Simplex Lattice Mixture Design Application for Biodiesel Production: Formulation and Characterization of Hybrid Oil as Feedstock

Purpose: The purpose of this study is to investigate the formulation and optimization of a hybrid oil for biodiesel production using a Simplex Lattice mixture design.

Five oil components were examined: waste kitchen oil (WKO), neem oil (NMO), shea butter (SHB), sesame oil (SEO), and palm kernel oil (PKO). Each experimental mixture had a total weight of 125 g.

The main responses examined in the mixture model analysis were cetane number (CN), density, higher calorific value (HCV), and viscosity.

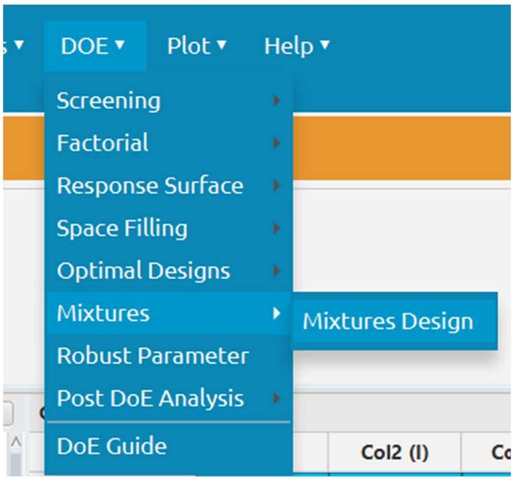
Isalos version used: 2.2.0

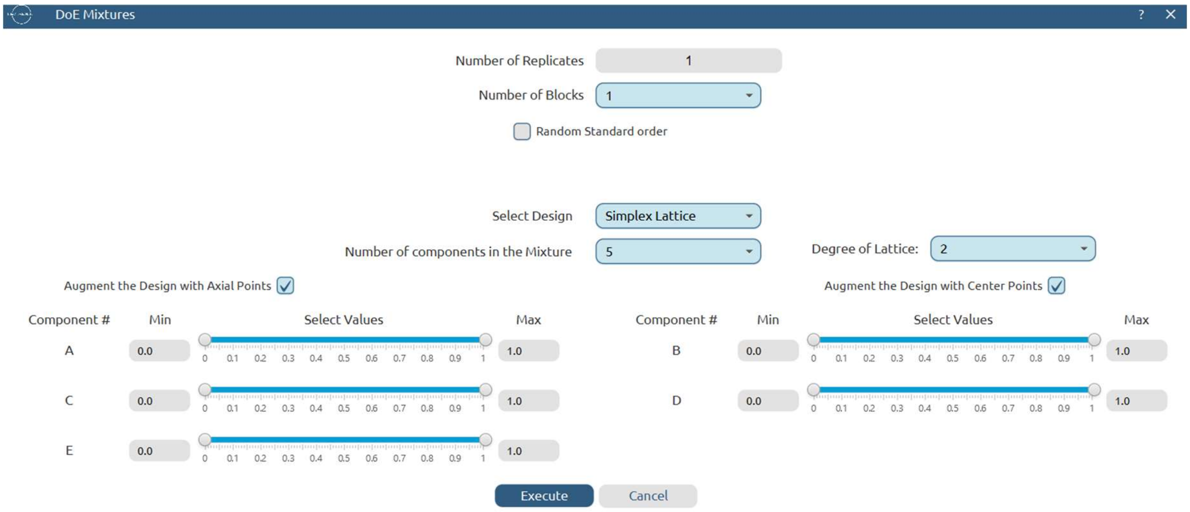
Scientific article:

Nouadjep, N. S., et al. (2019). *Simplex lattice mixture design application for biodiesel production: Formulation and characterization of hybrid oil as feedstock.* Fuel, 252, 135–142.

Step 1: Simplex Lattice Design

In the first tab named “Action”, rename it to “Simplex Lattice”. Then, go to DOE → Mixtures → Mixtures Design. Select Simplex Lattice, set the number of components to 5 and the degree to 2. Define the bounds of components A, B, C, D and E from 0 to 1. Select Axial Points and Center Points, and click Execute to generate the mixture design.





Results (right spreadsheet) :

Output

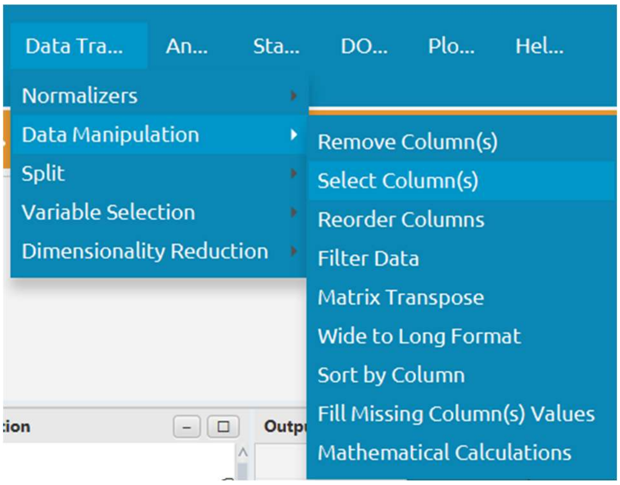
	Col1	Col2 (I)	Col3 (S)	Col4 (S)	Col5 (S)	Col6 (D)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	Standard Order	Block Number	Replicate Number	Point Type	A	B	C	D	E
1		1	Block: 1	Replicate: 1	Design Point	1.0	0.0	0.0	0.0	0.0
2		2	Block: 1	Replicate: 1	Design Point	0.0	1.0	0.0	0.0	0.0
3		3	Block: 1	Replicate: 1	Design Point	0.0	0.0	1.0	0.0	0.0
4		4	Block: 1	Replicate: 1	Design Point	0.0	0.0	0.0	1.0	0.0
5		5	Block: 1	Replicate: 1	Design Point	0.0	0.0	0.0	0.0	1.0
6		6	Block: 1	Replicate: 1	Design Point	0.0	0.0	0.0	0.5	0.5
7		7	Block: 1	Replicate: 1	Design Point	0.0	0.0	0.5	0.0	0.5
8		8	Block: 1	Replicate: 1	Design Point	0.0	0.0	0.5	0.5	0.0
9		9	Block: 1	Replicate: 1	Design Point	0.0	0.5	0.0	0.0	0.5
10		10	Block: 1	Replicate: 1	Design Point	0.0	0.5	0.0	0.5	0.0
11		11	Block: 1	Replicate: 1	Design Point	0.0	0.5	0.5	0.0	0.0
12		12	Block: 1	Replicate: 1	Design Point	0.5	0.0	0.0	0.0	0.5
13		13	Block: 1	Replicate: 1	Design Point	0.5	0.0	0.0	0.5	0.0
14		14	Block: 1	Replicate: 1	Design Point	0.5	0.0	0.5	0.0	0.0
15		15	Block: 1	Replicate: 1	Design Point	0.5	0.5	0.0	0.0	0.0
16		16	Block: 1	Replicate: 1	Design Point	0.2	0.2	0.2	0.2	0.2
17		17	Block: 1	Replicate: 1	Design Point	0.6	0.1	0.1	0.1	0.1
18		18	Block: 1	Replicate: 1	Design Point	0.1	0.6	0.1	0.1	0.1
19		19	Block: 1	Replicate: 1	Design Point	0.1	0.1	0.6	0.1	0.1
20		20	Block: 1	Replicate: 1	Design Point	0.1	0.1	0.1	0.6	0.1
21		21	Block: 1	Replicate: 1	Design Point	0.1	0.1	0.1	0.1	0.6

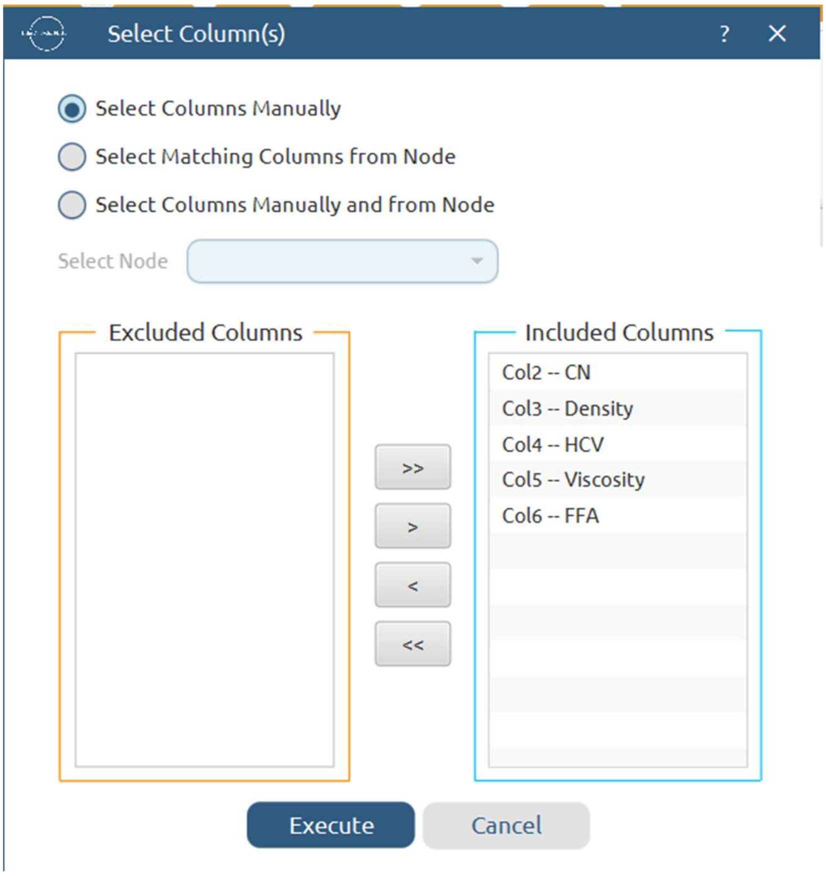
Step 2: Definition of Response Variables

Create a new spreadsheet and rename it "Responses". Enter the response values reported in the paper for the 26 experimental runs. The response variables are CN, Density, HCV, Viscosity and FFA. After entering the data, apply Data Transformation → Data Manipulation → Select Column(s) and include the CN, Density, HCV, Viscosity, and FFA response columns.

Input

	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)
User Header	User Row ID	CN	Density	HCV	Viscosity	FFA
1		54.6055	905.847	39.6791	32.2484	1.76364
2		70.308	907.25	42.501	27.015	4.5855
3		47.5319	909.2	39.9747	26.3612	2.4691
4		72.3327	900.11	45.3455	43.5892	3.17456
5		75.7377	902.85	43.4328	26.5067	8.11276
6		80.0153	908.613	43.7151	33.395	4.58547
7		75.4361	907.733	45.0211	28.4193	2.11637
8		60.662	910.147	41.3929	23.8744	0.705458
9		73.5769	908.799	43.9572	29.8432	2.4691
10		59.8482	903.233	40.2924	88.7468	6.34912
11		61.4078	902.047	37.9917	21.3157	5.29093
12		50.4382	909.407	42.3523	24.0258	1.05819
13		68.6448	900.497	45.759	49.3899	4.58547
14		62.6295	908.36	41.901	28.7015	8.11276
15		29.823	909.053	36.28	24.475	2.1164
16		71.5671	907.38	42.7455	61.9215	6.34912
17		56.959	896.89	38.8433	39.8722	7.76003
18		78.2371	907.56	43.4929	28.317	5.99639
19		60.2053	907.767	41.6217	45.4752	3.88002
20		75.071	907.313	43.0261	32.628	2.4691
21		70.0313	909.127	42.2693	23.7967	2.82183
22						

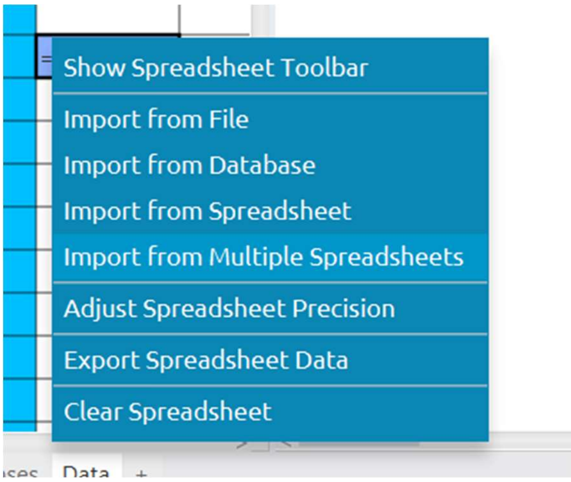


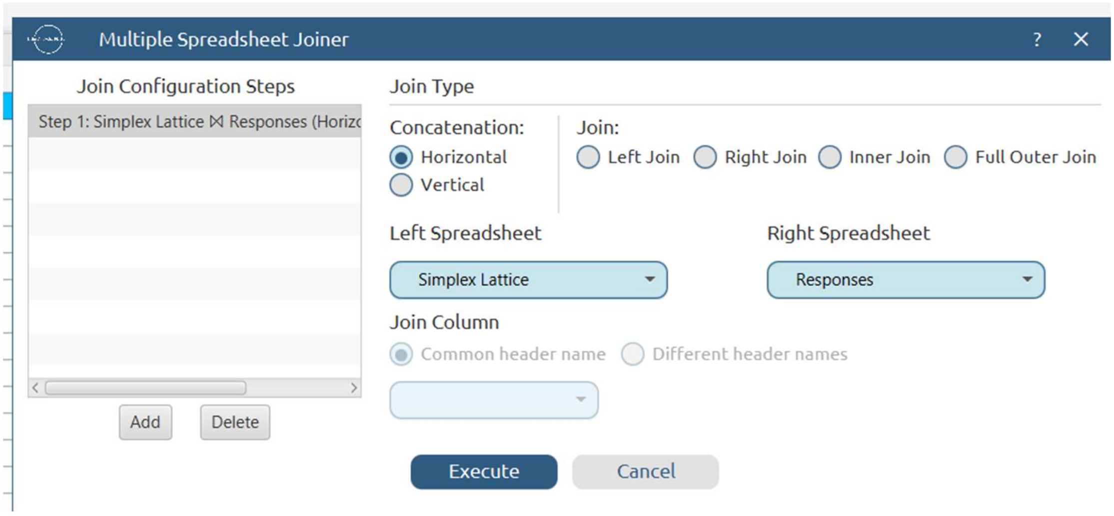


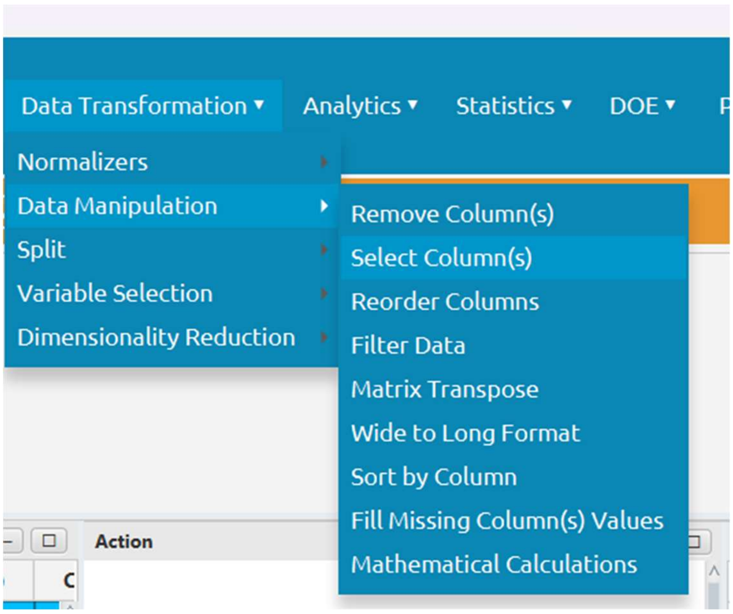
Step 3: Data Selection

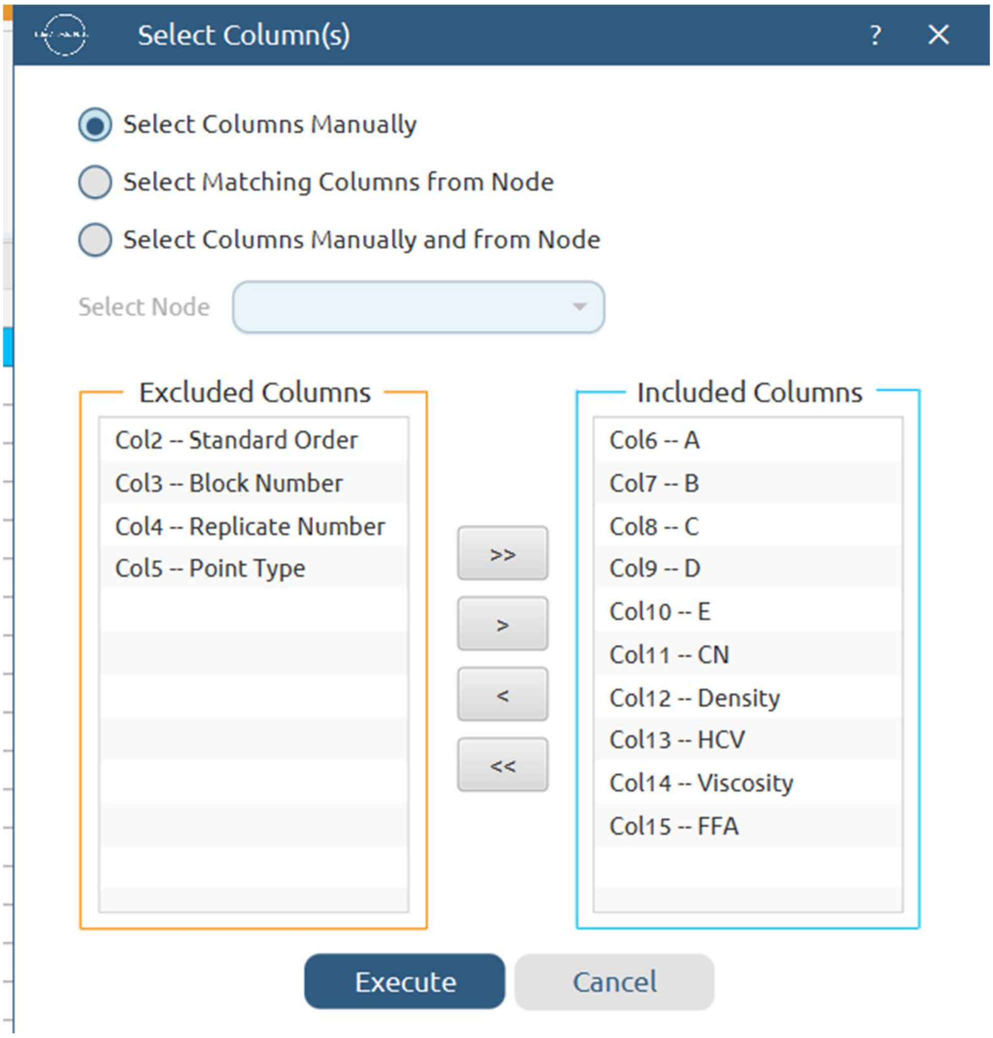
Create a tab named “Data”. To combine the mixture design with the response data, right-click on the spreadsheet and select Import from Multiple Spreadsheets. In the Multiple Spreadsheet Joiner, select Horizontal concatenation, with Simplex Lattice as the Left Spreadsheet and Responses as the Right Spreadsheet. Click Execute to combine the two spreadsheets into a single dataset.

Then, go to Data Transformation → Data Manipulation → Select Column(s). Exclude Standard Order, Block Number, Replicate Number, and Point Type, and include only A, B, C, D, E, CN, Density, HCV, Viscosity, and FFA. The resulting dataset contains the five mixture components and their corresponding response values.


Show Spreadsheet Toolbar
Import from File
Import from Database
Import from Spreadsheet
Import from Multiple Spreadsheets
Adjust Spreadsheet Precision
Export Spreadsheet Data
Clear Spreadsheet
Data


Multiple Spreadsheet Joiner
Join Configuration Steps
Step 1: Simplex Lattice ⋈ Responses (Horiz
Add
Delete
Join Type
Concatenation:
Horizontal
Vertical
Join:
Left Join
Right Join
Inner Join
Full Outer Join
Left Spreadsheet
Simplex Lattice
Right Spreadsheet
Responses
Join Column
Common header name
Different header names
Execute
Cancel


Data Transformation
Analytics
Statistics
DOE
Normalizers
Data Manipulation
Split
Variable Selection
Dimensionality Reduction
Remove Column(s)
Select Column(s)
Reorder Columns
Filter Data
Matrix Transpose
Wide to Long Format
Sort by Column
Fill Missing Column(s) Values
Mathematical Calculations
Action



Results :

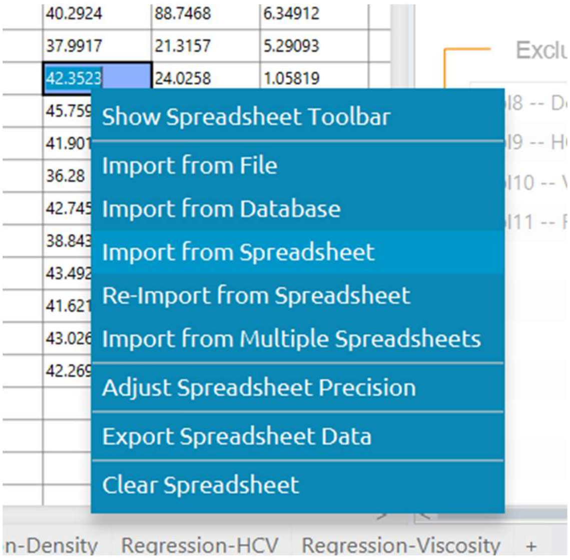
Output

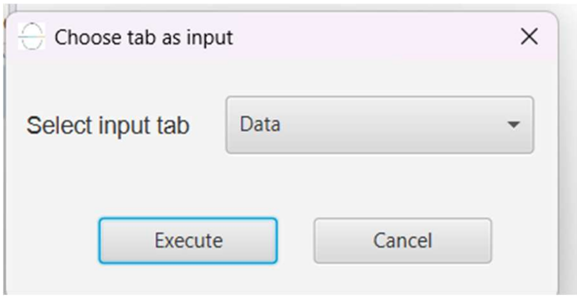
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)	Col11 (D)	Col12
User Header	User Row ID	A	B	C	D	E	CN	Density	HCV	Viscosity	FFA	
1		1.0	0.0	0.0	0.0	0.0	54.6055	905.847	39.6791	32.2484	1.76364	
2		0.0	1.0	0.0	0.0	0.0	70.308	907.25	42.501	27.015	4.5855	
3		0.0	0.0	1.0	0.0	0.0	47.5319	909.2	39.9747	26.3612	2.4691	
4		0.0	0.0	0.0	1.0	0.0	72.3327	900.11	45.3455	43.5892	3.17456	
5		0.0	0.0	0.0	0.0	1.0	75.7377	902.85	43.4328	26.5067	8.11276	
6		0.0	0.0	0.0	0.5	0.5	80.0153	908.613	43.7151	33.395	4.58547	
7		0.0	0.0	0.5	0.0	0.5	75.4361	907.733	45.0211	28.4193	2.11637	
8		0.0	0.0	0.5	0.5	0.0	60.662	910.147	41.3929	23.8744	0.705458	
9		0.0	0.5	0.0	0.0	0.5	73.5769	908.799	43.9572	29.8432	2.4691	
10		0.0	0.5	0.0	0.5	0.0	59.8482	903.233	40.2924	88.7468	6.34912	
11		0.0	0.5	0.5	0.0	0.0	61.4078	902.047	37.9917	21.3157	5.29093	
12		0.5	0.0	0.0	0.0	0.5	50.4382	909.407	42.3523	24.0258	1.05819	
13		0.5	0.0	0.0	0.5	0.0	68.6448	900.497	45.759	49.3899	4.58547	
14		0.5	0.0	0.5	0.0	0.0	62.6295	908.36	41.901	28.7015	8.11276	
15		0.5	0.5	0.0	0.0	0.0	29.823	909.053	36.28	24.475	2.1164	
16		0.2	0.2	0.2	0.2	0.2	71.5671	907.38	42.7455	61.9215	6.34912	
17		0.6	0.1	0.1	0.1	0.1	56.959	896.89	38.8433	39.8722	7.76003	
18		0.1	0.6	0.1	0.1	0.1	78.2371	907.56	43.4929	28.317	5.99639	
19		0.1	0.1	0.6	0.1	0.1	60.2053	907.767	41.6217	45.4752	3.88002	
20		0.1	0.1	0.1	0.6	0.1	75.071	907.313	43.0261	32.628	2.4691	
21		0.1	0.1	0.1	0.1	0.6	70.0313	909.127	42.2693	23.7967	2.82183	

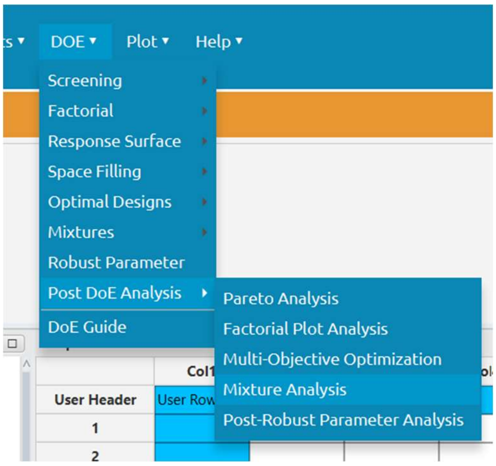
Step 4: Regression Analysis for CN

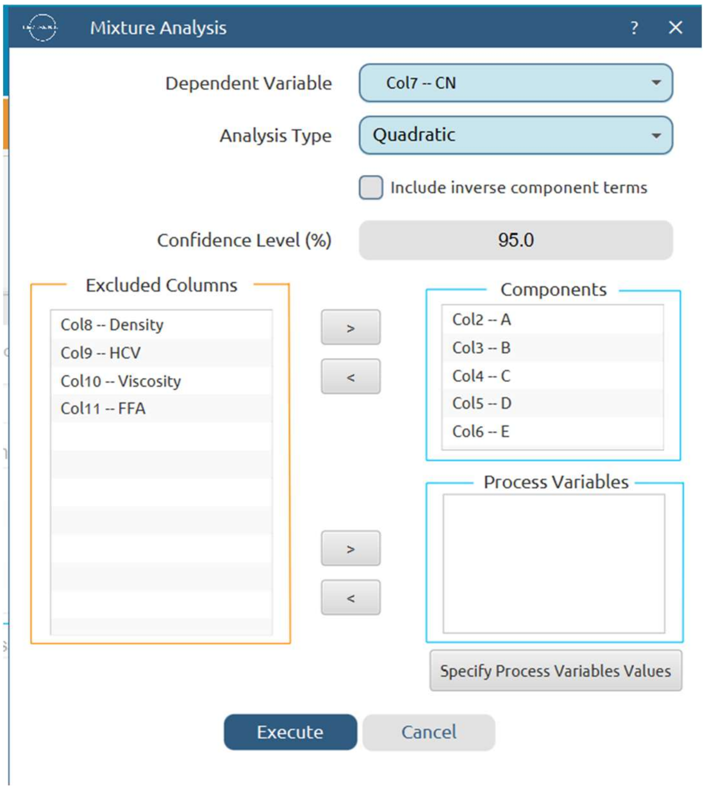
Create a new tab named "Regression-CN". Right-click on the spreadsheet, select Import from Spreadsheet, choose the Data tab as input, and click Execute.

Then, go to DOE → Post DOE Analysis → Mixture Analysis. Select CN as the dependent variable, select A, B, C, D, and E as the mixture components, and choose Quadratic as the analysis type. Keep the confidence level at 95% and click Execute to obtain the fitted mixture model and its statistical results.









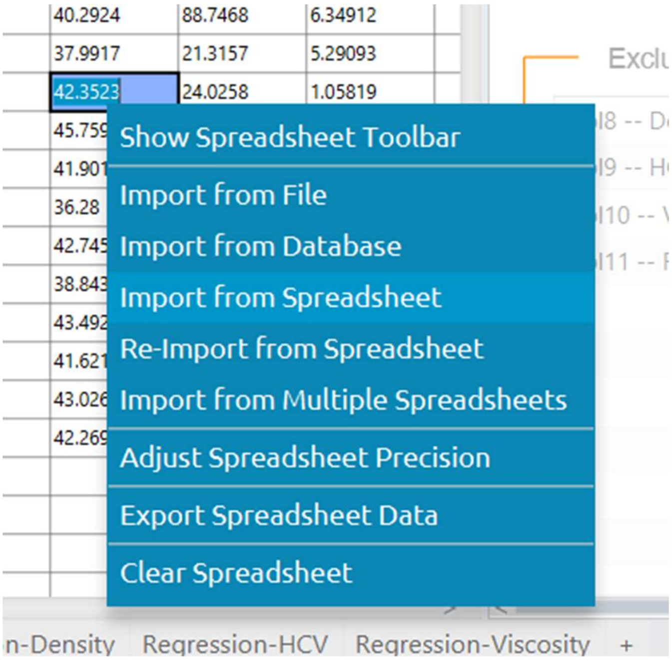
Output

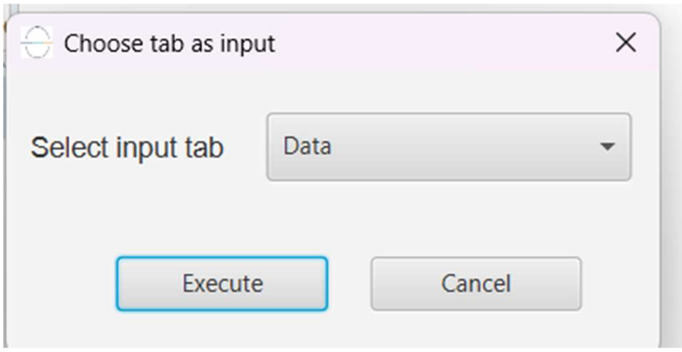
	Col1	Col2 (S)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value	VIF
1		A	53.0683950	7.9031903	33.7299850	72.4068050	6.7148067	1.0	0.0005302	2.3430014
2		B	71.4456398	7.9031903	52.1072298	90.7840498	9.0401012	1.0	0.0001027	2.3430014
3		C	45.1225605	7.9031903	25.7841505	64.4609705	5.7094109	1.0	0.0012495	2.3430014
4		D	71.3196640	7.9031903	51.9812540	90.6580740	9.0241613	1.0	0.0001037	2.3430014
5		E	73.3832950	7.9031903	54.0448850	92.7217050	9.2852750	1.0	0.0000883	2.3430014
6		A*B	-111.0543157	38.0246449	-204.0972700	-18.0113614	-2.9205878	1.0	0.0266109	1.5915534
7		A*C	58.6299257	38.0246449	-34.4130286	151.6728800	1.5418928	1.0	0.1740376	1.5915534
8		A*D	35.8821326	38.0246449	-57.1608217	128.9250869	0.9436546	1.0	0.3817756	1.5915534
9		A*E	-46.4370053	38.0246449	-139.4799596	46.6059489	-1.2212344	1.0	0.2678027	1.5915534
10		B*C	27.6876153	38.0246449	-65.3553390	120.7305696	0.7281492	1.0	0.4939474	1.5915534
11		B*D	-25.3597778	38.0246449	-118.4027321	67.6831765	-0.6669300	1.0	0.5296145	1.5915534
12		B*E	20.0622843	38.0246449	-72.9806700	113.1052386	0.5276127	1.0	0.6167009	1.5915534
13		C*D	16.3536636	38.0246449	-76.6892907	109.3966179	0.4300806	1.0	0.6821550	1.5915534
14		C*E	65.9573257	38.0246449	-27.0856286	159.0002800	1.7345941	1.0	0.1335044	1.5915534
15		D*E	37.4651326	38.0246449	-55.5778217	130.5080869	0.9852855	1.0	0.3625329	1.5915534
16										

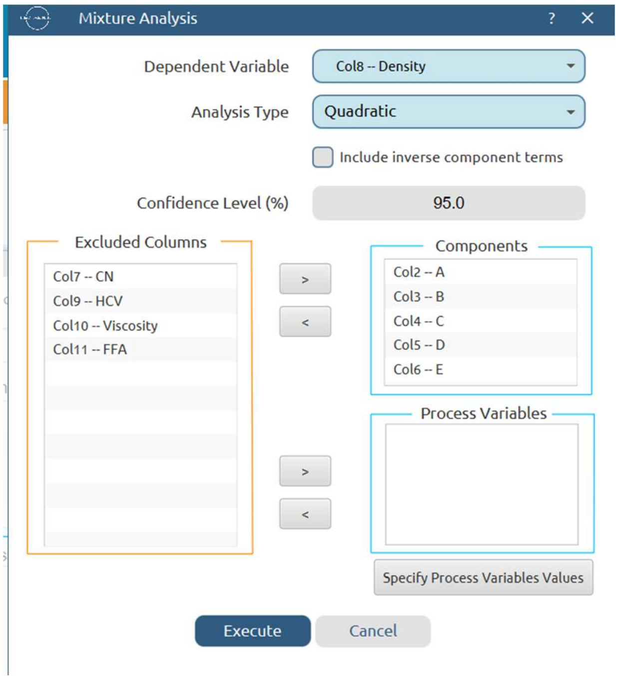
Step 5: Regression Analysis for Density

Create a new tab named “Regression-Density”. Right-click on the spreadsheet, select Import from Spreadsheet, choose the Data tab as input, and click Execute.

Then, go to DOE → Post DOE Analysis → Mixture Analysis. Select Density as the dependent variable, select A, B, C, D, and E as the mixture components, and choose Quadratic as the analysis type. Keep the confidence level at 95% and click Execute to obtain the fitted mixture model and its statistical results.







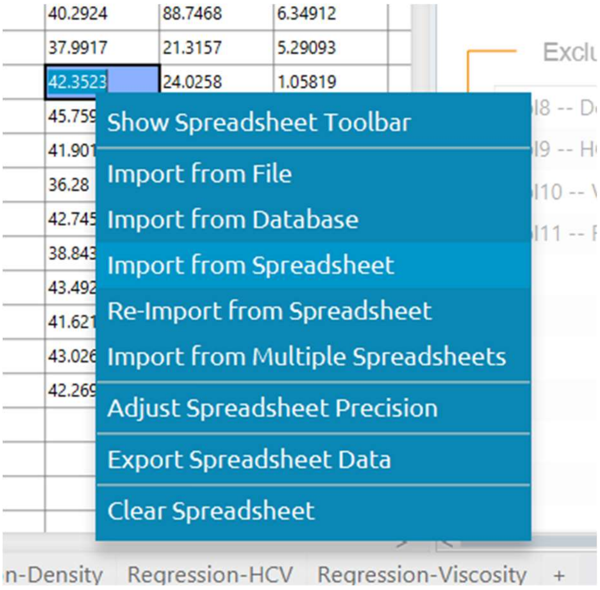
Output

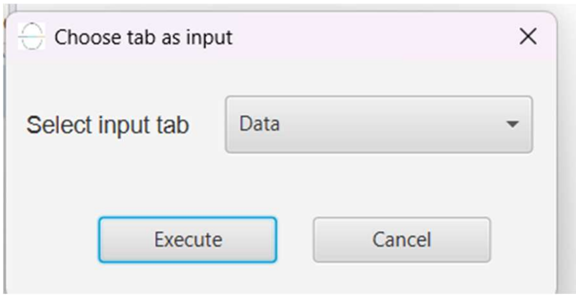
	Col1	Col2 (S)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value	VIF
1		A	904.4164815	3.9284163	894.8039932	914.0289699	230.2241965	1.0	0E-7	2.3430014
2		B	907.7550677	3.9284163	898.1425794	917.3675561	231.0740520	1.0	0E-7	2.3430014
3		C	909.4957574	3.9284163	899.8832690	919.1082457	231.5171541	1.0	0E-7	2.3430014
4		D	900.8408264	3.9284163	891.2283380	910.4533147	229.3139938	1.0	0E-7	2.3430014
5		E	903.3831712	3.9284163	893.7706828	912.9956595	229.9611616	1.0	0E-7	2.3430014
6		A*B	5.3550012	18.9008019	-40.8935950	51.6035974	0.2833214	1.0	0.7864522	1.5915534
7		A*C	-1.7356195	18.9008019	-47.9842157	44.5129767	-0.0918278	1.0	0.9298240	1.5915534
8		A*D	-14.1374816	18.9008019	-60.3860778	32.1111146	-0.7479832	1.0	0.4827469	1.5915534
9		A*E	15.6272081	18.9008019	-30.6213881	61.8758042	0.8268013	1.0	0.4399844	1.5915534
10		B*C	-25.9224471	18.9008019	-72.1710433	20.3261491	-1.3714999	1.0	0.2192965	1.5915534
11		B*D	-2.1283092	18.9008019	-48.3769053	44.1202870	-0.1126042	1.0	0.9140173	1.5915534
12		B*E	14.2603805	18.9008019	-31.9882157	60.5089767	0.7544855	1.0	0.4791132	1.5915534
13		C*D	21.2090701	18.9008019	-25.0395260	67.4576663	1.1221254	1.0	0.3046972	1.5915534
14		C*E	5.6777598	18.9008019	-40.5708364	51.9263560	0.3003978	1.0	0.7740102	1.5915534
15		D*E	28.2478977	18.9008019	-18.0006984	74.4964939	1.4945344	1.0	0.1856580	1.5915534
16										

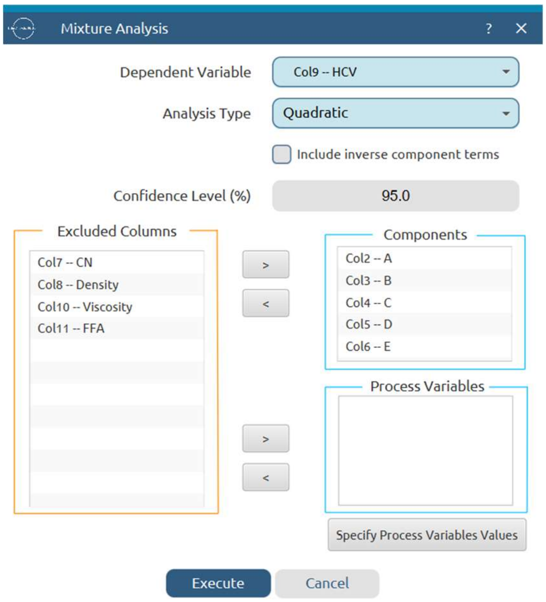
Step 6: Regression Analysis for HCV

Create a new tab named "Regression-HCV". Right-click on the spreadsheet, select Import from Spreadsheet, choose the Data tab as input, and click Execute.

Then, go to DOE → Post DOE Analysis → Mixture Analysis. Select HCV as the dependent variable, select A, B, C, D, and E as the mixture components, and choose Quadratic as the analysis type. Keep the confidence level at 95% and click Execute to obtain the fitted mixture model and its statistical results.







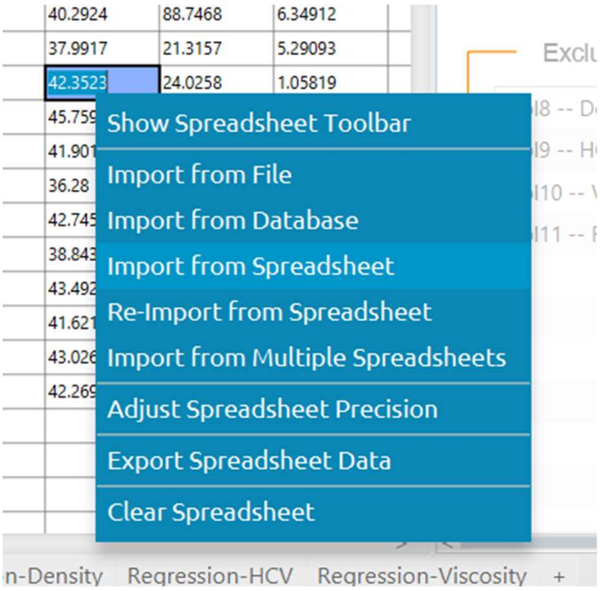
Output

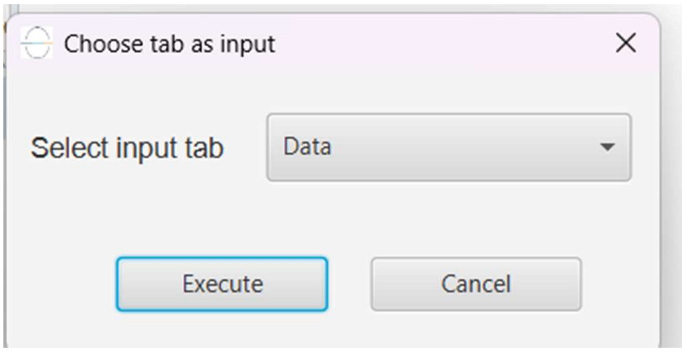
	Col1	Col2 (S)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value	VIF
1		A	39.1988119	1.6449985	35.1736456	43.2239782	23.8290868	1.0	4E-7	2.3430014
2		B	42.9930257	1.6449985	38.9678594	47.0181920	26.1356019	1.0	2E-7	2.3430014
3		C	39.9627567	1.6449985	35.9375904	43.9879231	24.2934914	1.0	3E-7	2.3430014
4		D	45.2231602	1.6449985	41.1979939	49.2483265	27.4913080	1.0	2E-7	2.3430014
5		E	43.1119223	1.6449985	39.0867559	47.1370886	26.2078795	1.0	2E-7	2.3430014
6		A*B	-18.1401413	7.9145866	-37.5064370	1.2261543	-2.2919885	1.0	0.0617753	1.5915534
7		A*C	8.3885207	7.9145866	-10.9777749	27.7548164	1.0598811	1.0	0.3299888	1.5915534
8		A*D	12.8581276	7.9145866	-6.5081680	32.2244233	1.6246114	1.0	0.1553710	1.5915534
9		A*E	2.6596518	7.9145866	-16.7066439	22.0259474	0.3360443	1.0	0.7482778	1.5915534
10		B*C	-10.9478517	7.9145866	-30.3141473	8.4184440	-1.3832500	1.0	0.2158581	1.5915534
11		B*D	-12.7074448	7.9145866	-32.0737404	6.6588508	-1.6055728	1.0	0.1594906	1.5915534
12		B*E	5.3800793	7.9145866	-13.9862163	24.7463750	0.6797676	1.0	0.5219994	1.5915534
13		C*D	-4.2607827	7.9145866	-23.6270784	15.1055129	-0.5383456	1.0	0.6097132	1.5915534
14		C*E	13.6803414	7.9145866	-5.6859542	33.0466371	1.7284973	1.0	0.1346342	1.5915534
15		D*E	-2.5060517	7.9145866	-21.8723473	16.8602440	-0.3166371	1.0	0.7622460	1.5915534

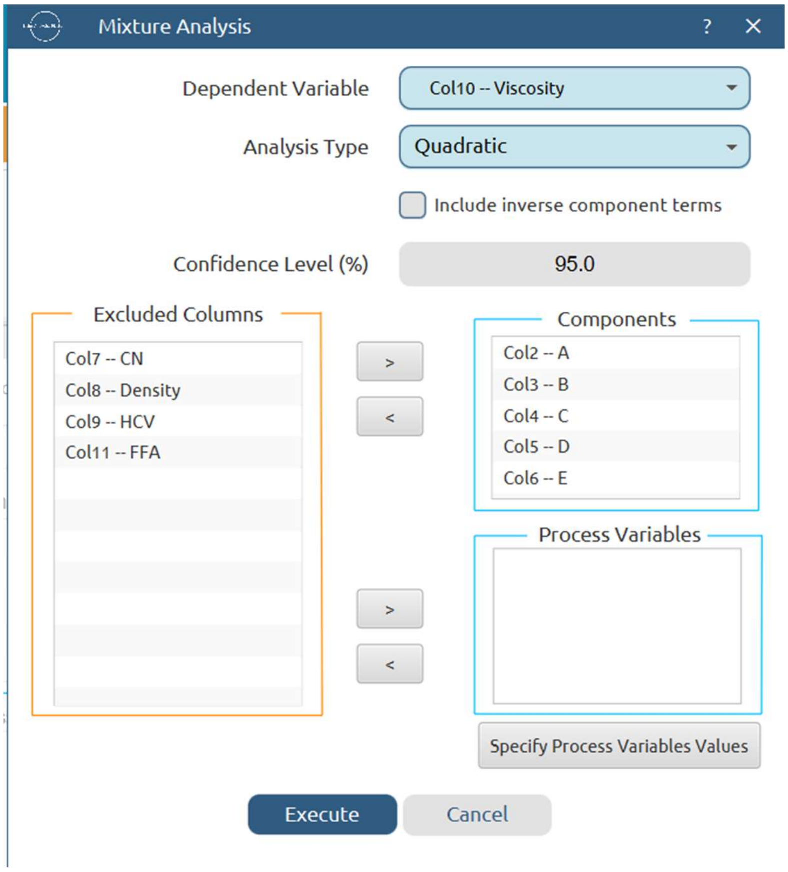
Step 7: Regression Analysis for Viscosity

Create a new tab named “Regression-Viscosity”. Right-click on the spreadsheet, select Import from Spreadsheet, choose the Data tab as input, and click Execute.

Then, go to DOE → Post DOE Analysis → Mixture Analysis. Select Viscosity as the dependent variable, select A, B, C, D, and E as the mixture components, and choose Quadratic as the analysis type. Keep the confidence level at 95% and click Execute to obtain the fitted mixture model and its statistical results.







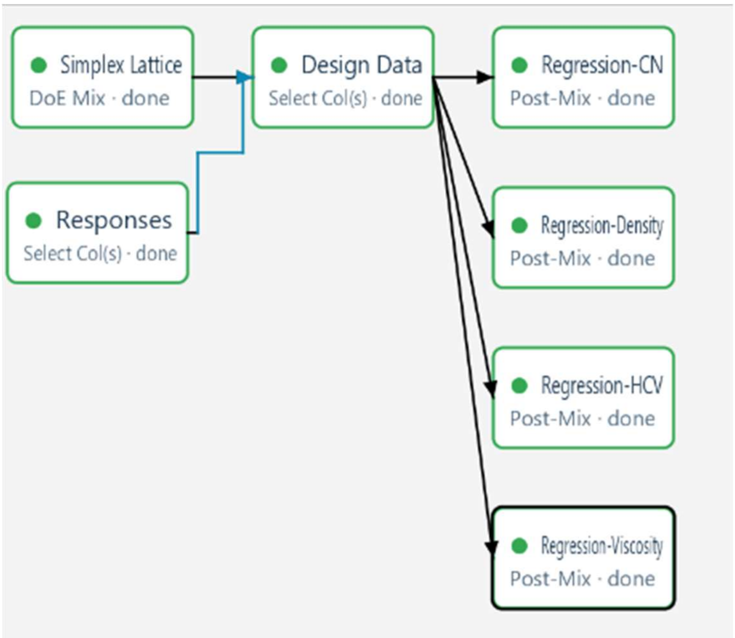
Output

	Col1	Col2 (S)	Col3 (D)	Col4 (D)	Col5 (D)	Col6 (D)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	Variable	Coefficient	Std. Error	Lower CI	Upper CI	Test Statistic	df	p-value	VIF
1		A	31.9055314	14.1424233	-2.6997318	66.5107945	2.2560159	1.0	0.0649024	2.3430014
2		B	23.5572658	14.1424233	-11.0479973	58.1625290	1.6657164	1.0	0.1468218	2.3430014
3		C	28.0246590	14.1424233	-6.5806042	62.6299221	1.9816023	1.0	0.0948131	2.3430014
4		D	39.2333762	14.1424233	4.6281131	73.8386393	2.7741622	1.0	0.0322447	2.3430014
5		E	23.9663521	14.1424233	-10.6389111	58.5716152	1.6946425	1.0	0.1410791	2.3430014
6		A*B	-9.1560646	68.0434867	-175.6524786	157.3403494	-0.1345620	1.0	0.8973586	1.5915534
7		A*C	19.2999216	68.0434867	-147.1964924	185.7963356	0.2836410	1.0	0.7862187	1.5915534
8		A*D	55.5589561	68.0434867	-110.9374579	222.0553701	0.8165213	1.0	0.4454025	1.5915534
9		A*E	-8.1014922	68.0434867	-174.5979062	158.3949218	-0.1190634	1.0	0.9091115	1.5915534
10		B*C	-6.0062094	68.0434867	-172.5026234	160.4902046	-0.0882702	1.0	0.9325344	1.5915534
11		B*D	217.2236251	68.0434867	50.7272111	383.7200391	3.1924235	1.0	0.0187788	1.5915534
12		B*E	19.4051768	68.0434867	-147.0912372	185.9015908	0.2851879	1.0	0.7850888	1.5915534
13		C*D	-30.7159887	68.0434867	-197.2124027	135.7804253	-0.4514170	1.0	0.6675465	1.5915534
14		C*E	25.2595630	68.0434867	-141.2368510	191.7559770	0.3712268	1.0	0.7232240	1.5915534
15		D*E	-1.3322025	68.0434867	-167.8286165	165.1642115	-0.0195787	1.0	0.9850143	1.5915534

Note : FFA was included in the experimental response data. However, no separate regression analysis was performed for FFA, since the paper reports fitted mixture models and ANOVA results only for CN, Density, HCV, and Viscosity.

Final Isalos Workflow

The final workflow is presented below :



References

Nouadjep, N. S., et al. (2019). *Simplex lattice mixture design application for biodiesel production: Formulation and characterization of hybrid oil as feedstock.* Fuel, 252, 135–142.