One-pot synthesis of titanium isophthalate and highly active catalytic glycolysis of waste PET

Ruiyang Wen, Guoliang Shen*, Meiqi Zhang, Yang Yu, Shijie Xu

School of Petrochemical Engineering, Shenyang University of Technology,

Liaoyang 111003, China

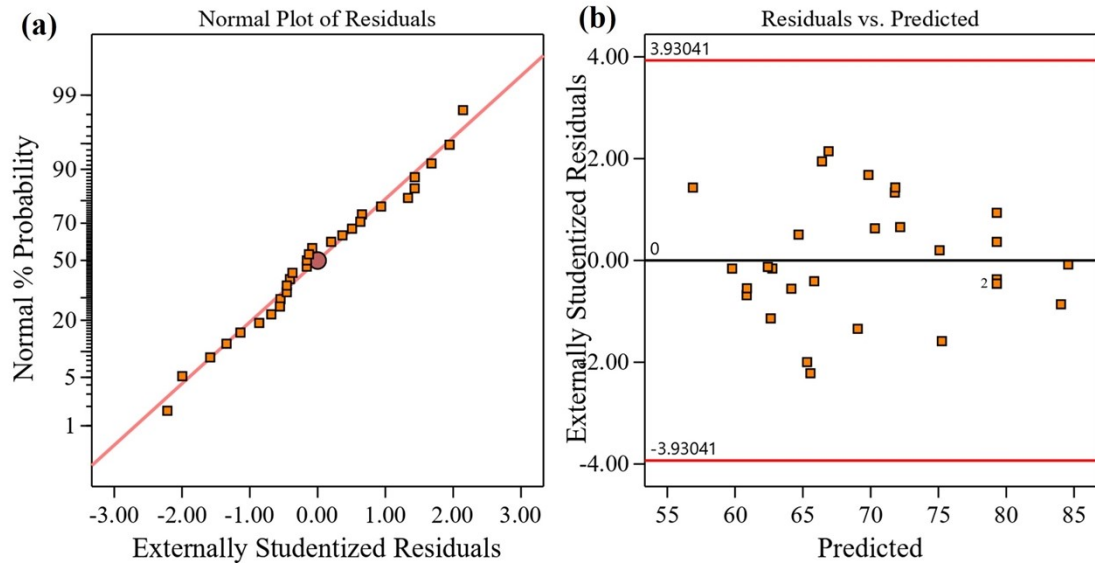**Tab. S1 Results of the experimental and predicted values**

Fig. S1 Tests of RSM model predictions and actual

Based on the preliminary experiments described above, the results of the full factorial BBD design with three levels of four factors and the BHET yields are presented in Tab. S1.

Tab. S1 Results of the experimental and predicted values

Run	A	B	C	D	Yield of BHET/%		Residual/%
					Actual	Predicted	
1	0	0	1	1	59.44	60.88	-1.44
2	0	-1	0	-1	65.70	69.05	-3.35
3	0	0	-1	1	59.36	59.78	-0.43
4	0	0	1	-1	75.36	71.82	3.54
5	1	1	0	0	75.11	71.79	3.32
6	1	0	0	1	64.76	65.84	-1.08
7	-1	1	0	0	71.80	66.90	4.90
8	0	0	0	0	82.64	79.30	3.34
9	-1	-1	0	0	84.36	84.57	-0.21
10	0	1	-1	0	60.54	65.56	-5.02
11	0	0	0	0	77.94	79.30	-1.36
12	0	0	0	0	77.64	79.30	-1.66
13	-1	0	0	-1	81.81	84.04	-2.23
14	-1	0	0	1	60.67	65.31	-4.64
15	0	0	0	0	80.64	79.30	1.34
16	-1	0	1	0	75.61	75.08	0.53
17	-1	0	-1	0	71.97	70.31	1.65
18	0	1	0	-1	71.39	75.25	-3.86
19	0	1	0	1	60.43	56.89	3.54
20	0	-1	1	0	73.89	72.18	1.71

Fig. S1(a) depicts the normal distribution of the residuals of the model. It can be observed that the residuals are uniformly distributed on both sides of the center value and exhibit a satisfactory fit. Fig. S1(b) presents a comparison of the residuals with the predicted values. The positive and negative residuals indicate the discrepancy between the predicted value and the actual value of the model. The residuals have been distributed within the allowable error line (±3.93041). The combination of the two graphs serves to illustrate the reliability and scientific validity of the model.

Fig. S1 Tests of RSM model predictions and actual

(a) normal plot of residuals; (b) residuals vs predicted.