Supplementary material

Kinetic modeling and optimization of sunflower oil methanolysis catalyzed by spherically-shaped $CaO/\gamma\text{-}Al_2O_3$ catalyst

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The obtained full quadratic model equations with codded and actual factors are as follows, respectively:

$$y = 93.87 - 0.62 \cdot X_1 + 19.76 \cdot X_2 + 24.22 \cdot X_3 - \\ -2.58 \cdot X_1 \cdot X_2 + 6.84 \cdot X_1 \cdot X_3 - 10.61 \cdot X_2 \cdot X_3 + \\ +0.0027 \cdot X_1^2 - 16.42 \cdot X_2^2 - 11.43 \cdot X_3^2 \quad \text{(S1)}$$

and

$$y = -211.37 - 3.76 \cdot X_1 + 693.56 \cdot X_2 + 40.27 \cdot 3 - \\ -4.31 \cdot X_1 \cdot X_2 + 1.14 \cdot X_1 \cdot X_3 - 26.51 \cdot X_2 \cdot X_3 + \\ +0.0003 \cdot X_1^2 - 410.50 \cdot X_2^2 - 2.86 \cdot X_3^2 \quad \text{(S2)}$$

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Table S1. CCCD matrix for the sunflower oil methanolysis over the $CaO/\gamma\text{-}Al_2O_3$ catalyst.

No	Coded factor			Actual factor			FAME content, %		RPD, %
	X_1	X_2	X_3	X_1	X_2	X_3	Actual	Modeled[a]	
1	-1	-1	-1	9	0.3	3	20.3	18.9	+6.9
2	1	-1	-1	15	0.3	3	4.1	4.0	+2.4
3	-1	1	-1	9	0.7	3	78.0	79.6	-2.1
4	1	1	-1	15	0.7	3	59.0	64.7	-9.7
5	-1	-1	1	9	0.3	7	75.3	74.9	+0.5
6	1	-1	1	15	0.3	7	94.0	87.3	+7.1
7	-1	1	1	9	0.7	7	98.1	93.2	+5.0
8	1	1	1	15	0.7	7	98.9	105.6	-6.8
9	-1.68	0	0	7	0.5	5	91.8	94.9	-3.4
10	1.68	0	0	17	0.5	5	96.1	92.8	+3.4
11	0	-1.68	0	12	0.164	5	9.0	14.2	-57.8
12	0	1.68	0	12	0.836	5	86.0	80.7	+6.2
13	0	0	-1.68	12	0.5	1.64	24.2	20.8	+14.1
14	0	0	1.68	12	0.5	8.36	99.0	102.3	-3.3
15	0	0	0	12	0.5	5	98.5	93.9	+4.7
16	0	0	0	12	0.5	5	96.2	93.9	+2.4
17	0	0	0	12	0.5	5	89.9	93.9	-4.5
18	0	0	0	12	0.5	5	98.1	93.9	+4.3
19	0	0	0	12	0.5	5	96.5	93.9	+2.7
20	0	0	0	12	0.5	5	84.0	93.9	-11.8
								MRPD, %	±2.0

[a]A reduced regression model is used for calculation. RPD - relative percentage deviation, MRPD – mean relative percentage deviation.

Table S2 ANOVA analysis for the full quadratic model.

Source	Sum of squares	Degrees of freedom	Mean squere	*F*-value	*p*-value
Model	20052.06	9	2228.01	61.75	< 0.0001
X_1 (Molar ratio)	5.23	1	5.23	0.14	0.712
X_2 (Catalyst loading)	5332.37	1	5332.37	147.79	< 0.0001
X_3 (Reaction time)	8009.88	1	8009.88	222.01	< 0.0001
X_1X_2	53.46	1	53.46	1.48	0.252
X_1X_3	374.28	1	374.28	10.37	0.0092
X_2X_3	899.73	1	899.73	24.94	0.0005
X_1^2	$1.052 \cdot e^{-4}$	1	$1.052 \cdot e^{-4}$	$6.00 \cdot e^{-6}$	0.999
X_2^2	3885.45	1	3885.45	107.69	< 0.0001
X_3^2	1883.74	1	1883.74	52.21	< 0.0001
Pure error	164.85	5	32.97		
Lack-of-fit	195.94	5	39.19	1.19	0.427
Total correction	20412.85	19			

R^2 = 0.982; R^2_{adj} = 0.966; R^2_{pred} = 0.913; *C.V.* = 8.0% and *Adequate Precision* = 22.7

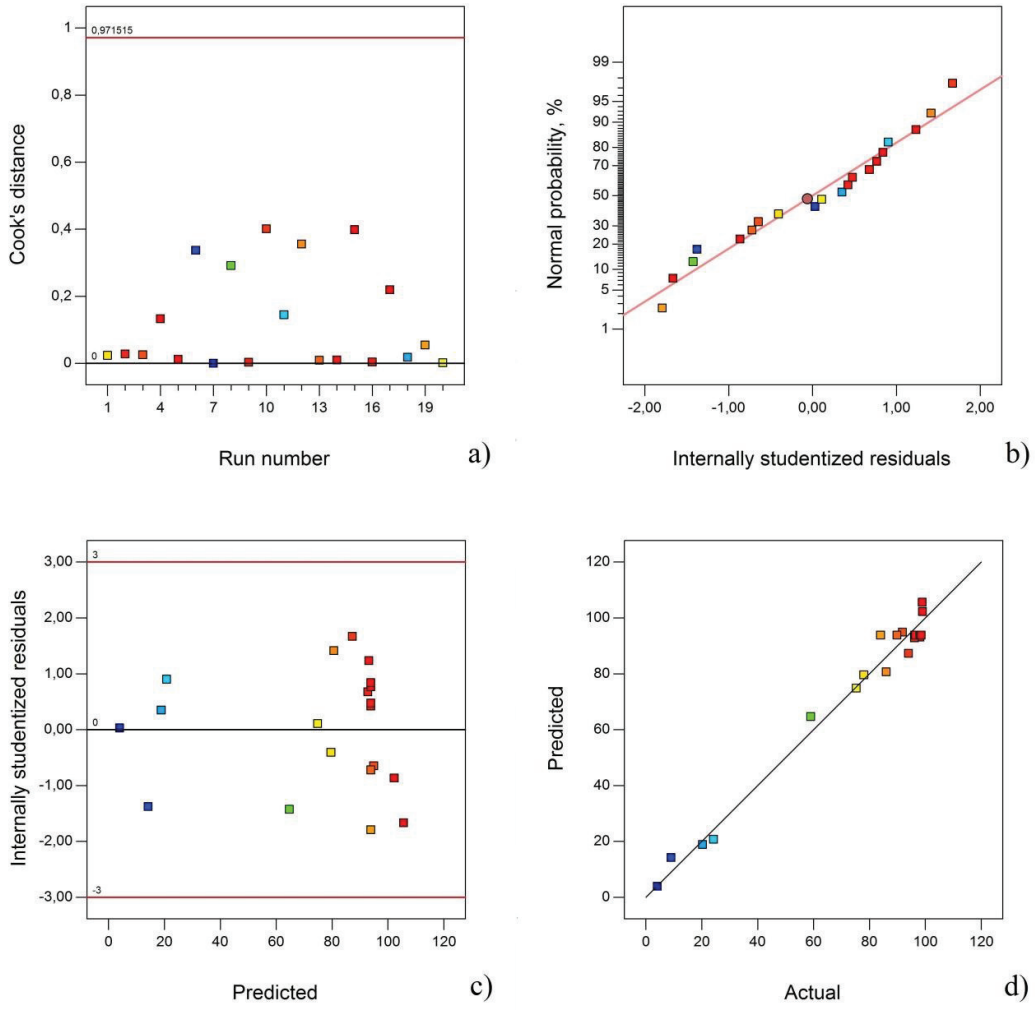

Figure S1 Statistical evaluations of the reduced quadratic model: (a) Cook's distance, (b) normal probability, (c) model outliers and (d) actual and predicted FAME content plot.