Application of CFD, statistical analysis and DoE for optimising H_2 generation through ammonia borane catalytic hydrolysis: A novel approach for multiobjective optimisation

The objective of this research paper is to study the hydrolysis of ammonia borane with a non-noble metal catalyst to produce H_2. Design of experiments (DoE) methodology is implemented to study the effects of the reaction parameters on the critical response variables. Afterwards, multi-objective optimization is carried out to calculate the factor values which lead the response variables to optimum results.

The factors (independent variables) examined are: X_1 = catalyst to substrate ratio, X_2 = reaction temperature (°C) and X_3 = ammonia borane concentration (mM). All the factors are continuous. The responses (dependent variables) examined are: Y_1 = reaction time (min), Y_2 = turnover frequency (sec^{-1}) and Y_3 = H_2 yield (%). The applied DoE method is Box Behnken design.

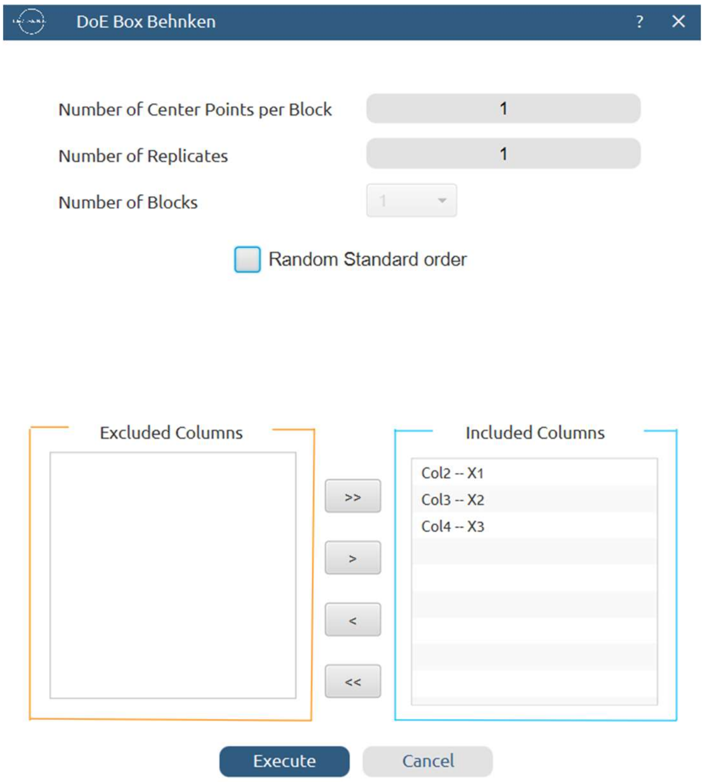
Isalos version used: 2.1.0

Scientific article: https://www.sciencedirect.com/science/article/abs/pii/S1385894725116173

Step 1: Box Behnken 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 “Box Behnken.” Afterwards, apply the Box Behnken method: *DOE → Response Surface → Box Behnken*

	Col1	Col2 (I)	Col3 (I)	Col4 (I)
User Header	User Row ID	X1	X2	X3
1		1000	30	74
2		2000	50	111



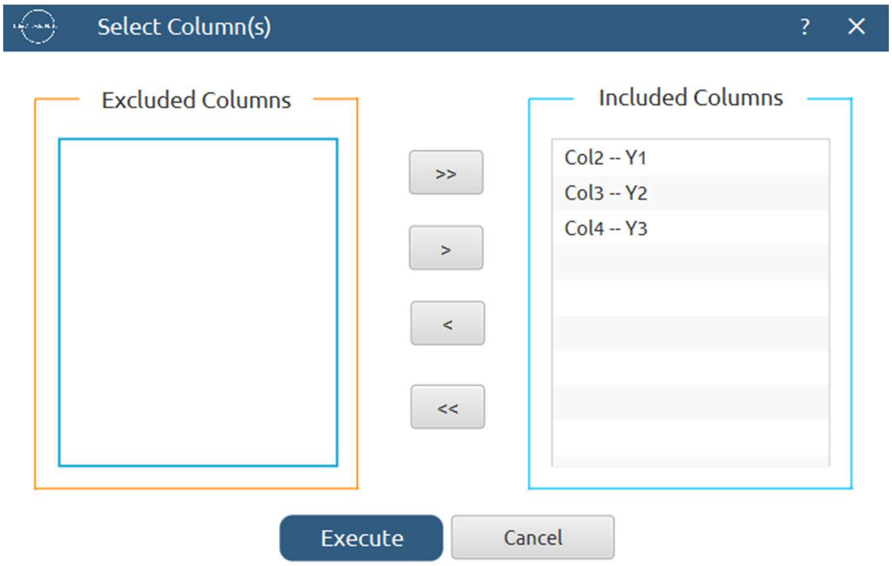
Results (right spreadsheet):

	Col2 (I)	Col3 (S)	Col4 (S)	Col5 (S)	Col6 (D)	Col7 (D)	Col8 (D)
User Header	Standard Order	Block Number	Replicate Number	Point Type	X1	X2	X3
1	1	Block: 1	Replicate: 1	Design Point	1000.0	30.0	92.5
2	2	Block: 1	Replicate: 1	Design Point	2000.0	30.0	92.5
3	3	Block: 1	Replicate: 1	Design Point	1000.0	50.0	92.5
4	4	Block: 1	Replicate: 1	Design Point	2000.0	50.0	92.5
5	5	Block: 1	Replicate: 1	Design Point	1000.0	40.0	74.0
6	6	Block: 1	Replicate: 1	Design Point	2000.0	40.0	74.0
7	7	Block: 1	Replicate: 1	Design Point	1000.0	40.0	111.0
8	8	Block: 1	Replicate: 1	Design Point	2000.0	40.0	111.0
9	9	Block: 1	Replicate: 1	Design Point	1500.0	30.0	74.0
10	10	Block: 1	Replicate: 1	Design Point	1500.0	50.0	74.0
11	11	Block: 1	Replicate: 1	Design Point	1500.0	30.0	111.0
12	12	Block: 1	Replicate: 1	Design Point	1500.0	50.0	111.0
13	13	Block: 1	----	Center Point	1500.0	40.0	92.5

Step 2: Definition of response variables

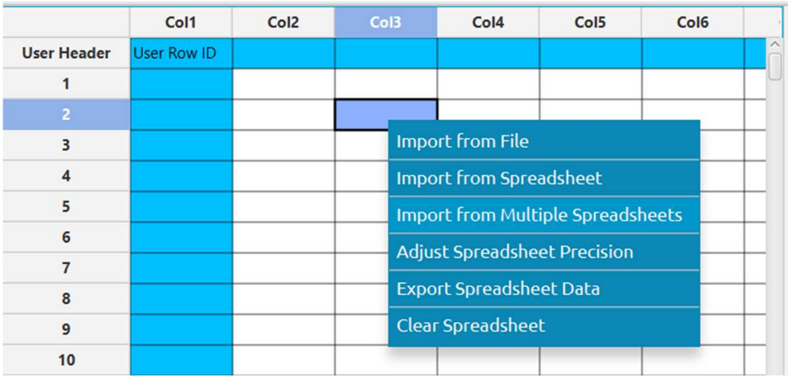
Create a new tab named “Responses” and define the responses in the column headers. Fill each column with the values of the corresponding responses that were observed and make sure the values follow the order of the experiments as given by the Box Behnken method. Then, select all columns to be transferred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

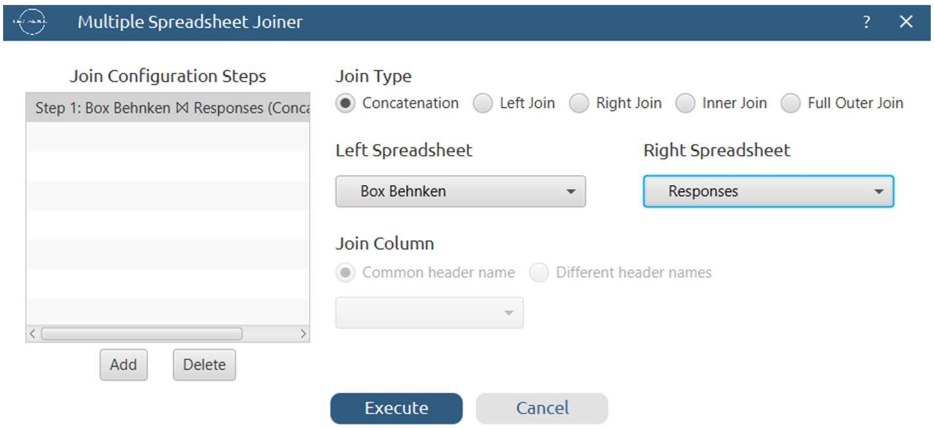
	Col1	Col2 (D)	Col3 (I)	Col4 (D)
User Header	User Row ID	Y1	Y2	Y3
1		95.35	3035	68
2		166.76	2936	55.2
3		15.96	3755	70
4		41.07	2185	67
5		42.1	2526	69
6		83.57	3480	57.7
7		31.64	3075	65.1
8		71.79	2280	54.7
9		206.6	4519	52.7
10		31.4	2754	70.2
11		141.85	3022	70.8
12		23.55	2974	67.7
13		68.8	19375	61.1

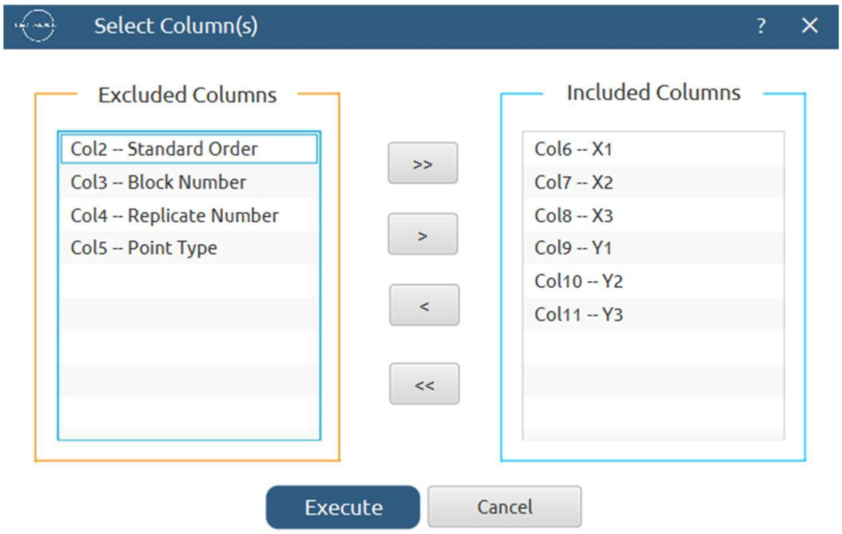


Step 3: Data isolation

Create a new tab named "Data" and import the results from the "Box Behnken" 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)*





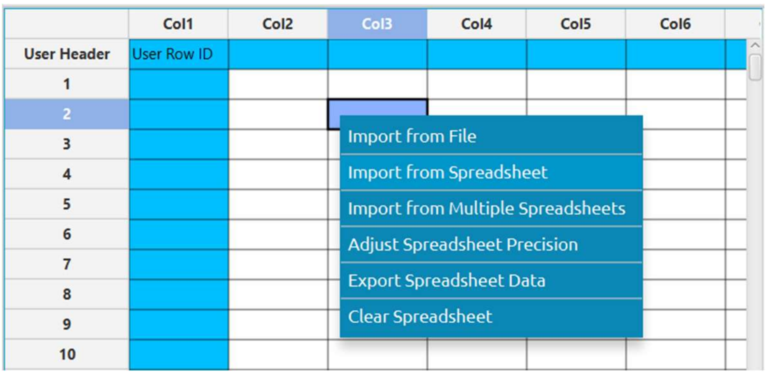


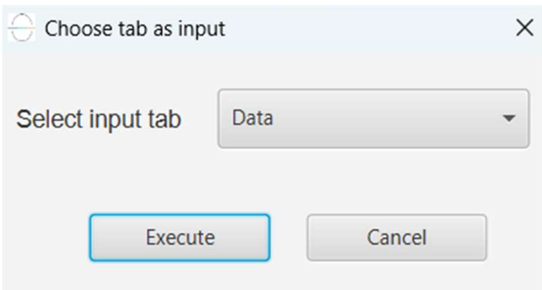
Results:

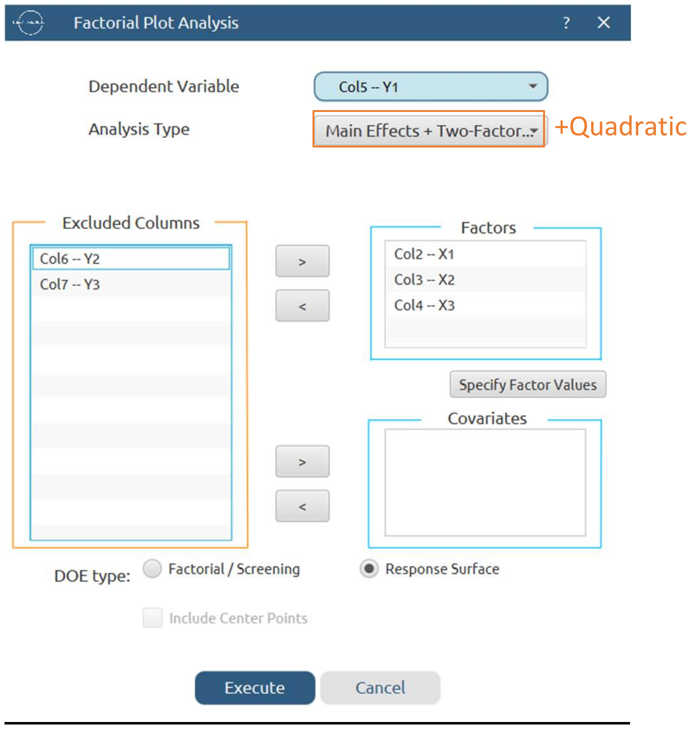
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (I)	Col7 (D)
User Header	User Row ID	X1	X2	X3	Y1	Y2	Y3
1		1000.0	30.0	92.5	95.35	3035	68
2		2000.0	30.0	92.5	166.76	2936	55.2
3		1000.0	50.0	92.5	15.96	3755	70
4		2000.0	50.0	92.5	41.07	2185	67
5		1000.0	40.0	74.0	42.1	2526	69
6		2000.0	40.0	74.0	83.57	3480	57.7
7		1000.0	40.0	111.0	31.64	3075	65.1
8		2000.0	40.0	111.0	71.79	2280	54.7
9		1500.0	30.0	74.0	206.6	4519	52.7
10		1500.0	50.0	74.0	31.4	2754	70.2
11		1500.0	30.0	111.0	141.85	3022	70.8
12		1500.0	50.0	111.0	23.55	2974	67.7
13		1500.0	40.0	92.5	68.8	19375	61.1

Step 4: Factorial Analysis

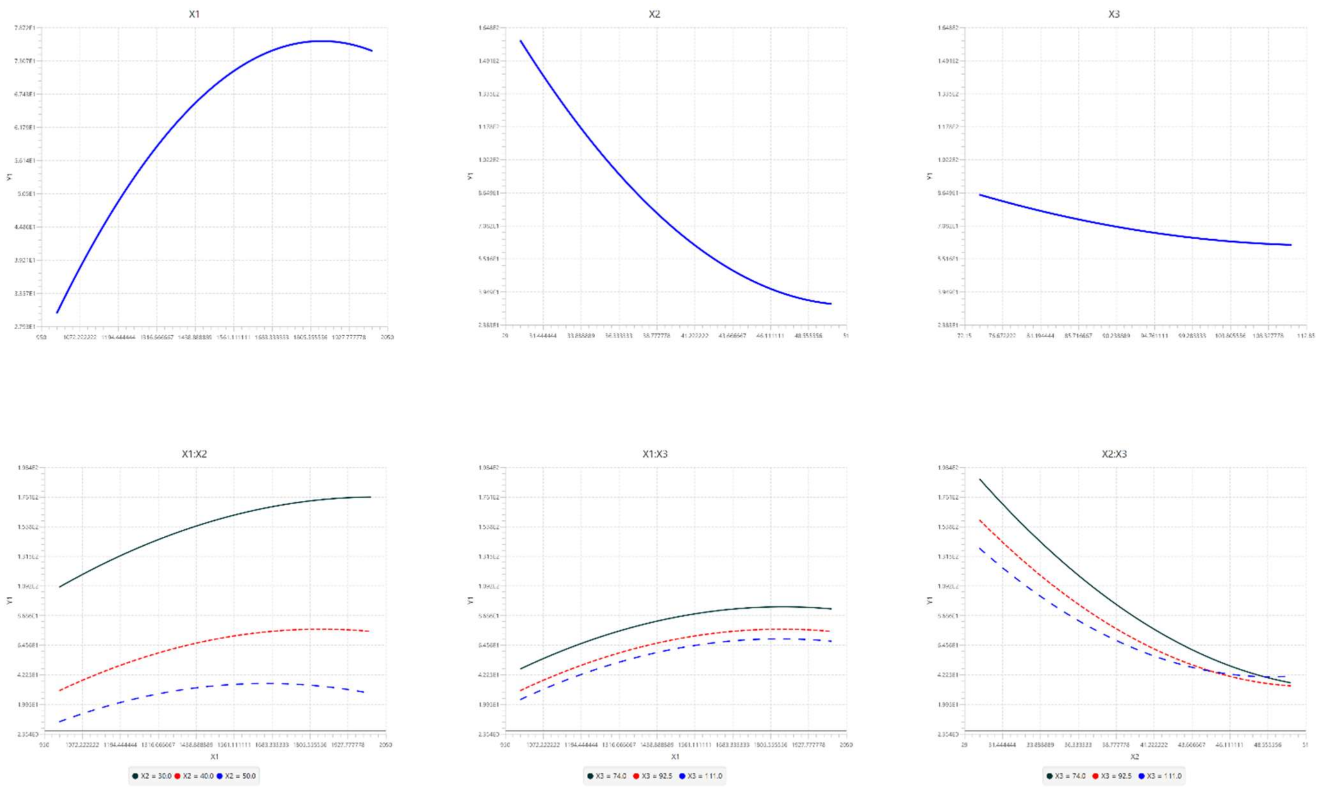
Create a new tab named “Factorial analysis – Y1” and import the results from the “Data” spreadsheet. Afterwards, conduct factorial analysis for the first response variable, Y_1, to produce main effects and interaction plots: *DOE → Post DoE Analysis → Factorial Plot Analysis*



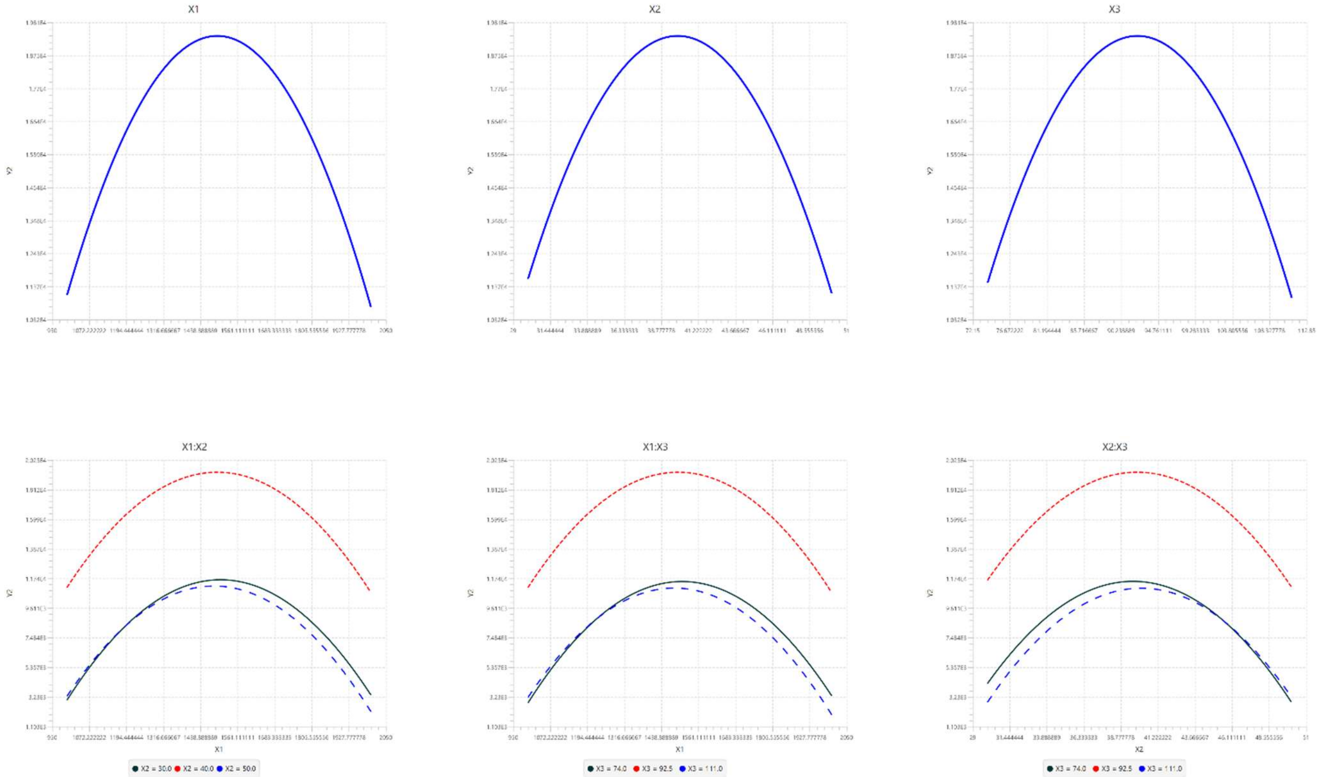




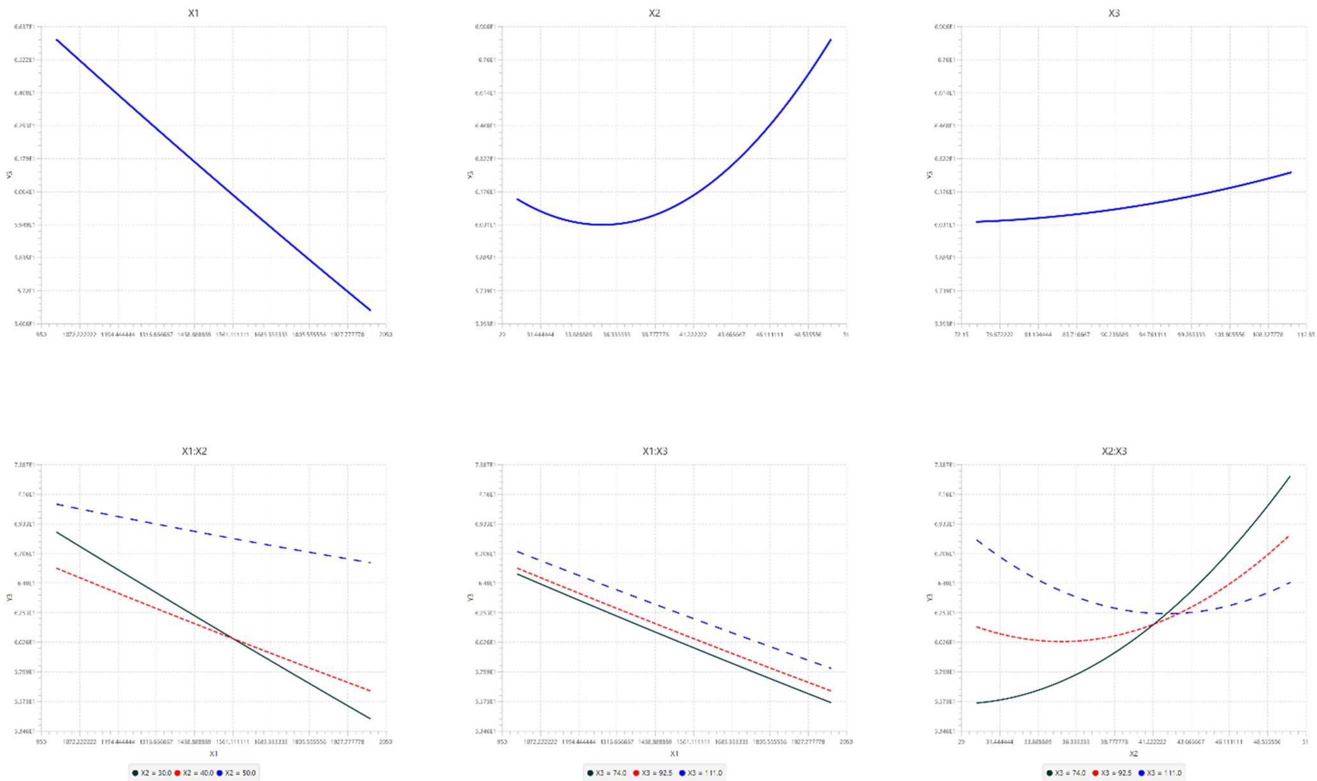
Results (also given in table format, not displayed here):



Repeat this step for the rest of the response variables. Results, Y_2:

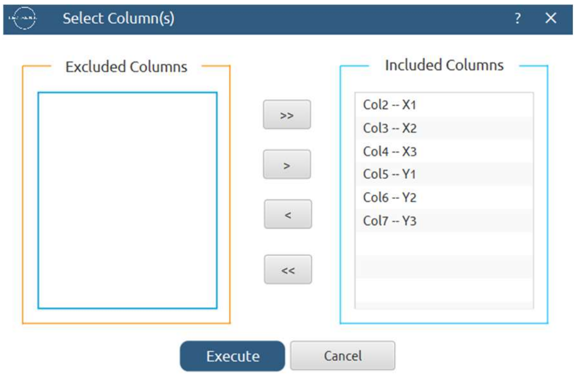


Results, Y_3:



Step 5: Define additional experimental points

Create a new tab named “Full data” and import the results from the “Data” spreadsheet. Then, add in each column the values of the additional experimental runs that were executed and select all the columns to be transferred to the right spreadsheet: <u>*Data Transformation → Data Manipulation → Select Column(s)*</u>

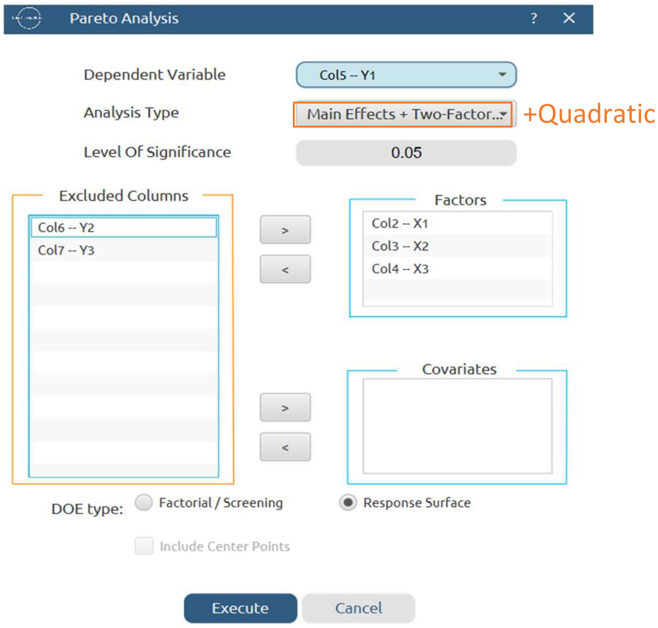


Results:

	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (I)	Col7 (D)
User Header	User Row ID	X1	X2	X3	Y1	Y2	Y3
1		1000.0	30.0	92.5	95.35	3035	68
2		2000.0	30.0	92.5	166.76	2936	55.2
3		1000.0	50.0	92.5	15.96	3755	70
4		2000.0	50.0	92.5	41.07	2185	67
5		1000.0	40.0	74.0	42.1	2526	69
6		2000.0	40.0	74.0	83.57	3480	57.7
7		1000.0	40.0	111.0	31.64	3075	65.1
8		2000.0	40.0	111.0	71.79	2280	54.7
9		1500.0	30.0	74.0	206.6	4519	52.7
10		1500.0	50.0	74.0	31.4	2754	70.2
11		1500.0	30.0	111.0	141.85	3022	70.8
12		1500.0	50.0	111.0	23.55	2974	67.7
13		1500.0	40.0	92.5	68.8	19375	61.1
14		1000	50	74	20.48	2628	74
15		1000	50	111	22.4	2951	61.9
16		2000	50	74	40.97	2749	74.7
17		1000	30	74	67.02	637	65.8
18		1000	35	74	57.21	1775	76
19		1000	45	74	27.79	2080	73.5
20		2000	50	111	45.4	1008	64.7
21		1000	30	111	87.7	2913	60.8

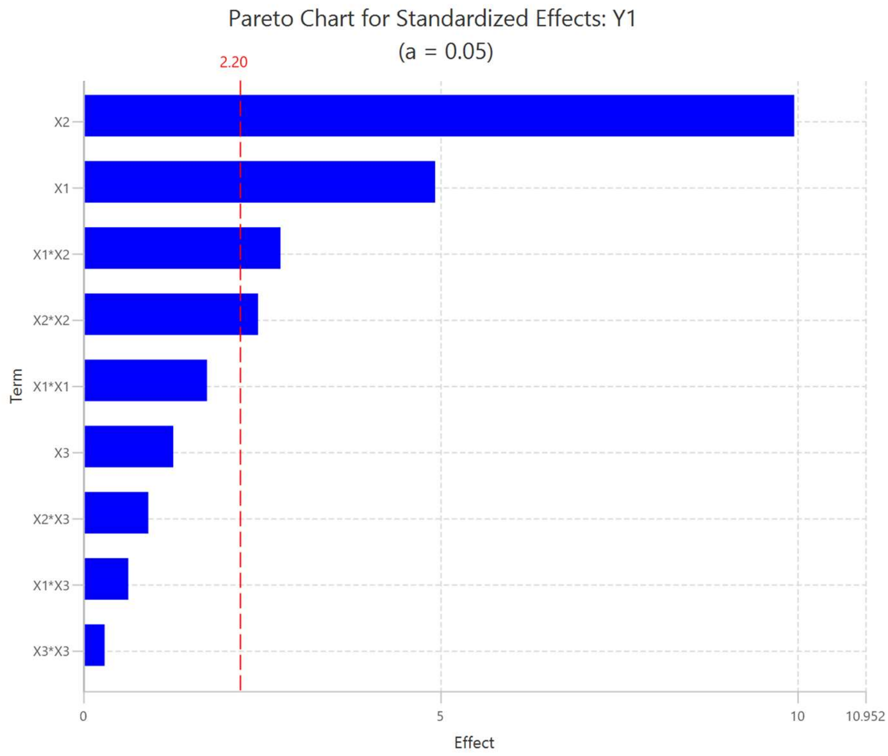
Step 6: Pareto Analysis

Create a new tab named “Pareto analysis – Y1” and import the results from the “Full data” spreadsheet. Afterwards, conduct pareto analysis for the first response variable, Y_1: *DOE → Post DoE Analysis → Pareto Analysis*



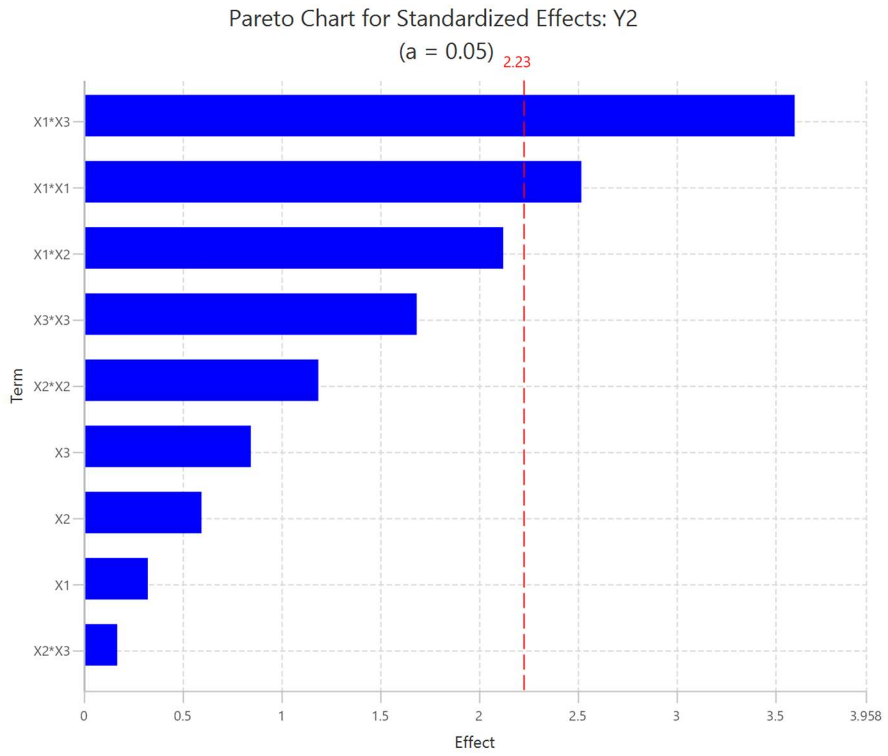
Results:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		X2	9.9562015
3		X1	4.9272968
4		X1*X2	2.7611431
5		X2*X2	2.4477405
6		X1*X1	1.7325479
7		X3	1.2596017
8		X2*X3	0.9104352
9		X1*X3	0.6306287
10		X3*X3	0.2984454
11		Significance Value	2.2009852



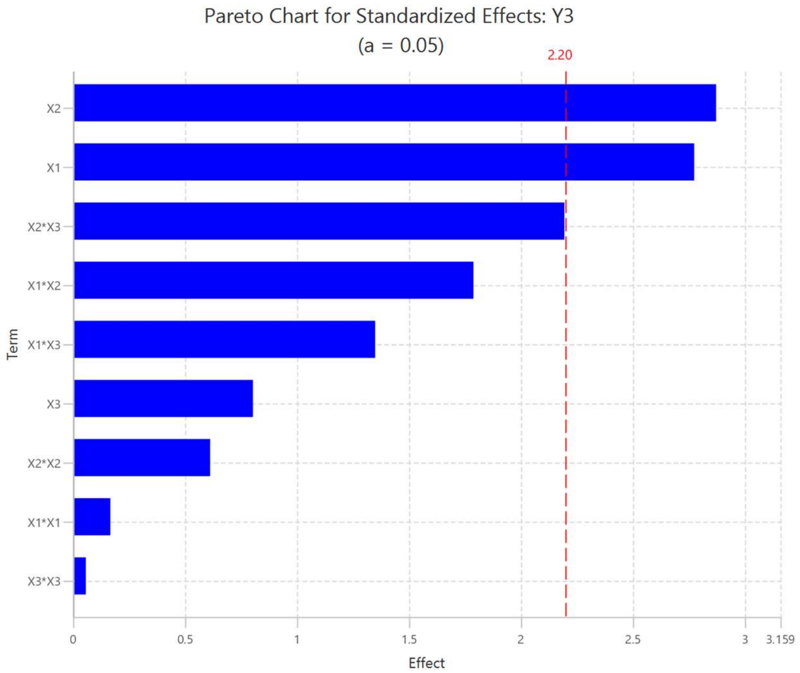
Repeat this step for the rest of the response variables. The experimental point (1500, 40, 92.5) is not included in the analysis of Y_2. Results, Y_2:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		X1*X3	3.5978633
3		X1*X1	2.5183154
4		X1*X2	2.1227279
5		X3*X3	1.6849455
6		X2*X2	1.1867544
7		X3	0.8451740
8		X2	0.5954917
9		X1	0.3239851
10		X2*X3	0.1689221
11		Significance Value	2.2281389



Results, Y_3:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		X2	2.8715101
3		X1	2.7737042
4		X2*X3	2.1939092
5		X1*X2	1.7877166
6		X1*X3	1.3488904
7		X3	0.8032723
8		X2*X2	0.6122096
9		X1*X1	0.1664083
10		X3*X3	0.0569245
11		Significance Value	2.2009852

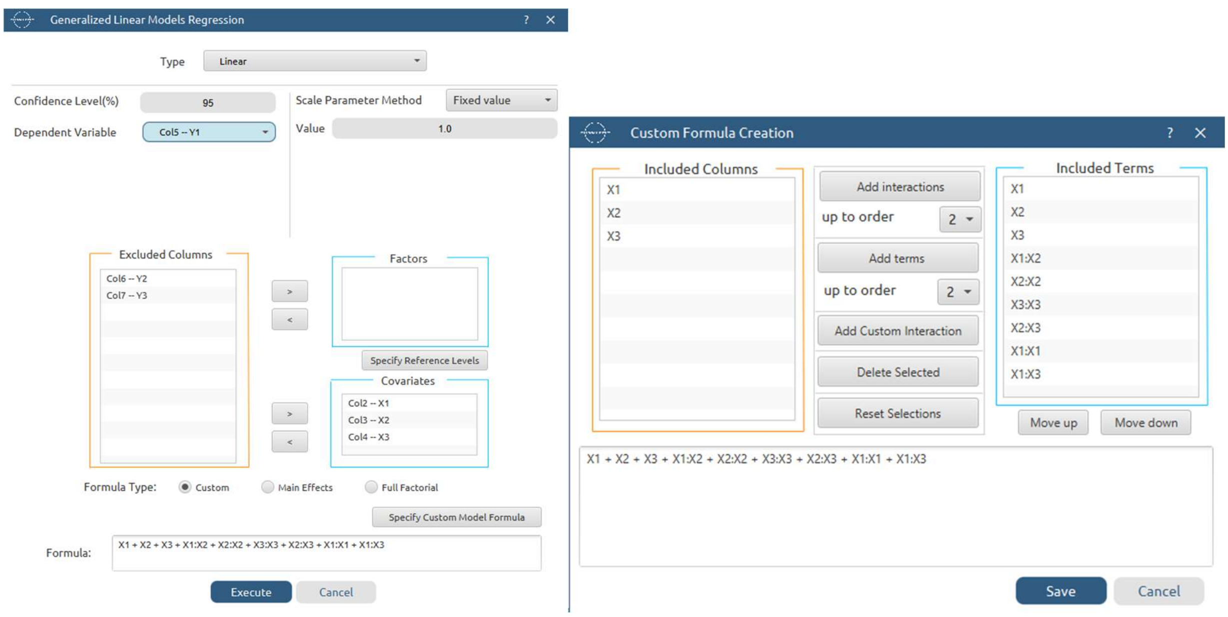


Step 7: Regression

The goal here is to produce a regression equation that includes main effects, two-factor interactions, and quadratic effects for Y_1:

$$Y = b_0 + b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{11}{X_1}^2 + b_{22}{X_2}^2 + b_{33}{X_3}^2$$

Create a new tab named “Regression – Y1” and import the results from the spreadsheet “Full data”. Afterwards, fit a generalized linear model to the data: _Analytics → Regression → Statistical fitting → Generalized Linear Models_



Results:

Y1	Prediction
95.35	89.2177719
166.76	178.7443840
15.96	15.4639319
41.07	32.2093374
42.1	33.6057753
83.57	94.4561775
31.64	28.1189956
71.79	73.5406111
206.6	167.3378175
31.4	45.8110682
141.85	142.7543384
23.55	43.9922011
68.8	72.3045748
20.48	15.6115763
22.4	21.5071025
40.97	40.0713752
67.02	100.7477223
57.21	61.0332803
27.79	18.4652073
45.4	30.5381147
87.7	83.8786366

Goodness of Fit	
	Value
Deviance	4146.2045278
Scaled Deviance	4146.2045278
Pearson Chi-Square	4146.2045278
Scaled Pearson Chi-Square	4146.2045278
Log Likelihood	-2092.399973 1
Akaike's Information Criterion (AIC)	4204.7999462
Finite Sample Corrected AIC (AICC)	4226.7999462
Bayesian Information Criterion (BIC)	4215.2451705
Consistent AIC (CAIC)	4225.2451705

Parameter Estimates							
Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value
intercept	392.3547113	18.6186338	355.8628595	428.8465630	444.0809286	1	0.0
X1	0.4529055	0.0071356	0.4389200	0.4668910	4028.6161623	1	0.0
X2	-22.5533074	0.4407998	-23.4172591	-21.6893556	2617.8074820	1	0.0
X3	-2.6350099	0.2972705	-3.2176493	-2.0523706	78.5707707	1	0.0
X1*X3	-0.0004170	0.0000341	-0.0004837	-0.0003502	149.9013141	1	0.0
X1*X2	-0.0036391	0.0000679	-0.0037721	-0.0035060	2873.6632037	1	0.0
X2*X3	0.0307630	0.0017404	0.0273519	0.0341741	312.4324160	1	0.0
X1*X1	-0.0000719	0.0000021	-0.0000761	-0.0000677	1131.4322093	1	0.0
X2*X2	0.2457387	0.0051711	0.2356037	0.2558738	2258.3371856	1	0.0
X3*X3	0.0090443	0.0015609	0.0059849	0.0121036	33.5728150	1	0E-7

Repeat this step for the rest of the response variables. The experimental point (1500, 40, 92.5) is not included in the analysis of Y_2. Results, Y_2:

Y2	Prediction
3035	2696.0043892
2936	3465.4795703
3755	3368.2504530
2185	2381.2655875
2526	2270.3732991
3480	3511.5630470
3075	3348.6932852
2280	1889.9938528
4519	3523.6857780
2754	3382.4388261
3022	3316.7981815
2974	3046.0772145
2628	2175.0423474
2951	3188.6253260
2749	2538.0020720
637	1438.0592760
1775	1970.1719094
2080	2338.6634451
1008	851.6958703
2913	2581.1162697

Goodness of Fit	
	Value
Deviance	3541832.0924195
Scaled Deviance	3541832.0924195
Pearson Chi-Square	3541832.0924195
Scaled Pearson Chi-Square	3541832.0924195
Log Likelihood	-1770934.4249804
Akaike's Information Criterion (AIC)	3541888.8499608
Finite Sample Corrected AIC (AICC)	3541913.2944053
Bayesian Information Criterion (BIC)	3541898.8072836
Consistent AIC (CAIC)	3541908.8072836

Parameter Estimates							
Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value
intercept	-44134.5085994	26.9079658	-44187.2472433	-44081.7699556	2690263.7312914	1	0.0
X1	22.4648876	0.0084613	22.4483037	22.4814715	7049092.9334033	1	0.0
X2	508.6775473	0.5372784	507.6245011	509.7305936	896368.1553165	1	0.0
X3	480.1483655	0.3780336	479.4074332	480.8892978	1613206.6235688	1	0.0
X1*X1	-0.0041037	0.0000027	-0.0041090	-0.0040983	2246198.9621478	1	0.0
X2*X2	-4.6382249	0.0065672	-4.6510963	-4.6253535	498826.6379509	1	0.0
X3*X3	-2.0056000	0.0020001	-2.0095201	-2.0016800	1005540.7389801	1	0.0
X1*X2	-0.0878230	0.0000695	-0.0879593	-0.0876867	1595940.2598834	1	0.0
X1*X3	-0.0729700	0.0000341	-0.0730368	-0.0729032	4584767.2486655	1	0.0
X2*X3	-0.1749649	0.0017404	-0.1783760	-0.1715538	10106.4983269	1	0.0

Results, Y_3:

Y3	Prediction
68	67.3607889
55.2	53.2337082
70	69.5287257
67	67.8510157
69	69.9567461
57.7	57.6949867
65.1	63.3732505
54.7	59.8302191
52.7	58.0861479
70.2	73.7251030
70.8	63.1083492
67.7	64.2546384
61.1	63.3257615
74	76.2876595
61.9	62.4578309
74.7	70.2505855
65.8	66.8733898
76	68.0091233
73.5	72.7162582
64.7	65.1394849
60.8	67.5362271

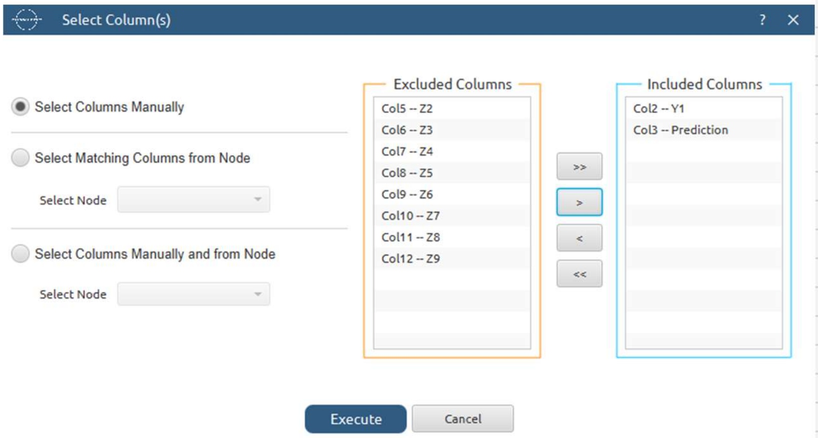
Goodness of Fit	
	Value
Deviance	289.3926652
Scaled Deviance	289.3926652
Pearson Chi-Square	289.3926652
Scaled Pearson Chi-Square	289.3926652
Log Likelihood	-163.9940418
Akaike's Information Criterion (AIC)	347.9880836
Finite Sample Corrected AIC (AICC)	369.9880836
Bayesian Information Criterion (BIC)	358.4333080
Consistent AIC (CAIC)	368.4333080

Parameter Estimates							
Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value
intercept	79.5115722	18.6186338	43.0197205	116.0034239	18.2374897	1	0.0000195
X1	-0.0491262	0.0071356	-0.0631117	-0.0351407	47.3987499	1	0E-7
X2	-0.0015113	0.4407998	-0.8654630	0.8624404	0.0000118	1	0.9972644
X3	0.4541275	0.2972705	-0.1285119	1.0367669	2.3337381	1	0.1265975
X1*X3	0.0002356	0.0000341	0.0001689	0.0003024	47.8683153	1	0E-7
X1*X2	0.0006225	0.0000679	0.0004894	0.0007555	84.0798952	1	0.0
X2*X3	-0.0195847	0.0017404	-0.0229958	-0.0161736	126.6286996	1	0.0
X1*X1	-0.0000018	0.0000021	-0.0000060	0.0000024	0.7285252	1	0.3933616
X2*X2	0.0162378	0.0051711	0.0061027	0.0263729	9.8604136	1	0.0016887
X3*X3	-0.0004558	0.0015609	-0.0035151	0.0026036	0.0852496	1	0.7703054

Step 8: Data isolation for Regression Metrics

Create a tab named "Metrics Data – Y1" and import the results from the spreadsheet "Regression – Y1". Next, assign names to all unnamed columns containing data, using names such as Z1–Z9. Then, select only the response column (Y1) 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	Y1	Prediction	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9
1		95.35	89.2177719		Goodness of Fit							
2		166.76	178.7443840			Value						
3		15.96	15.4639319		Deviance	4146.2045278						
4		41.07	32.2093374		Scaled Deviance	4146.2045278						
5		42.1	33.6057753		Pearson Chi-Square	4146.2045278						
6		83.57	94.4561775		Scaled Pearson Chi-Square	4146.2045278						
7		31.64	28.1189956		Log Likelihood	-2092.3999731						
8		71.79	73.5406111		Akaike's Information Criterion (AIC)	4204.7999462						
9		206.6	167.3378175		Finite Sample Corrected AIC (AICC)	4226.7999462						
10		31.4	45.8110682		Bayesian Information Criterion (BIC)	4215.2451705						
11		141.85	142.7543384		Consistent AIC (CAIC)	4225.2451705						
12		23.55	43.9922011									
13		68.8	72.3045748									
14		20.48	15.6115763		Parameter Estimates							
15		22.4	21.5071025		Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value



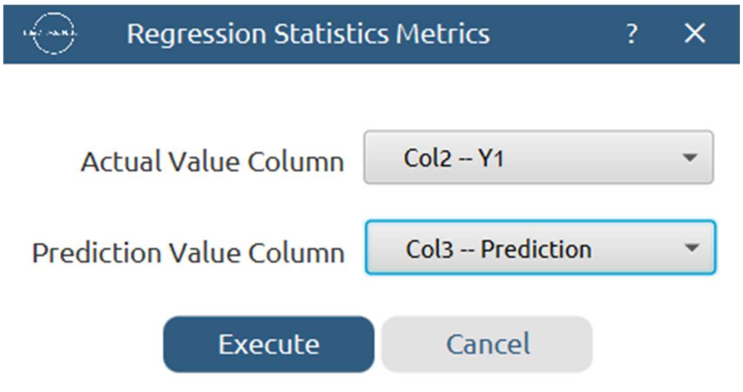
Results:

	Col1	Col2 (D)	Col3 (D)
User Header	User Row ID	Y1	Prediction
1		95.35	89.2177719
2		166.76	178.7443840
3		15.96	15.4639319
4		41.07	32.2093374
5		42.1	33.6057753
6		83.57	94.4561775
7		31.64	28.1189956
8		71.79	73.5406111
9		206.6	167.3378175
10		31.4	45.8110682
11		141.85	142.7543384
12		23.55	43.9922011
13		68.8	72.3045748
14		20.48	15.6115763
15		22.4	21.5071025
16		40.97	40.0713752
17		67.02	100.7477223
18		57.21	61.0332803
19		27.79	18.4652073
20		45.4	30.5381147
21		87.7	83.8786366

Repeat this step for the rest of the response variables.

Step 9: Regression Metrics

Create a tab named "Metrics – Y1" and import the results from the spreadsheet "Metrics Data – Y1". Then, produce the regression metrics for the Y_1 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		197.4383108	14.0512743	9.6604150	0.9199492

Repeat this step for the rest of the response variables. Results, Y_2:

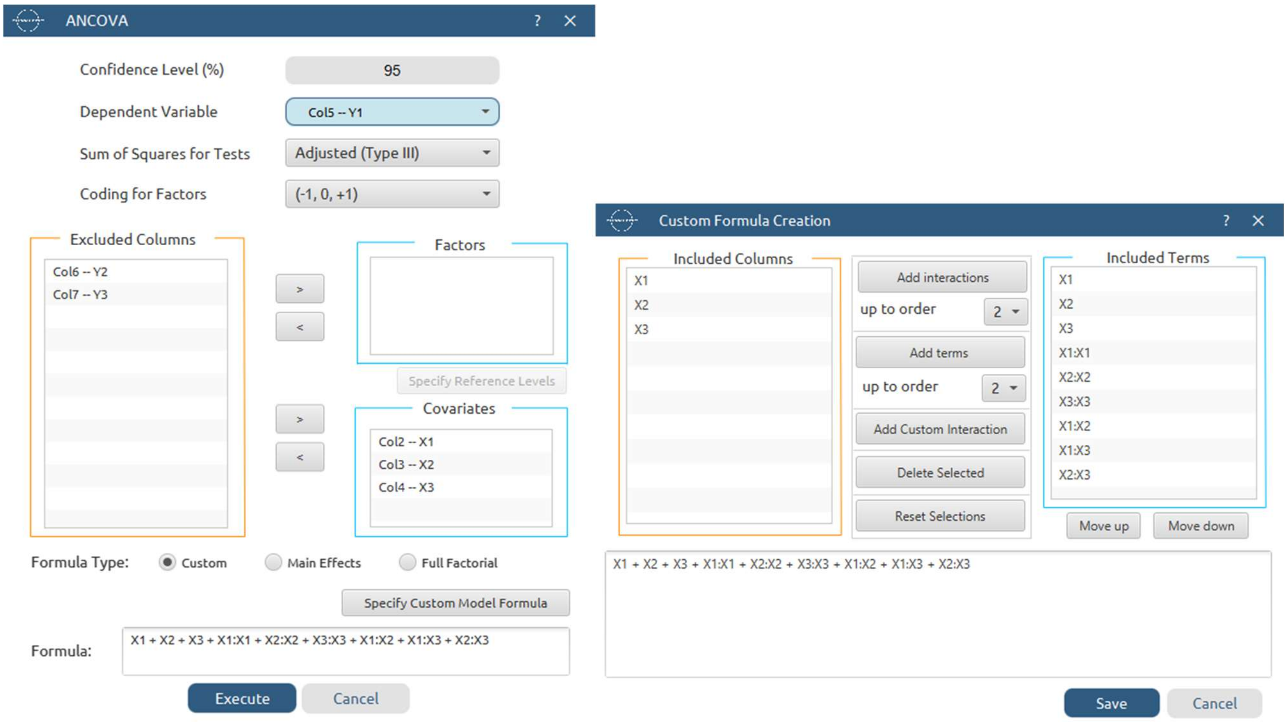
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	Mean Squared Error	Root Mean Squared Error	Mean Absolute Error	R Squared
1		177091.6046210	420.8225334	351.8835668	0.7547436

Results, Y_3:

	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		13.7806031	3.7122235	2.7780558	0.6883665

Step 10: Analysis of Covariance

Create a new tab named “ANCOVA – Y1” and import the results from the spreadsheet “Full data”. Afterwards perform analysis of covariance for Y_1: *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		X1	1	4028.6161623	4028.6161623	10.6880347	0.0074751
2		X2	1	2617.8074820	2617.8074820	6.9451186	0.0231844
3		X3	1	78.5707707	78.5707707	0.2084505	0.6568679
4		X1*X1	1	1131.4322093	1131.4322093	3.0017222	0.1110818
5		X2*X2	1	2258.3371856	2258.3371856	5.9914336	0.0323753
6		X3*X3	1	33.5728150	33.5728150	0.0890696	0.7709254
7		X1*X2	1	2873.6632037	2873.6632037	7.6239112	0.0185180
8		X2*X3	1	312.4324160	312.4324160	0.8288922	0.3821102
9		X1*X3	1	149.9013141	149.9013141	0.3976925	0.5411636
10		Error	11	4146.2045278	376.9276843		
11		Total	20	51794.6763810			

Repeat this step for the rest of the response variables. Results, Y_2:

	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		X1	1	7049092.9333906	7049092.9333906	19.9023916	0.0012139
2		X2	1	896368.1553144	896368.1553144	2.5308036	0.1427276
3		X3	1	1613206.6235647	1613206.6235647	4.5547236	0.0586071
4		X1*X1	1	2246198.9621435	2246198.9621435	6.3419126	0.0304752
5		X2*X2	1	498826.6379497	498826.6379497	1.4083859	0.2627524
6		X3*X3	1	1005540.7389776	1005540.7389776	2.8390412	0.1229010
7		X1*X2	1	1595940.2598835	1595940.2598835	4.5059738	0.0597486
8		X2*X3	1	10106.4983269	10106.4983269	0.0285347	0.8692259
9		X1*X3	1	4584767.2486652	4584767.2486652	12.9446205	0.0048651
10		Error	10	3541832.0924196	354183.2092420		
11		Total	19	14441345.8			

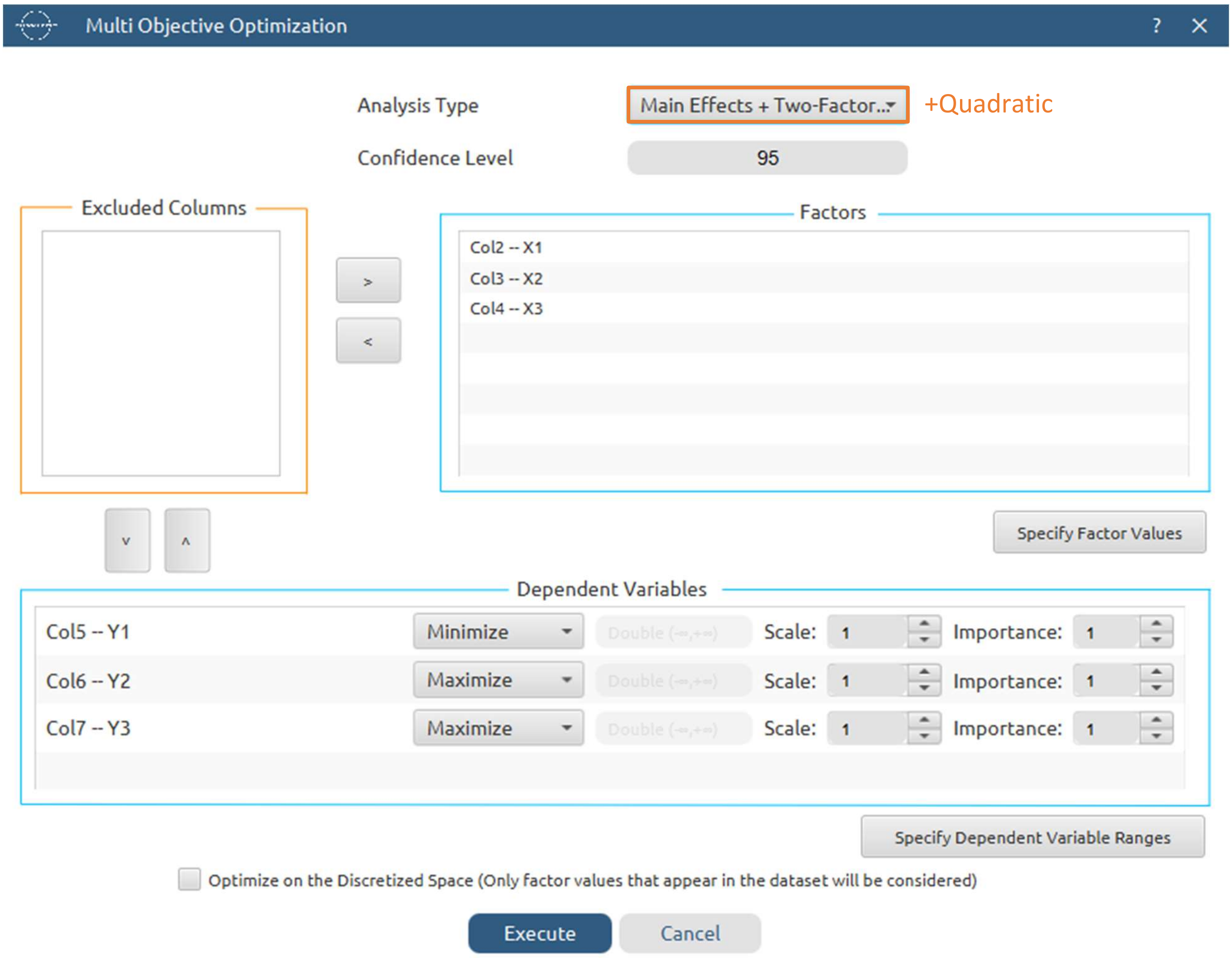
Results, Y_3:

	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		X1	1	47.3987499	47.3987499	1.8016568	0.2065587
2		X2	1	0.0000118	0.0000118	4E-7	0.9994786
3		X3	1	2.3337381	2.3337381	0.0887069	0.7713775
4		X1*X1	1	0.7285252	0.7285252	0.0276917	0.8708550
5		X2*X2	1	9.8604136	9.8604136	0.3748006	0.5528435
6		X3*X3	1	0.0852496	0.0852496	0.0032404	0.9556262
7		X1*X2	1	84.0798952	84.0798952	3.1959305	0.1013706
8		X2*X3	1	126.6286996	126.6286996	4.8132377	0.0506216
9		X1*X3	1	47.8683153	47.8683153	1.8195052	0.2044852
10		Error	11	289.3926652	26.3084241		
11		Total	20	928.6314286			

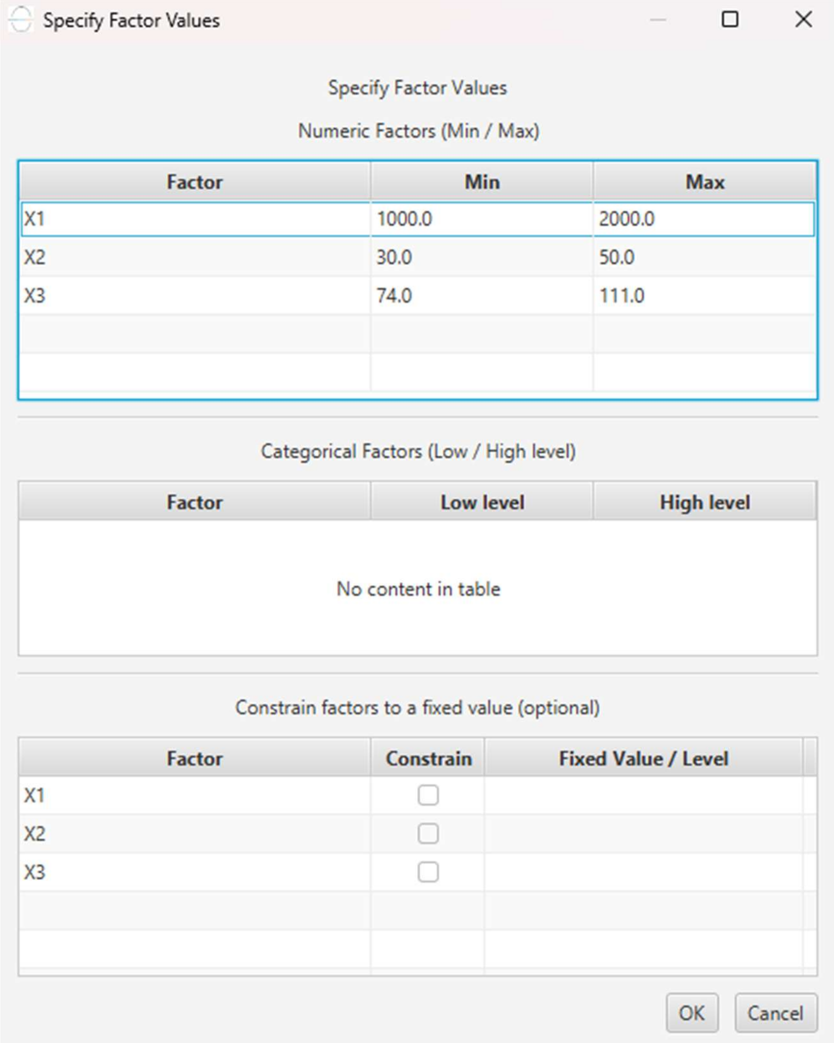
Step 11: Multi-Objective Optimization

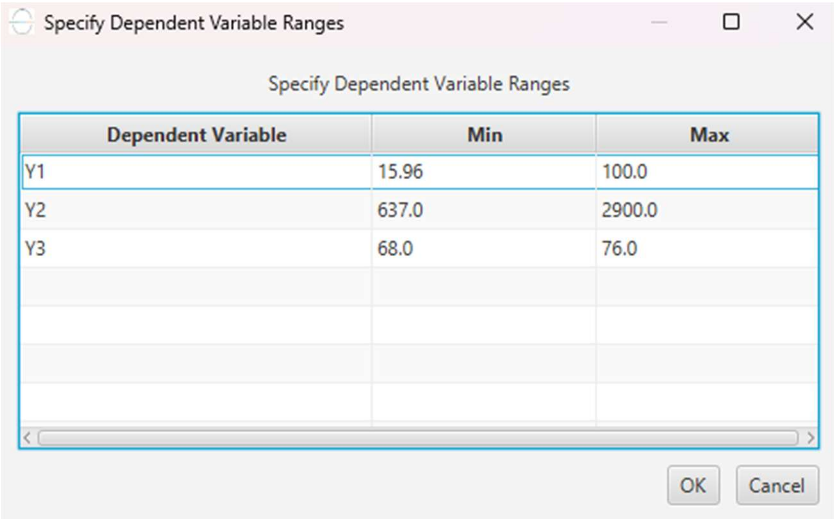
Create a new tab named "Multi-objective optimization" and import the results from the spreadsheet "Full data". The goal of this step is to evaluate the factor values which will optimize all the response variables simultaneously. To perform multi-objective optimization, click on: *DOE → Post DoE Analysis → Multi-Objective Optimization*

Select all three factors to be included in the optimization, and choose which response variables should be minimized and maximized. Reaction time, Y_1, is the only response variable which should be minimized. Leave scale and importance values at 1.



Specify the range for the factor values and the dependent variables as shown below.


Specify Factor Values
Specify Factor Values
Numeric Factors (Min / Max)
Factor
Min
Max
X1
1000.0
2000.0
X2
30.0
50.0
X3
74.0
111.0
Categorical Factors (Low / High level)
Factor
Low level
High level
No content in table
Constrain factors to a fixed value (optional)
Factor
Constrain
Fixed Value / Level
X1
X2
X3
OK
Cancel

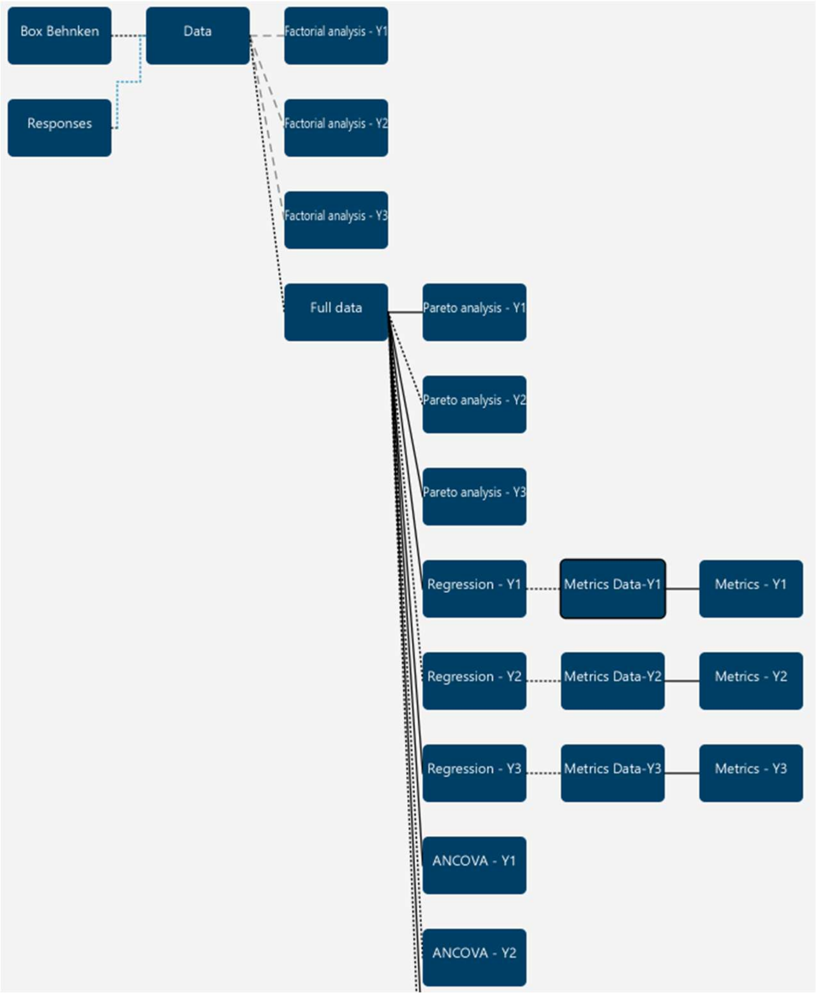

Specify Dependent Variable Ranges
Specify Dependent Variable Ranges
Dependent Variable
Min
Max
Y1
15.96
100.0
Y2
637.0
2900.0
Y3
68.0
76.0
OK
Cancel

Results:

	Col1	Col2 (S)	Col3 (S)	Col4 (S)	Col5 (S)	Col6 (S)	Col7 (S)	Col8 (S)
User Header	User Row ID							
1		Optimal Settings - Solution						
2		X1	X2	X3				
3		1127.6667237	50.0	76.5416699				
4								
5		Response Prediction						
6		Response	Predicted Value	Standard Error	(95.0%) CI Lower	(95.0%) CI Upper	(95.0%) PI Lower	(95.0%) PI Upper
7		Y1	26.5121753	13.7191066	-4.0558992	57.0802498	-28.0500654	81.0744159
8		Y2	2900.0000000	402.5196779	2003.1302670	3796.8697330	1299.1395282	4500.8604718
9		Y3	75.0740088	3.5568681	67.1488129	82.9992048	60.9279935	89.2200241
10								
11		Desirabilities						
12		Y1	Y2	Y3	Overall			
13		0.8744387	1.0000000	0.8842511	0.9178428			

Final Isalos Workflow

The final workflow is presented below:



References

(1) Michael, A.; Adamou, P.; Harkou, E.; Christodoulou, C.; Barlocco, I.; Mintis, D.; Afantitis, A.; Delgado, J. J.; Chen, X.; Manos, G.; Dimitratos, N.; Villa, A.; Constantinou, A. Application of CFD, Statistical Analysis and DoE for Optimising H2 Generation through Ammonia Borane Catalytic Hydrolysis: A Novel Approach for Multiobjective Optimisation. *Chemical Engineering Journal* **2025**, *525*, 170772. https://doi.org/10.1016/j.cej.2025.170772.