

## Supplementary material to

### PROCESS MODELING AND KINETIC ESTIMATION FOR DESULFURIZATION OF DIESEL FUEL USING NANO - ZnO/ Al<sub>2</sub>O<sub>3</sub>

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*Chem. Ind. Chem. Eng. Q.* 30 (2) 151–159 (2024)

*Table S1. The most accurate model parameters of ODS reaction for 3% ZnO/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.*

Parameter	Value	Unit
n	1.998	–
EA	27.736	KJ/mol.
A <sub>0</sub>	5020.569	wt <sup>-0.998</sup> .min <sup>-1</sup>
SSE	3.334 × 10 <sup>-5</sup>	–

*Table S2. The most accurate model parameters of ODS reaction for 6% ZnO/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.*

Parameter	Value	Unit
n	1.982	–
EA	26.028	KJ/mol.
A <sub>0</sub>	5138.720	wt <sup>-0.982</sup> .min <sup>-1</sup>
SSE	1.934 × 10 <sup>-5</sup>	–

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Table S3. The most accurate model parameters of ODS reaction for 9% ZnO/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Parameter	Value	Unit
n	1.952	–
EA	24.000	KJ/mol.
A <sub>0</sub>	6999.992	wt <sup>-0.952</sup> .min <sup>-1</sup>
SSE	4.387 × 10 <sup>-6</sup>	–

Table S4. Experimental and simulation results for 3% ZnO/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Temperature (°C)	Reaction time (min)	DBT content (ppm)		DBT conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	534	554.564	12.602	9.237	3.851
30	40	488	507.665	20.131	16.912	4.030
30	60	450	468.076	26.350	23.392	4.017
30	80	419	434.210	31.424	28.935	3.630
50	20	488	508.639	20.131	16.753	4.229
50	40	435	435.637	28.805	28.701	0.146
50	60	385	380.950	36.989	37.651	1.052
50	80	339	338.455	44.517	44.606	0.161
70	20	426	446.781	30.278	26.877	4.878
70	40	368	352.106	39.771	42.372	4.319
70	60	305	290.524	50.082	52.451	4.746
70	80	260	247.267	57.447	59.531	4.897
90	20	393	375.250	35.679	38.584	4.517
90	40	283	270.730	53.682	55.691	4.336
90	60	211	211.733	65.466	65.346	0.347
90	80	175	173.839	71.358	71.548	0.663

Table S5. Experimental and simulation results for 6% ZnO/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Temperature (°C)	Reaction time (min)	DBT content (ppm)		DBT conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	485	502.780	20.622	17.712	3.666
30	40	409	426.920	33.061	30.128	4.381
30	60	360	370.818	41.080	39.310	3.005
30	80	315	327.625	48.445	46.379	4.008
50	20	415	433.731	32.079	29.013	4.513
50	40	340	335.790	44.354	45.043	1.238
50	60	285	273.728	53.355	55.200	3.955
50	80	221	230.908	63.830	62.208	4.483
70	20	360	355.088	41.080	41.884	1.364
70	40	261	249.691	57.283	59.134	4.333
70	60	185	192.304	69.722	68.526	3.948
70	80	150	156.245	75.450	74.428	4.163
90	20	268	278.380	56.137	54.439	3.873
90	40	187	179.597	69.394	70.606	3.959
90	60	132	132.334	78.396	78.341	0.253
90	80	109	104.660	82.160	82.871	3.982

Table S6. Experimental and simulation results for 9% ZnO/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Temperature (°C)	Reaction time (min)	DBT content (ppm)		DBT conversion %		Error %
		Experimental	Predicted	Experimental	Predicted	
30	20	360	354.775	41.080	41.935	1.451
30	40	261	248.406	57.283	59.344	4.825
30	60	191	190.460	68.740	68.828	0.283
30	80	149	154.103	75.614	74.779	3.425
50	20	265	264.038	56.628	56.786	0.363
50	40	170	166.620	72.177	72.730	1.988
50	60	119	121.114	80.524	80.178	1.776
50	80	92	94.878	84.943	84.472	3.128
70	20	180	188.798	70.540	69.100	4.888
70	40	114	109.962	81.342	82.003	3.542
70	60	86	87.109	85.925	85.743	1.290
70	80	57	56.166	90.671	90.808	1.463
90	20	137	132.884	77.578	78.251	3.004
90	40	75	73.141	87.725	88.029	2.479
90	60	52	50.100	91.489	91.800	3.654
90	80	38	37.958	93.781	93.788	0.111

Table S7. Optimal values of operating conditions for ODS operation employing 3% ZnO/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Parameter	Value	Unit
C <sub>DBT,t</sub>	734.193	ppm
Temperature	82	°C
Time	200	min
Conversion	86	%

Table S8. Optimal values of operating conditions for ODS operation employing 6% ZnO/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Parameter	Value	Unit
C <sub>DBT,t</sub>	849.736	ppm
Temperature	77	°C
Time	190	min
Conversion	92.100	%

Table S9. Optimal values of operating conditions for ODS operation employing 9% ZnO/  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

Parameter	Value	Unit
C <sub>DBT,t</sub>	862,703	ppm
Temperature	87	°C
Time	200	min
Conversion	98.099	%

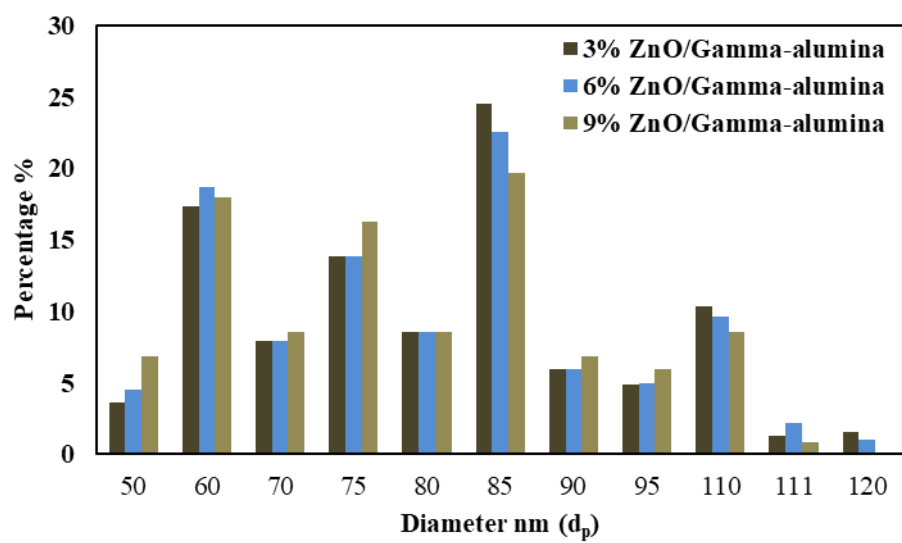


Figure S1. Particle size distribution for the synthesized nano-catalyst.