

Supporting information

Prediction Model for Optimal Efficiency of the Green Corrosion Inhibitor Oleoylsarcosine: Optimization by Statistical Testing of the Relevant Influencing Factors

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Table S1. The complete response table for the four independent variables and their three levels. The efficiency is the output of 27 individual runs based on the Box-Behnken design (BBD).

No	IE (%)	A			B			C			D		
		-1	0	+1	-1	0	+1	-1	0	+1	-1	0	+1
1	85.20	85.20			85.20				85.20			85.20	
2	77.99	77.99					77.99		77.99			77.99	
3	66.77			66.77	66.77				66.77			66.77	
4	69.87			69.87			69.87		69.87			69.87	
5	89.11		89.11			89.11		89.11			89.11		
6	92.06		92.06			92.06		92.06					92.06
7	39.94		39.94			39.94				39.94	39.94		
8	37.86		37.86			37.86				37.86			37.86
9	70.05	70.05				70.05			70.05		70.05		
10	52.40	52.40				52.40			52.40				52.40
11	85.57			85.57		85.57			85.57		85.57		
12	74.59			74.59		74.59			74.59				74.59
13	92.86		92.86		92.86			92.86				92.86	
14	50.15		50.15		50.15					50.15		50.15	
15	91.96		91.96				91.96	91.96					01.96
16	41.80		41.80				41.80			41.80		41.80	
17	91.98	91.98				91.98		91.35					91.98
18	54.26	54.26				54.26				54.26		54.26	
19	94.35			94.35		94.35		94.35				94.35	
20	46.03			46.03		46.03				46.03		46.03	
21	86.46		86.46		86.46				86.46		86.46		
22	80.63		80.63		80.63				80.63				80.63
23	76.51		76.51				76.51		76.51		76.51		
24	73.55		73.55				73.55		73.55				73.55
25	74.23		74.23			74.23			74.23			74.23	
26	74.23		74.23			74.23			74.23			74.23	
27	74.23		74.23			74.23			74.23			74.23	
Value	27	6	15	6	6	15		6	15	6	6	15	6
Av.	72.02	71.98	71.70	72.86	77.01	70.06		92.05	74.82	45.01	74.61	72.39	68.52
Effect = High-Low			1.158			6.952			47.046			6.091	

No	IE (%)	AB			AC			AD			BC		
		-1	0	+1	-1	0	+1	-1	0	+1	-1	0	+1
1	85.20			85.20		85.20			85.20			85.20	
2	77.99	77.99				77.99			77.99			77.99	
3	66.77	66.77				66.77			66.77			66.77	
4	69.87			69.87		69.87			69.87			69.87	
5	89.11		89.11			89.11			89.11			89.11	
6	92.06		92.06			92.06			92.06			92.06	
7	39.94		39.94			39.94			39.94			39.94	
8	37.86		37.86			37.86			37.86			37.86	
9	70.05		70.05			70.05				70.05		70.05	
10	52.40		52.40			52.40		52.40				52.40	
11	85.57		85.57			85.57		85.57				85.57	
12	74.59		74.59			74.59				74.59		74.59	
13	92.86		92.86			92.86			92.86				92.86
14	50.15		50.15			50.15			50.15		50.15		
15	91.96		91.96			91.96			91.96		91.96		
16	41.80		41.80			41.80			41.80				41.80
17	91.98		91.98				91.98		91.98			91.98	
18	54.26		54.26		54.26				54.26			54.26	
19	94.35		94.35		94.35				94.35			94.35	
20	46.03		46.03				46.03		46.03			46.03	
21	86.46		86.46			86.46			86.46			86.46	
22	80.63		80.63			80.63			80.63			80.63	
23	76.51		76.51			76.51			76.51			76.51	
24	73.55		73.55			73.55			73.55			73.55	
25	74.23		74.23			74.23			74.23			74.23	
26	74.23		74.23			74.23			74.23			74.23	
27	74.23		74.23			74.23			74.23			74.23	
Value	27	2	23	2	2	23	2	2	23	2	2	23	2
Av.	72.02	72.38	71.51	77.54	74.31	72.09	69.01	68.99	72.26	72.32	71.06	72.52	67.33
Effect = High-Low			6.021			5.300			3.335			5.186	

No	IE (%)	BD			CD			ABC			ABD		
		-1	0	+1	-1	0	+1	-1	0	+1	-1	0	+1
1	85.20		85.20			85.20			85.20			85.20	
2	77.99		77.99			77.99			77.99			77.99	
3	66.77		66.77			66.77			66.77			66.77	
4	69.87		69.87			69.87			69.87			69.87	
5	89.11		89.11				89.11		89.11			89.11	
6	92.06		92.06		92.06				92.06			92.06	
7	39.94		39.94		39.94				39.94			39.94	
8	37.86		37.86				37.86		37.86			37.86	
9	70.05		70.05			70.05			70.05			70.05	
10	52.40		52.40			52.40			52.40			52.40	
11	85.57		85.57			85.57			85.57			85.57	
12	74.59		74.59			74.59			74.59			74.59	
13	92.86		92.86			92.86			92.86			92.86	
14	50.15		50.15			50.15			50.15			50.15	
15	91.96		91.96			91.96			91.96			91.96	
16	41.80		41.80			41.80			41.80			41.80	
17	91.98		91.98			91.98			91.98			91.98	
18	54.26		54.26			54.26			54.26			54.26	
19	94.35		94.35			94.35			94.35			94.35	
20	46.03		46.03			46.03			46.03			46.03	
21	86.46			86.46		86.46			86.46			86.46	
22	80.63	80.63				80.63			80.63			80.63	
23	76.51	76.51				76.51			76.51			76.51	
24	73.55			73.55		73.55			73.55			73.55	
25	74.23		74.23			74.23			74.23			74.23	
26	74.23		74.23			74.23			74.23			74.23	
27	74.23		74.23			74.23			74.23			74.23	
Value	27	2	23	2	2	23	2	0	27	0	0	27	0
Av.	72.02	78.57	70.76	80.01	66.00	73.29	63.49		72.02			72.02	
Effect = High-Low			9.244			9.805							

No	IE (%)	ACD			CBD			ABCD		
		-1	0	+1	-1	0	+1	-1	0	+1
1	85.20		85.20			85.20			85.20	
2	77.99		77.99			77.99			77.99	
3	66.77		66.77			66.77			66.77	
4	69.87		69.87			69.87			69.87	
5	89.11		89.11			89.11			89.11	
6	92.06		92.06			92.06			92.06	
7	39.94		39.94			39.94			39.94	
8	37.86		37.86			37.86			37.86	
9	70.05		70.05			70.05			70.05	
10	52.40		52.40			52.40			52.40	
11	85.57		85.57			85.57			85.57	
12	74.59		74.59			74.59			74.59	
13	92.86		92.86			92.86			92.86	
14	50.15		50.15			50.15			50.15	
15	91.96		91.96			91.96			91.96	
16	41.80		41.80			41.80			41.80	
17	91.98		91.98			91.98			91.98	
18	54.26		54.26			54.26			54.26	
19	94.35		94.35			94.35			94.35	
20	46.03		46.03			46.03			46.03	
21	86.46		86.46			86.46			86.46	
22	80.63		80.63			80.63			80.63	
23	76.51		76.51			76.51			76.51	
24	73.55		73.55			73.55			73.55	
25	74.23		74.23			74.23			74.23	
26	74.23		74.23			74.23			74.23	
27	74.23		74.23			74.23			74.23	
Valu e	27	0	27	0	0	27	0	0	27	0
Av.	72.02		72.02			72.02			72.02	
Effect = High-Low										

S2: Details of optimization by implementing the response surface method (RSM) in Minitab17 based on the Box-Behnken Design (BBD)

Box-Behnken Design

Factors: 4 Replicates: 1
Base runs: 27 Total runs: 27
Base blocks: 1 Total blocks: 1

Center points: 3

Response Surface Regression: Eff.% versus A, B, C, D

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	14	7264.74	518.91	7.10	0.001
Linear	4	6830.80	1707.70	23.37	0.000
A	1	2.34	2.34	0.03	0.861
B	1	76.96	76.96	1.05	0.325
C	1	6640.17	6640.17	90.89	0.000
D	1	111.33	111.33	1.52	0.241
Square	4	345.89	86.47	1.18	0.367
A*A	1	0.28	0.28	0.00	0.951
B*B	1	43.50	43.50	0.60	0.455
C*C	1	196.37	196.37	2.69	0.127
D*D	1	12.35	12.35	0.17	0.688
2-Way Interaction	6	88.05	14.67	0.20	0.970
A*B	1	26.57	26.57	0.36	0.558
A*C	1	28.09	28.09	0.38	0.547
A*D	1	11.12	11.12	0.15	0.703
B*C	1	13.88	13.88	0.19	0.671
B*D	1	2.06	2.06	0.03	0.869
C*D	1	6.33	6.33	0.09	0.774
Error	12	876.72	73.06		
Lack-of-Fit	10	876.72	87.67	*	*
Pure Error	2	0.00	0.00		
Total	26	8141.45			

Model Summary

S R-sq
8.54750 89.23%

The above analysis is used to determine the acceptance of the selected method for the factor optimization. The square regression coefficient R-sq indicates the acceptance of the RSM and yields 89.2%, which turns out to be a good choice.

To determine the coefficient values of the second-order model according to Eq. 4, in Minitab 17 the following step was implemented and thereafter applied the values in the Eq. 4 as described below:

S3: Coded Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	74.23	4.93	15.04	0.000	
A	0.44	2.47	0.18	0.861	1.00
B	-2.53	2.47	-1.03	0.325	1.00
C	-23.52	2.47	-9.53	0.000	1.00
D	-3.05	2.47	-1.23	0.241	1.00
A*A	-0.23	3.70	-0.06	0.951	1.25
B*B	2.86	3.70	0.77	0.455	1.25
C*C	-6.07	3.70	-1.64	0.127	1.25
D*D	-1.52	3.70	-0.41	0.688	1.25
A*B	2.58	4.27	0.60	0.558	1.00
A*C	-2.65	4.27	-0.62	0.547	1.00
A*D	1.67	4.27	0.39	0.703	1.00
B*C	-1.86	4.27	-0.44	0.671	1.00
B*D	0.72	4.27	0.17	0.869	1.00
C*D	-1.26	4.27	-0.29	0.774	1.00

Regression Equation in uncoded units

$$\begin{aligned}\text{Eff.}\% = & 74.23 + 0.44 A - 2.53 B - 23.52 C - 3.05 D - 0.23 A*A + 2.86 B*B \\ & - 6.07 C*C - 1.52 D*D + 2.58 A*B - 2.65 A*C + 1.67 A*D - 1.86 B*C \\ & + 0.72 B*D - 1.26 C*D\end{aligned}$$

The above equation is used to predict the optimal efficiency that can be achieved by choosing the best level for each variable.