11		0.045
12		1.485
13		0.098
14		2.352
15		1.405
16		1.385
17		1.37
18		1.345
19		1.32
20		1.29

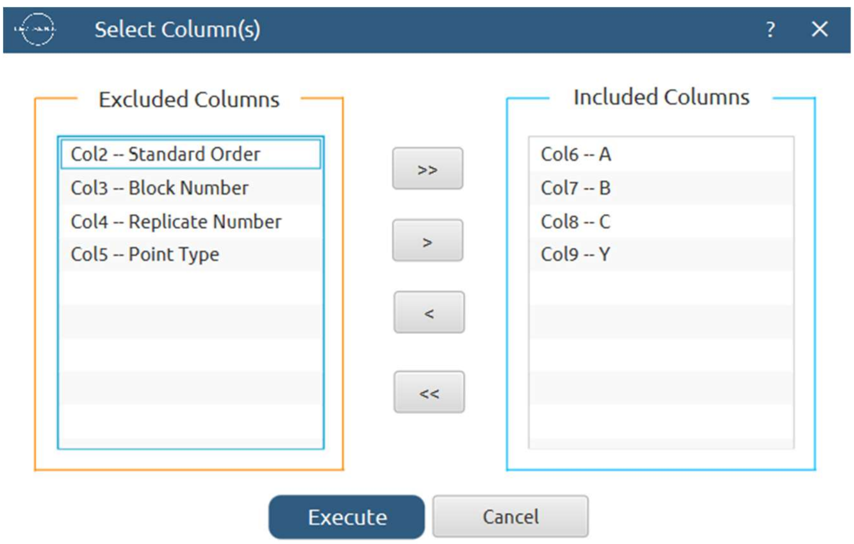


Step 3: Data isolation

Create a new tab named “Data” and import the results from the “CCC” and “Responses” spreadsheets by right clicking on the left spreadsheet. Then, select only the factors and responses columns to be transferred to the right spreadsheet: *Data Transformation → Data Manipulation → Select Column(s)*





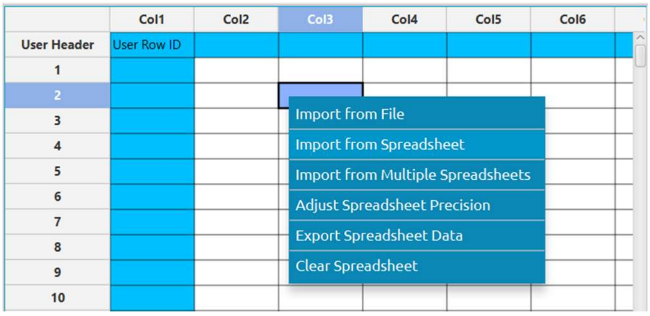


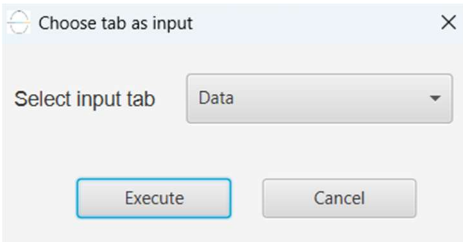
Results:

	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	A	B	C	Y
1		60.0	6.0	15.0	0.32
2		120.0	6.0	15.0	0.36
3		60.0	8.0	15.0	0.69
4		120.0	8.0	15.0	0.682
5		60.0	6.0	50.0	1.075
6		120.0	6.0	50.0	1.04
7		60.0	8.0	50.0	2.33
8		120.0	8.0	50.0	2.355
9		39.5462151	7.0	32.5	1.12
10		140.4537849	7.0	32.5	0.61
11		90.0	5.3182072	32.5	0.045
12		90.0	8.6817928	32.5	1.485
13		90.0	7.0	3.0686255	0.098
14		90.0	7.0	61.9313745	2.352
15		90.0	7.0	32.5	1.405
16		90.0	7.0	32.5	1.385
17		90.0	7.0	32.5	1.37
18		90.0	7.0	32.5	1.345
19		90.0	7.0	32.5	1.32
20		90.0	7.0	32.5	1.29

Step 4: Normalization

Create a new tab named "Normalized data" and import the results from the "Data" spreadsheet. Afterwards, normalize the factor columns to take values in the range [-1.682, 1.682]: *Data Transformation → Normalizers → Min-Max*





Results:

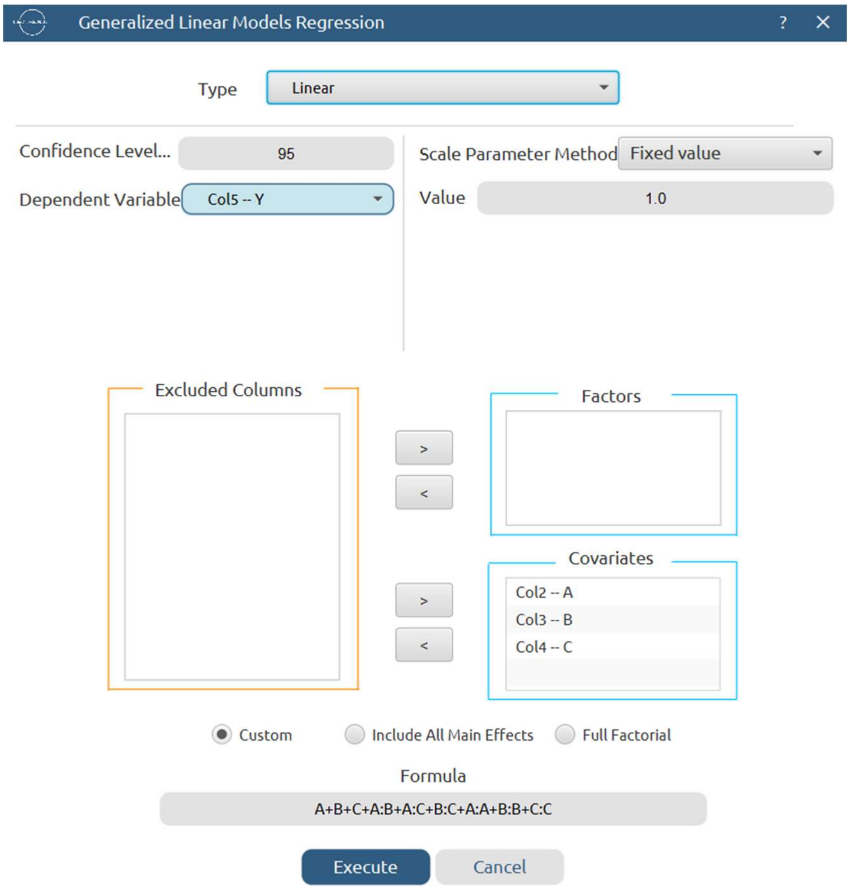
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	A	B	C	Y
1		-1.0001232	-1.0001232	-1.0001232	0.32
2		1.0001232	-1.0001232	-1.0001232	0.36
3		-1.0001232	1.0001232	-1.0001232	0.69
4		1.0001232	1.0001232	-1.0001232	0.682
5		-1.0001232	-1.0001232	1.0001232	1.075
6		1.0001232	-1.0001232	1.0001232	1.04
7		-1.0001232	1.0001232	1.0001232	2.33
8		1.0001232	1.0001232	1.0001232	2.355
9		-1.682	0E-7	0E-7	1.12
10		1.682	0E-7	0E-7	0.61
11		0E-7	-1.682	0E-7	0.045
12		0E-7	1.682	0E-7	1.485
13		0E-7	0E-7	-1.682	0.098
14		0E-7	0E-7	1.682	2.352
15		0E-7	0E-7	0E-7	1.405
16		0E-7	0E-7	0E-7	1.385
17		0E-7	0E-7	0E-7	1.37
18		0E-7	0E-7	0E-7	1.345
19		0E-7	0E-7	0E-7	1.32
20		0E-7	0E-7	0E-7	1.29

Step 5: Regression

The goal here is to produce a regression equation that includes main effects, two-factor interactions and quadratic effects for the response variable Y:

$$Y = b_0 + b_1 A + b_2 B + b_3 C + b_{12} AB + b_{13} AC + b_{23} BC + b_{11} A^2 + b_{22} B^2 + b_{33} C^2$$

Create a new tab named "Regression – Y" and import the results from the spreadsheet "Normalized data". Afterwards, fit a generalized linear model to the data: *Analytics → Regression → Statistical fitting → Generalized Linear Models*



Results:

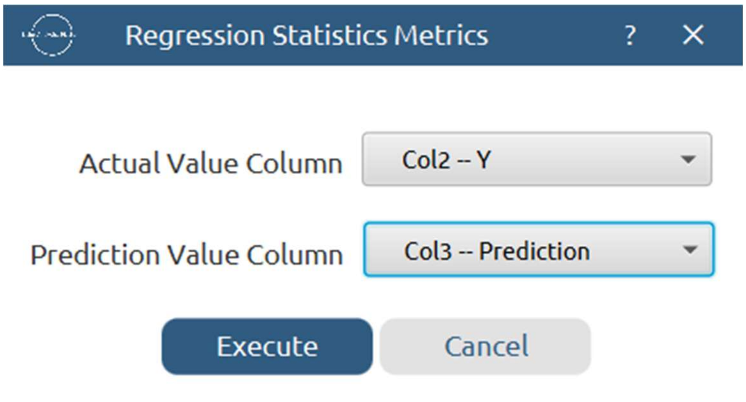
Y	Prediction
0.32	0.2857534
0.36	0.1708658
0.69	0.6456239
0.682	0.5367364
1.075	1.0772260
1.04	0.9413384
2.33	2.3760965
2.355	2.2462090
1.12	1.0690581
0.61	0.8632277
0.045	0.1662055
1.485	1.5660803
0.098	0.2746250
2.352	2.3776608
1.405	1.3467155
1.385	1.3467155
1.37	1.3467155
1.345	1.3467155
1.32	1.3467155
1.29	1.3467155

Goodness of Fit	
	Value
Deviance	0.2128920
Scaled Deviance	0.2128920
Pearson Chi-Square	0.2128920
Scaled Pearson Chi-Square	0.2128920
Log Likelihood	-18.4852167
Akaike's Information Criterion (AIC)	56.9704333
Finite Sample Corrected AIC (AICC)	81.4148777
Bayesian Information Criterion (BIC)	66.9277560
Consistent AIC (CAIC)	76.9277560

Parameter Estimates							
Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value
intercept	1.3467155	0.4078483	0.5473476	2.1460835	10.9032120	1	0.0009600
A	-0.0611862	0.2705647	-0.5914833	0.4691109	0.0511405	1	0.8210905
B	0.4161340	0.2705647	-0.1141631	0.9464311	2.3655063	1	0.1240437
C	0.6251593	0.2705647	0.0948622	1.1554564	5.3387434	1	0.0208565
A*A	-0.1345196	0.2633550	-0.6506859	0.3816467	0.2609084	1	0.6094968
A*B	0.0014996	0.3534663	-0.6912816	0.6942809	0.0000180	1	0.9966149
A*C	-0.0052487	0.3534663	-0.6980299	0.6875325	0.0002205	1	0.9881525
B*B	-0.1698662	0.2633550	-0.6860326	0.3463001	0.4160361	1	0.5189216
B*C	0.2346922	0.3534663	-0.4580890	0.9274734	0.4408605	1	0.5067074
C*C	-0.0072717	0.2633550	-0.5234381	0.5088946	0.0007624	1	0.9779717

Step 6: Regression Metrics

Create a tab named "Metrics – Y" and import the results from the spreadsheet "Regression – Y". Then, produce the regression metrics for the linear regression equation: *Statistics → Model Metrics → Regression Metrics*

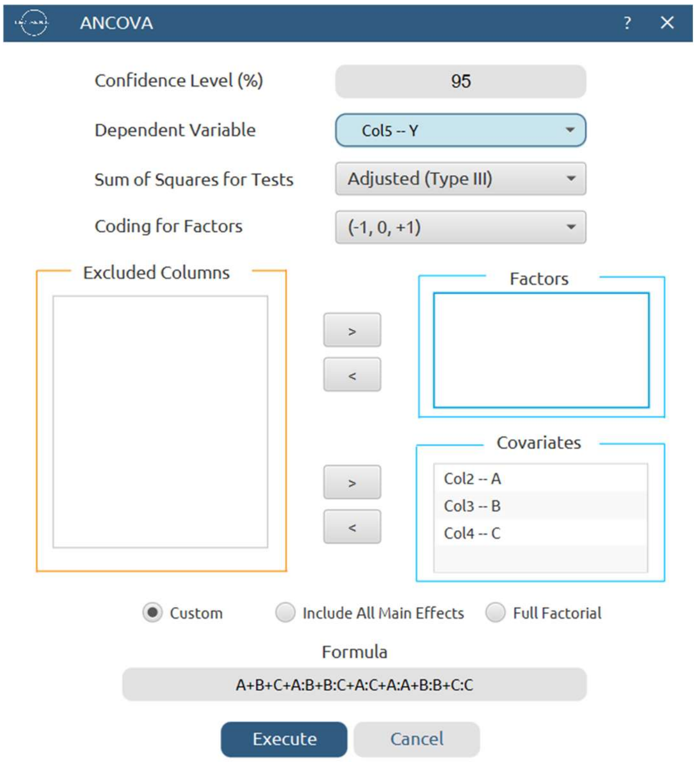


Results:

	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	Mean Squared Error	Root Mean Squared Error	Mean Absolute Error	R Squared
1		0.0106446	0.1031727	0.0791268	0.9764317

Step 7: Analysis of Covariance

Create a new tab named "ANCOVA – Y" and import the results from the spreadsheet "Normalized data". Afterwards perform analysis of covariance for Y using the formula for the quadratic equation: *Statistics → Analysis of (Co)Variance → ANCOVA*

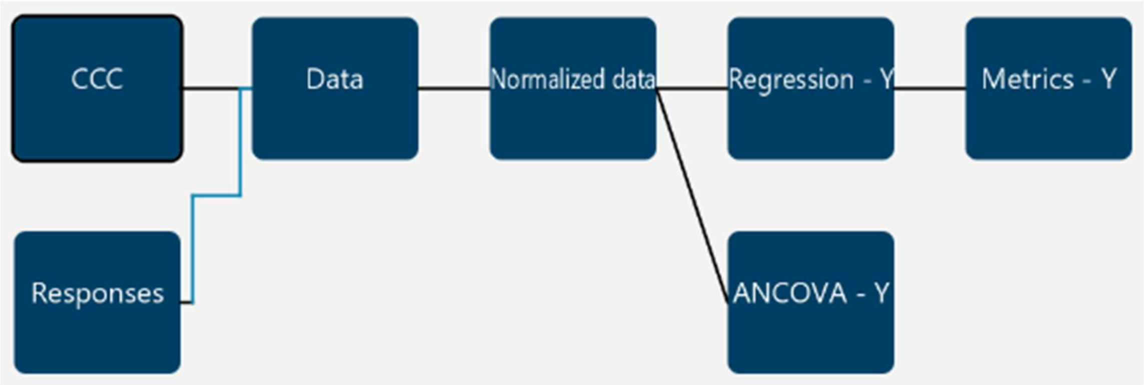


Results:

	Col1	Col2 (S)	Col3 (I)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)
User Header	User Row ID	Source	DF	Adj SS	Adj MS	F-Value	P-Value
1		A	1	0.0511405	0.0511405	2.4021811	0.1522099
2		B	1	2.3655063	2.3655063	111.1129827	0.0000010
3		C	1	5.3387434	5.3387434	250.7724082	0E-7
4		A*B	1	0.0000180	0.0000180	0.0008455	0.9773749
5		B*C	1	0.4408605	0.4408605	20.7081782	0.0010573
6		A*C	1	0.0002205	0.0002205	0.0103574	0.9209501
7		A*A	1	0.2609084	0.2609084	12.2554351	0.0057191
8		B*B	1	0.4160361	0.4160361	19.5421207	0.0012928
9		C*C	1	0.0007624	0.0007624	0.0358124	0.8536891
10		Error	10	0.2128920	0.0212892		
11		Total	19	9.0329905			

Final Isalos Workflow

The final workflow is presented below:



References

(1) Bayuo, J.; Abukari, M. A.; Pelig-Ba, K. B. Optimization Using Central Composite Design (CCD) of Response Surface Methodology (RSM) for Biosorption of Hexavalent Chromium from Aqueous Media. *Appl Water Sci* **2020**, *10* (6), 135. https://doi.org/10.1007/s13201-020-01213-3.