Modeling the biodiesel production using the wheat straw ash as a catalyst

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Table S-1. Experimental matrix (Replicates: runs 13/14, 27/28, 41/42, 55/56, and 69/7.)

Run	Factor A	Factor B	Factor C	Factor D	Content of FAME, % (Y)
1	55	15	18	60	23.7
2	65	15	18	60	67.4
3	55	15	24	60	37.2
4	65	15	24	60	36.5
5	55	10	21	60	49.4
6	65	10	21	60	41.6
7	55	20	21	60	15.6
8	65	20	21	60	11.2
9	60	10	18	60	73.8
10	60	10	24	60	40.9
11	60	20	18	60	32.2
12	60	20	24	60	18.2
13	60	15	21	60	74.0
14	60	15	21	60	81.9
15	55	15	18	90	45.3
16	65	15	18	90	84.8
17	55	15	24	90	68.1
18	65	15	24	90	85.9
19	55	10	21	90	73.5
20	65	10	21	90	68.4
21	55	20	21	90	35.7
22	65	20	21	90	25.9
23	60	10	18	90	91.7
24	60	10	24	90	64.2
25	60	20	18	90	59.7
26	60	20	24	90	35.2
27	60	15	21	90	91.1
28	60	15	21	90	93.1
29	55	15	18	120	57.8
30	65	15	18	120	92.4
31	55	15	24	120	76.0
32	65	15	24	120	94.9
33	55	10	21	120	85.3
34	65	10	21	120	76.9
35	55	20	21	120	51.9
36	65	20	21	120	23.0
37	60	10	18	120	95.8
38	60	10	24	120	82.3
39	60	20	18	120	74.8
40	60	20	24	120	52.5
41	60	15	21	120	95.0
42	60	15	21	120	95.7
43	55	15	18	180	79.9
44	65	15	18	180	97.5
45	55	15	24	180	93.4

| Run	Factor *A*	Factor *B*	Factor *C*	Factor *D*	Content of FAME, % (*Y*)
46	65	15	24	180	98.4
47	55	10	21	180	95.4
48	65	10	21	180	94.1
49	55	20	21	180	79.3
50	65	20	21	180	63.9
51	60	10	18	180	98.1
52	60	10	24	180	91.4
53	60	20	18	180	91.3
54	60	20	24	180	78.6
55	60	15	21	180	97.5
56	60	15	21	180	96.5
57	55	15	18	240	93.1
58	65	15	18	240	97.5
59	55	15	24	240	98.2
60	65	15	24	240	98.4
61	55	10	21	240	97.8
62	65	10	21	240	94.1
63	55	20	21	240	90.6
64	65	20	21	240	78.5
65	60	10	18	240	98.6
66	60	10	24	240	94.9
67	60	20	18	240	96.1
68	60	20	24	240	91.2
69	60	15	21	240	98.4
70	60	15	21	240	96.7
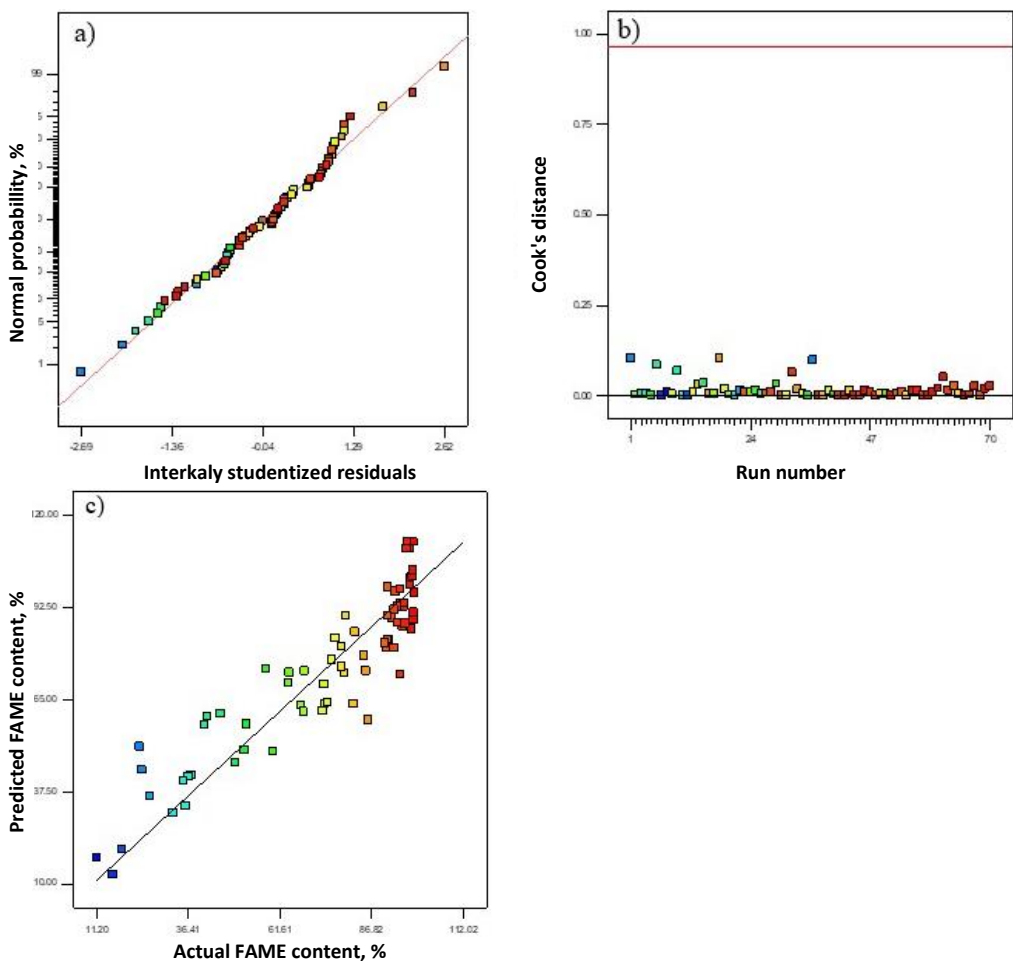
Fig. S-1. Normal probability plot of residuals (a), Cook's distance (b), and predicted versus actual values of FAME content for the developed quadratic model
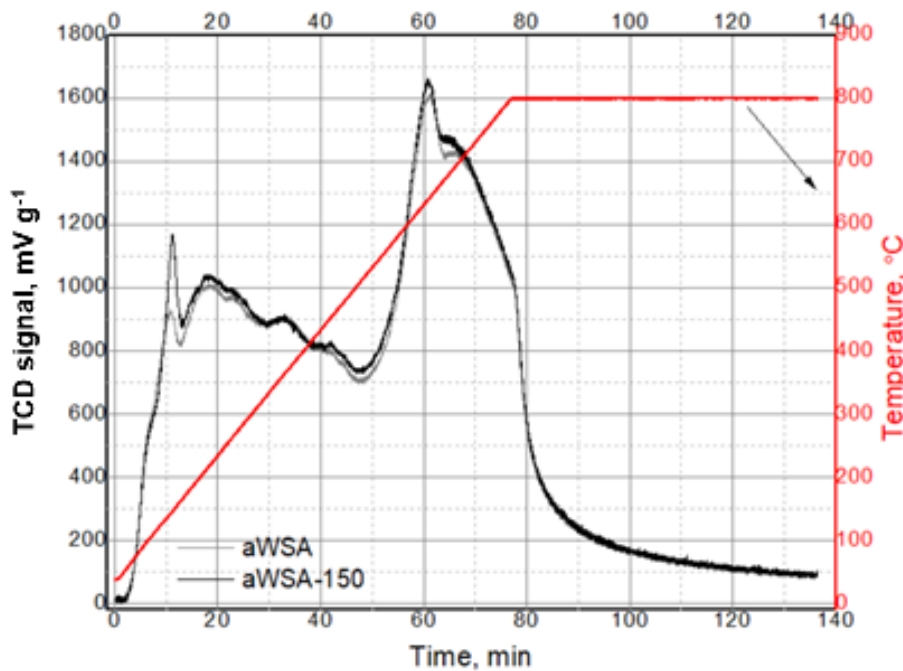
Fig. S-2 Checking the reproducibility of TCD for the differently aged fWSA sample; aWSA aging time 40 days and aWSA-150 aging time 150 days

Adequacy of the historical data design-based models

Table S-2. Results of sequential model sum of squares test

Source	Sum of squares	df	Mean square	*F*-value	*p*-value	Remark
Mean *vs:* Total	380351.0	1	380351.0			
Linear *vs.* Mean	27342.1	4	6835.5	24.7	< 0.0001	
2FI *vs.* Linear	2104.2	6	350.7	1.3	0.271	
Quadratic vs 2FI	8765.7	4	2191.4	16.9	< 0.0001	**Suggested**
Cubic *vs.* Quadratic	5597.1	13	430.5	11.6	< 0.0001	Aliased
Residual	1553.7	42	37.0			
Total	425713.7	70	6081.6			

The test selects the highest order polynomial, where the additional terms are significant, and the model is not aliased.

Table S-3. Results of lack of fit test

Source	Sum of squares	df	Mean square	F value	p value	Remark
Linear	17985.3	60	299.8	42.3	0.0003	
2FI	15881.1	54	294.1	41.5	0.0003	
Quadratic	7115.4	50	142.3	20.1	0.0016	**Suggested**
Cubic	1518.3	37	41.0	5.8	0.0288	Aliased
Pure Error	35.4	5	7.1			

It wants the selected model to have insignificant lack-of-fit.

Table S-4. Results of model summary statistics test. This test focuses on the model maximizing the R^2_{adj}. PRESS - Predicted Residual Sum of Squares for the model

Source	Standard deviation	R^2	R^2_{adj}	R^2_{pred}	PRESS	Remark
Linear	16.7	0.603	0.578	0.546	20592.8	
2FI	16.4	0.649	0.590	0.528	21389.1	
Quadratic	11.4	0.842	0.802	0.754	11161.3	**Suggested**
Cubic	6.1	0.966	0.944	0.876	5643.3	Aliased

ANOVA results for the quadratic model

Final quadratic equation in terms of coded and actual factors

Coded factors:

$Y = 103.68 + 1.70A - 11.60B - 2.43C + 24.21D - 2.22AB - 4.93AC - 3.03AD + 0.30BC + 7.31BD +$
$+ 3.32CD - 13.07A^2 - 16.32B^2 - 2.60C^2 - 15.86D^2$ (S 1)

Actual factors:

$Y = 2578.59 + 72.32A + 19.73B + 28.90C + 0.759D - 0.089AB - 0.329AC - 0.007AD + 0.020BC +$
$+0.016BD + 0.012CD - 0.523A^2 - 0.653B^2 - 0.289C^2 - 0.002D^2$ (S 2)

Statistical criteria:

$R^2 = 0.842$, $R^2_{adj} = 0.802$, $R^2_{pred} = 0.745$, MRPD = ±14.6 %, C.V. = 15.5 %, and Adeq. Prec. = 18.8.

Table S-5. Optimal process conditions based on the quadratic equation

A	B	C	D	Y / %
60.3	**11.6**	**18.3**	**124**	**98.6** [a]
61.1	12.3	18.4	118	98.6
60.5	16.6	18.5	149	98.6
63.2	15.2	18.5	138	98.6
60.1	11.3	18.6	127	98.6
56.4	14.3	18.8	167	98.6
57.3	10.3	20.2	220	98.6
64.0	12.3	21.1	149	98.6
64.5	13.3	22.0	170	98.6
62.4	10.8	22.2	151	98.6
64.1	14.6	22.8	183	98.6
58.6	13.8	22.8	138	98.6
62.3	15.1	22.9	155	98.6
63.1	16.2	23.0	185	98.6
57.1	13.4	23.1	149	98.6
62.9	13.9	23.6	162	98.6
55.4	16.1	23.6	188	98.6
63.2	11.4	23.9	219	98.6
56.9	11.6	24.0	165	98.6

[a]The selected optimal process conditions: temperature of 60.3 ℃, catalyst loading of 11.6 % (based on the oil mass), methanol-to-oil molar ratio of 18.3, and reaction time of 124 min. Desirability = 1 in all runs.