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.

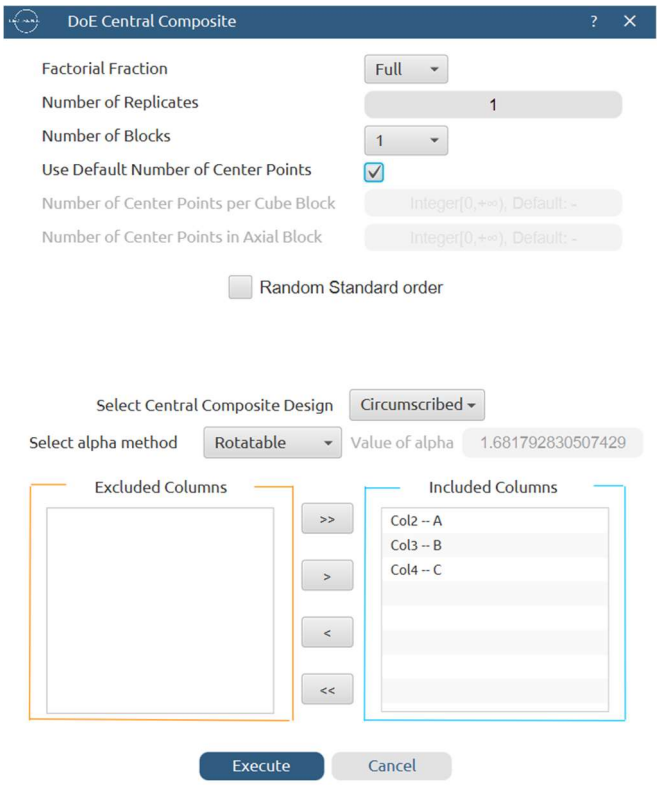
Isalos version used: 2.1.2

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



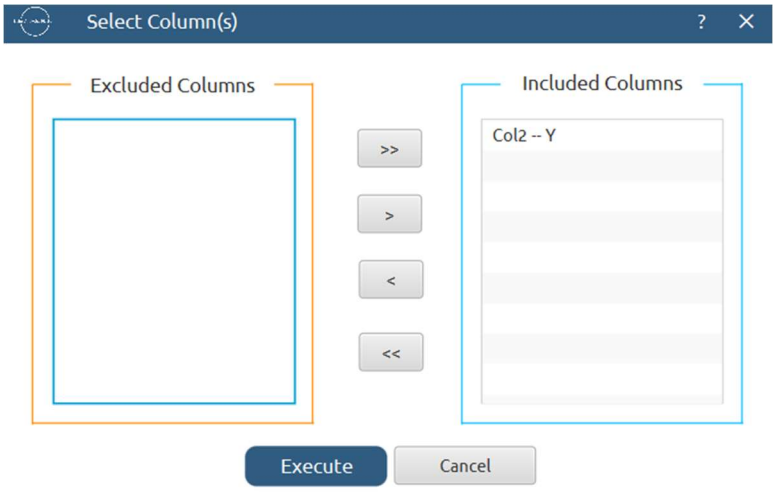
Results (right spreadsheet):

	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	Cube Point	60.0	6.0	15.0
2		2	Block: 1	Replicate: 1	Cube Point	120.0	6.0	15.0
3		3	Block: 1	Replicate: 1	Cube Point	60.0	8.0	15.0
4		4	Block: 1	Replicate: 1	Cube Point	120.0	8.0	15.0
5		5	Block: 1	Replicate: 1	Cube Point	60.0	6.0	50.0
6		6	Block: 1	Replicate: 1	Cube Point	120.0	6.0	50.0
7		7	Block: 1	Replicate: 1	Cube Point	60.0	8.0	50.0
8		8	Block: 1	Replicate: 1	Cube Point	120.0	8.0	50.0
9		9	Block: 1	----	Center Point	90.0	7.0	32.5
10		10	Block: 1	----	Center Point	90.0	7.0	32.5
11		11	Block: 1	----	Center Point	90.0	7.0	32.5
12		12	Block: 1	----	Center Point	90.0	7.0	32.5
13		13	Block: 1	----	Center Point	90.0	7.0	32.5
14		14	Block: 1	----	Center Point	90.0	7.0	32.5
15		15	Block: 1	Replicate: 1	Axial Point	39.5462151	7.0	32.5
16		16	Block: 1	Replicate: 1	Axial Point	140.4537849	7.0	32.5
17		17	Block: 1	Replicate: 1	Axial Point	90.0	5.3182072	32.5
18		18	Block: 1	Replicate: 1	Axial Point	90.0	8.6817928	32.5
19		19	Block: 1	Replicate: 1	Axial Point	90.0	7.0	3.0686255
20		20	Block: 1	Replicate: 1	Axial Point	90.0	7.0	61.9313745

Step 2: Definition of response variables

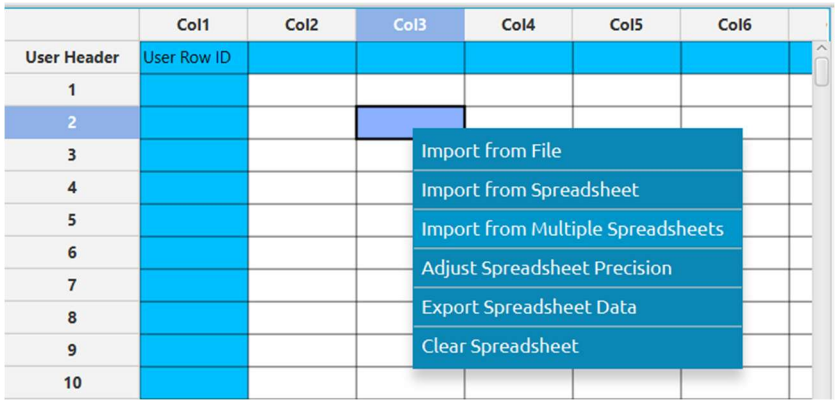
Create a new tab named “Responses” and define the response in the column headers. Fill each column with the values of the response that was observed and make sure the values follow the order of the experiments as given by the Circumscribed Central Composite method. Then, select all columns to be transferred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

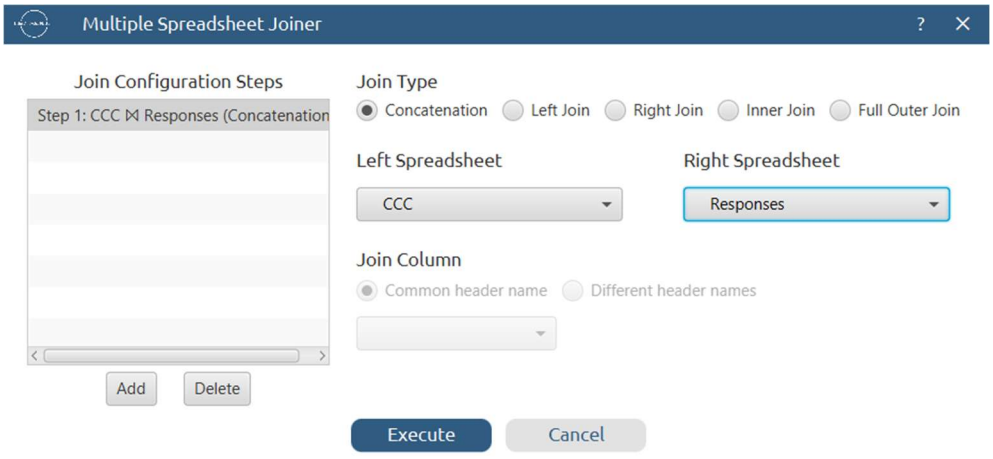
	Col1	Col2 (D)
User Header	User Row ID	Y
1		0.32
2		0.36
3		0.69
4		0.682
5		1.075
6		1.04
7		2.33
8		2.355
9		1.405
10		1.385
11		1.37
12		1.345
13		1.32
14		1.29
15		1.12
16		0.61
17		0.045
18		1.485
19		0.098
20		2.352

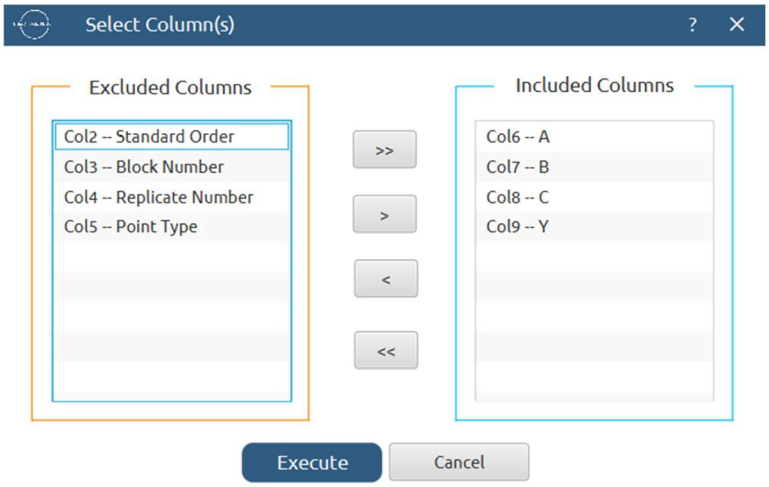


Step 3: Data selection

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)*





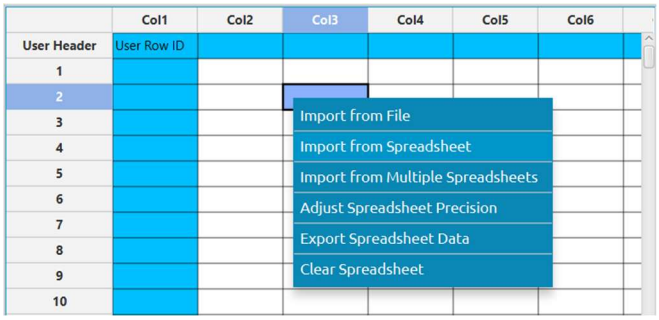


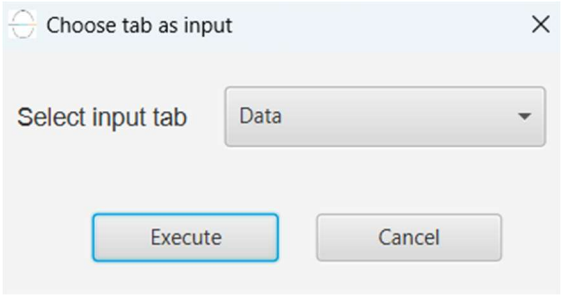
Results:

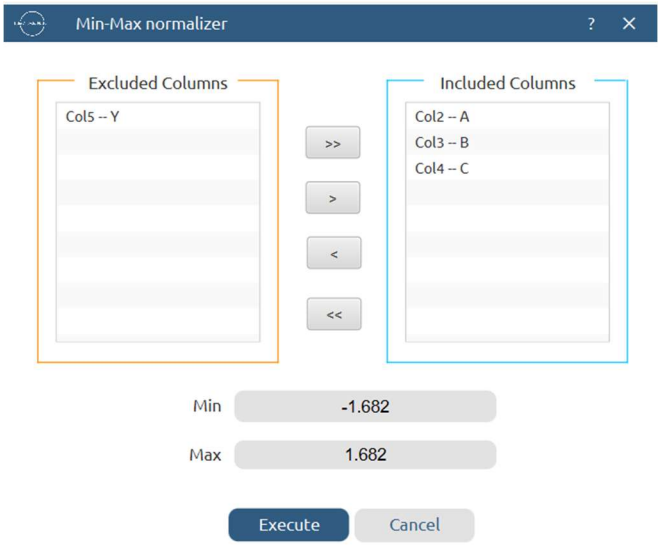
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	A	B	C	Y
1		60.0	6.0	15.0	0.32
2		120.0	6.0	15.0	0.36
3		60.0	8.0	15.0	0.69
4		120.0	8.0	15.0	0.682
5		60.0	6.0	50.0	1.075
6		120.0	6.0	50.0	1.04
7		60.0	8.0	50.0	2.33
8		120.0	8.0	50.0	2.355
9		90.0	7.0	32.5	1.405
10		90.0	7.0	32.5	1.385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

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:

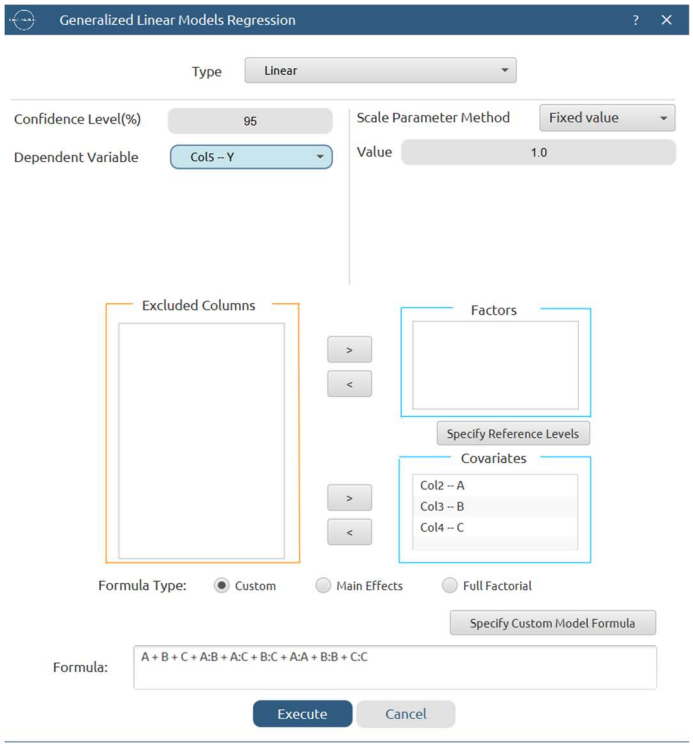
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	A	B	C	Y
1		-1.0001232	-1.0001232	-1.0001232	0.32
2		1.0001232	-1.0001232	-1.0001232	0.36
3		-1.0001232	1.0001232	-1.0001232	0.69
4		1.0001232	1.0001232	-1.0001232	0.682
5		-1.0001232	-1.0001232	1.0001232	1.075
6		1.0001232	-1.0001232	1.0001232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

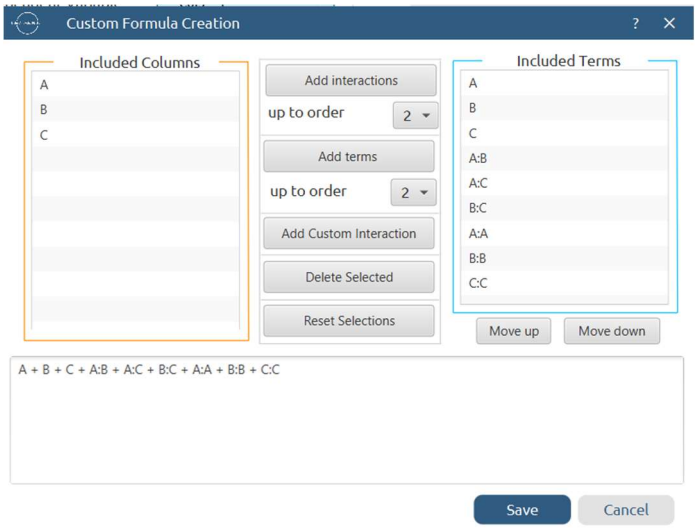
Step 5: Regression

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

$$Y = b_0 + b_1A + b_2B + b_3C + b_{12}AB + b_{13}AC + b_{23}BC + b_{11}A^2 + b_{22}B^2 + b_{33}C^2$$

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
1.405	1.3467155
1.385	1.3467155
1.37	1.3467155
1.345	1.3467155
1.32	1.3467155
1.29	1.3467155
1.12	1.0690581
0.61	0.8632277
0.045	0.1662055
1.485	1.5660803
0.098	0.2746250
2.352	2.3776608

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

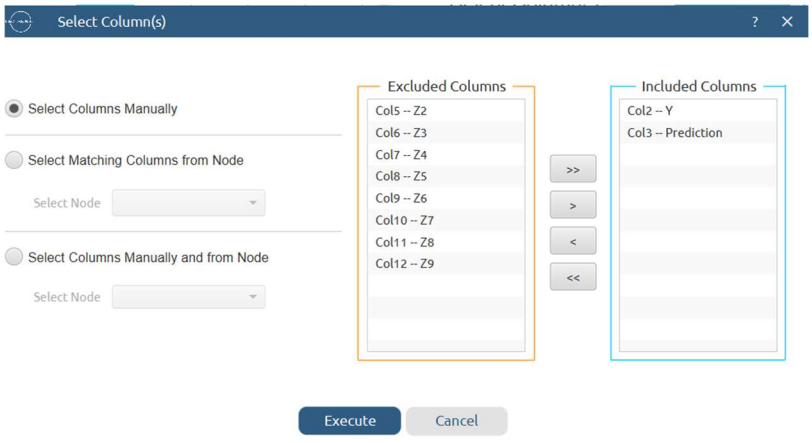
Parameter Estimates							
Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value
intercept	1.3467155	0.4078483	0.5473476	2.1460835	10.9032120	1	0.0009600
A	-0.0611862	0.2705647	-0.5914833	0.4691109	0.0511405	1	0.8210905
B	0.4161340	0.2705647	-0.1141631	0.9464311	2.3655063	1	0.1240437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

Step 6: Data selection for Regression Metrics

Create a tab named “Metrics Data – Y” and import the results from the spreadsheet “Regression – Y”. Next, assign names to all unnamed columns containing data, using names such as Z1–Z9. Then, select only the response column (Y) and the “Prediction” column to be transferred to the right spreadsheet: *Data Transformation* → *Data Manipulation* → *Select Column(s)*

	Col1	Col2 (D)	Col3 (D)	Col4	Col5 (S)	Col6 (S)	Col7 (S)	Col8 (S)	Col9 (S)	Col10 (S)	Col11 (S)	Col12 (S)
User Header	User Row ID	Y	Prediction	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9
1		0.32	0.2857534		Goodness of Fit							
2		0.36	0.1708658			Value						
3		0.69	0.6456239		Deviance	0.2128920						
4		0.682	0.5367364		Scaled Deviance	0.2128920						
5		1.075	1.0772260		Pearson Chi-Square	0.2128920						
6		1.04	0.9413384		Scaled Pearson Chi-Square	0.2128920						
7		2.33	2.3760965		Log Likelihood	-18.4852167						
8		2.355	2.2462090		Akaike's Information Criterion (AIC)	56.9704333						
9		1.405	1.3467155		Finite Sample Corrected AIC (AICC)	81.4148777						
10		1.385	1.3467155		Bayesian Information Criterion (BIC)	66.9277560						
11		1.37	1.3467155		Consistent AIC (CAIC)	76.9277560						
12		1.345	1.3467155									
13		1.32	1.3467155									
14		1.29	1.3467155		Parameter Estimates							
15		1.12	1.0690581		Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value
16		0.61	0.8632277		intercept	1.3467155	0.4078483	0.5473476	2.1460835	10.9032120	1	0.0009600

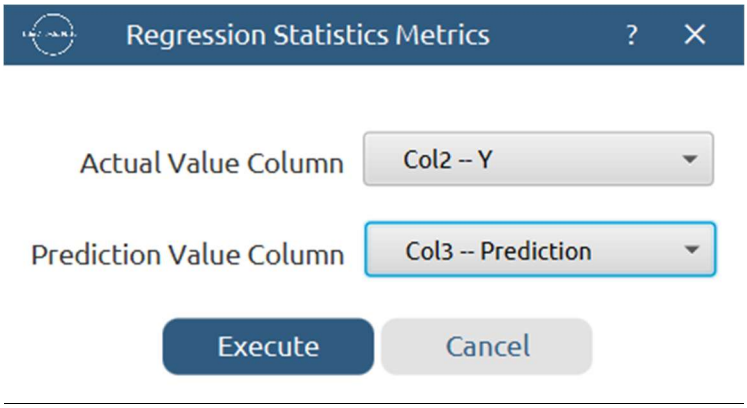
Results:



	Col1	Col2 (D)	Col3 (D)
User Header	User Row ID	Y	Prediction
1		0.32	0.2857534
2		0.36	0.1708658
3		0.69	0.6456239
4		0.682	0.5367364
5		1.075	1.0772260
6		1.04	0.9413384
7		2.33	2.3760965
8		2.355	2.2462090
9		1.405	1.3467155
10		1.385	1.3467155
11		1.37	1.3467155
12		1.345	1.3467155
13		1.32	1.3467155
14		1.29	1.3467155
15		1.12	1.0690581
16		0.61	0.8632277
17		0.045	0.1662055
18		1.485	1.5660803
19		0.098	0.2746250
20		2.352	2.3776608

Step 7: Regression Metrics

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

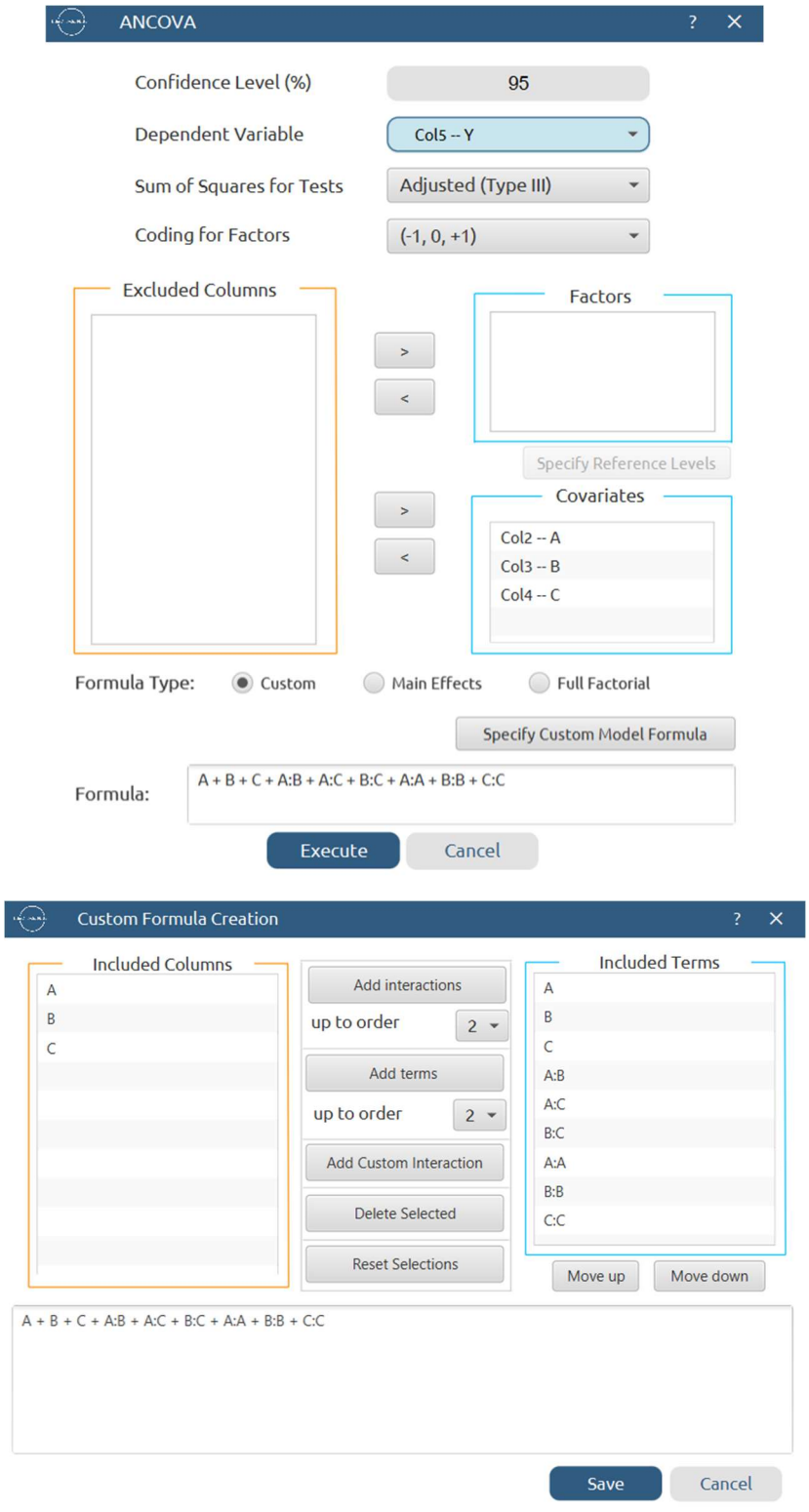


Results:

	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 8: 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*

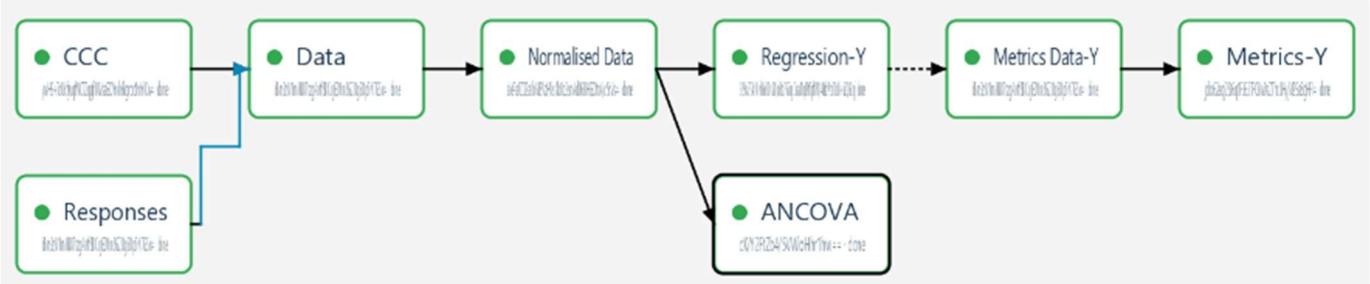


Results:

	Col1	Col2 (S)	Col3 (I)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (S)
User Header	User Row ID	Source	DF	Adj SS	Adj MS	F-Value	P-Value	Significant
1		A	1	0.0511405	0.0511405	2.4021811	0.1522099	No
2		B	1	2.3655063	2.3655063	111.1129827	0.0000010	Yes
3		C	1	5.3387434	5.3387434	250.7724082	0E-7	Yes
4		A*B	1	0.0000180	0.0000180	0.0008455	0.9773749	No
5		A*C	1	0.0002205	0.0002205	0.0103574	0.9209501	No
6		B*C	1	0.4408605	0.4408605	20.7081782	0.0010573	Yes
7		A*A	1	0.2609084	0.2609084	12.2554351	0.0057191	Yes
8		B*B	1	0.4160361	0.4160361	19.5421207	0.0012928	Yes
9		C*C	1	0.0007624	0.0007624	0.0358124	0.8536891	No
10		Error	10	0.2128920	0.0212892			
11		Total	19	9.0329906				

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.