Electronic Supplementary Information

Study on performance and mechanism for aerobic oxidative desulfurization based on the dual-functional material possessing catalytic and adsorptive properties

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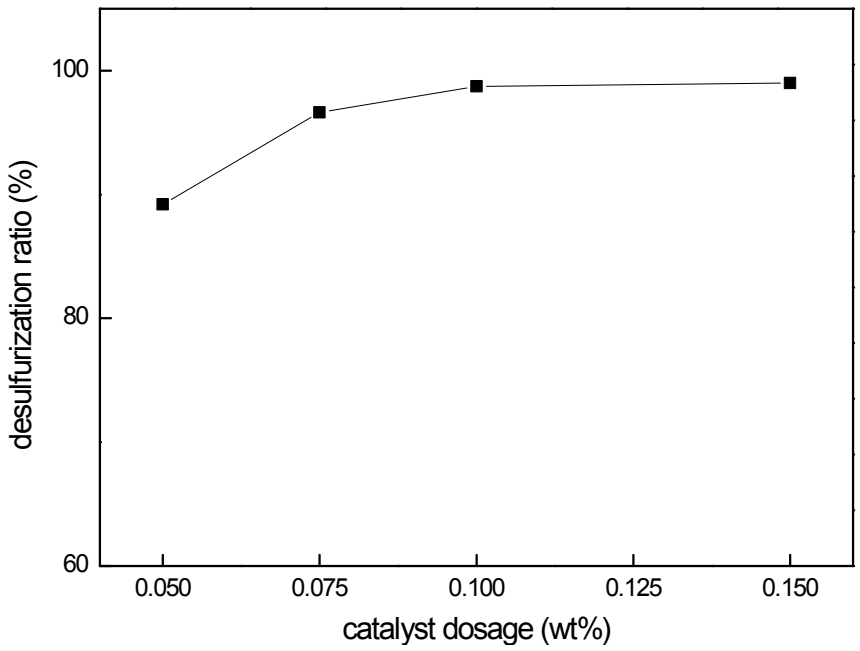
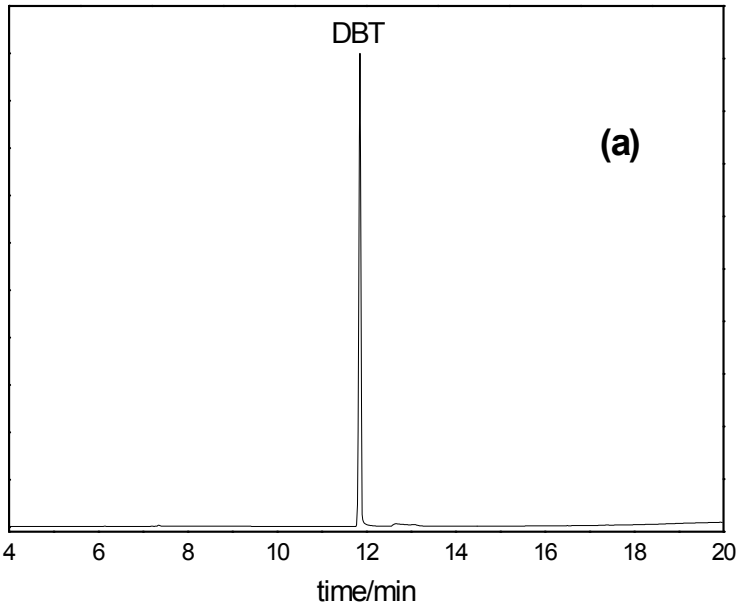


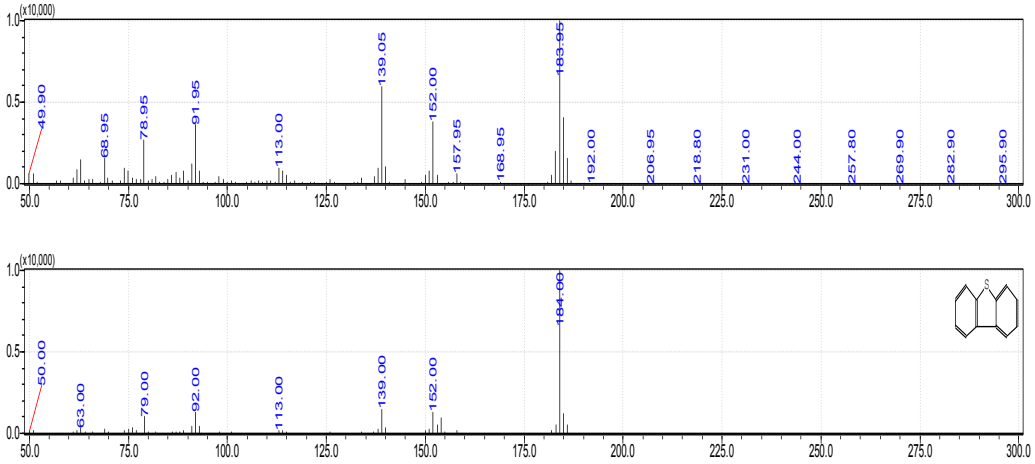
Fig. S1. The desulfurization ratio curves over catalyst dosage. (The condition was as that described in Fig. 3, and the reaction time was determined as 120 min).

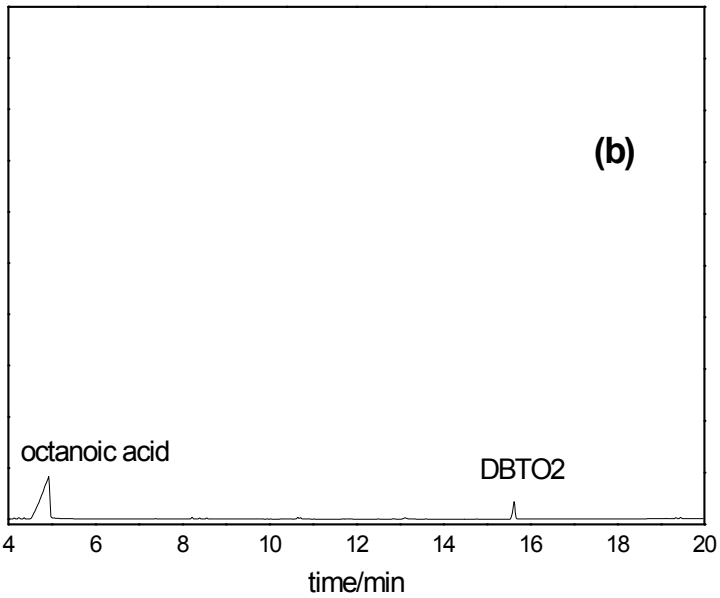
Table S1. The evaluation of selectivity to the supported catalysts for ODS.

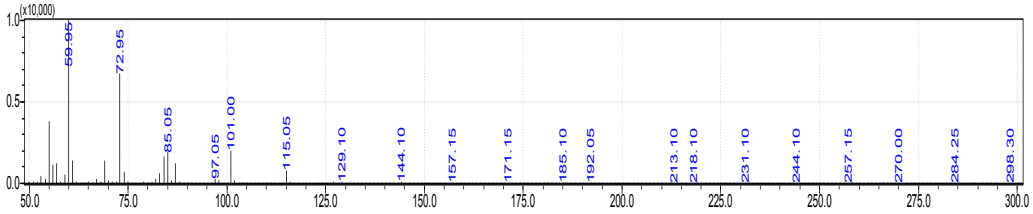
Model oil	Desulfurization ratio/%	
	After ODS treatment	After ODS treatment with extration
Sample 1	96.10	100
Sample 2	43.25	94.31
Sample 3	24.10	84.45

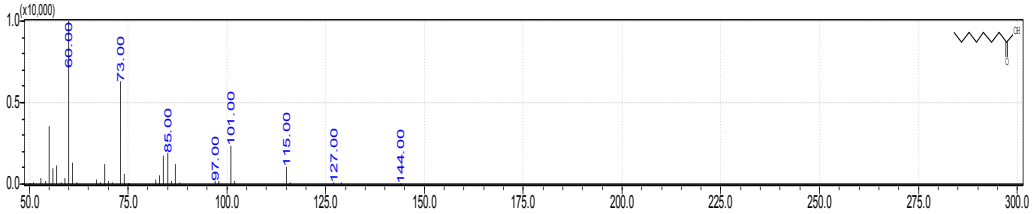
Note: Sample 1 refers to the model oil containing 250 ppmw DBT, Sample 2 refers to the simulated oil containing 250 ppmw DBT and 10% n-octylene, Sample 3 refers to the model oil containing 250 ppmw DBT and 10% xylene; the condition is as described in figure. 12.


DBT
(a)
4
6
8
10
12
14
16
18
20
time/min


(x10,000)
1.0
0.5
0.0
49.90
68.95
78.95
91.95
113.00
139.05
152.00
157.95
168.95
183.95
192.00
206.95
218.80
231.00
244.00
257.80
269.90
282.90
295.90
50.0
75.0
100.0
125.0
150.0
175.0
200.0
225.0
250.0
275.0
300.0
(x10,000)
1.0
0.5
0.0
50.00
63.00
79.00
92.00
113.00
139.00
152.00
184.00
S
50.0
75.0
100.0
125.0
150.0
175.0
200.0
225.0
250.0
275.0
300.0


(b)
octanoic acid
DBTO2
4
6
8
10
12
14
16
18
20
time/min


(x10,000)
69.95
72.95
85.05
97.05
101.00
115.05
129.10
144.10
157.15
171.15
185.10
192.05
213.10
218.10
231.10
244.10
257.15
270.00
284.25
298.30


(x10,000)
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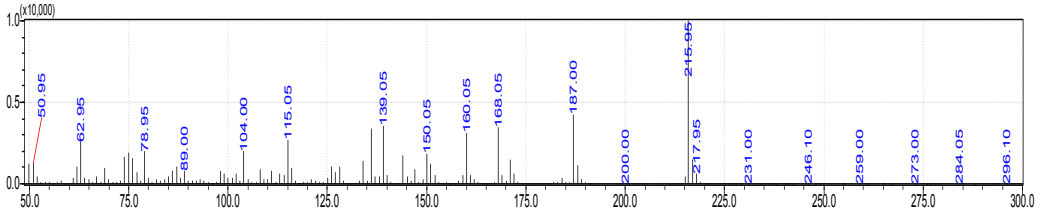
73.00
85.00
97.00
101.00
115.00
127.00
144.00


(x10,000)
50.95
62.95
78.95
89.00
104.00
115.05
139.05
150.05
160.05
168.05
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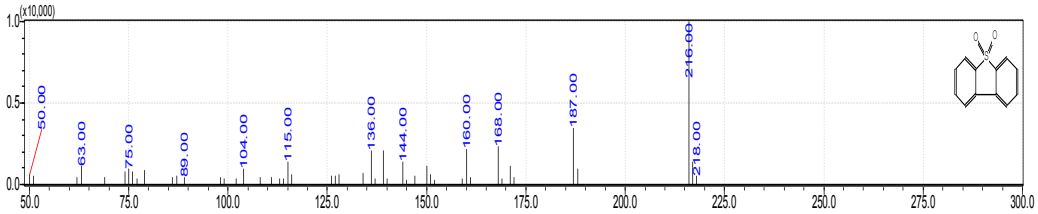
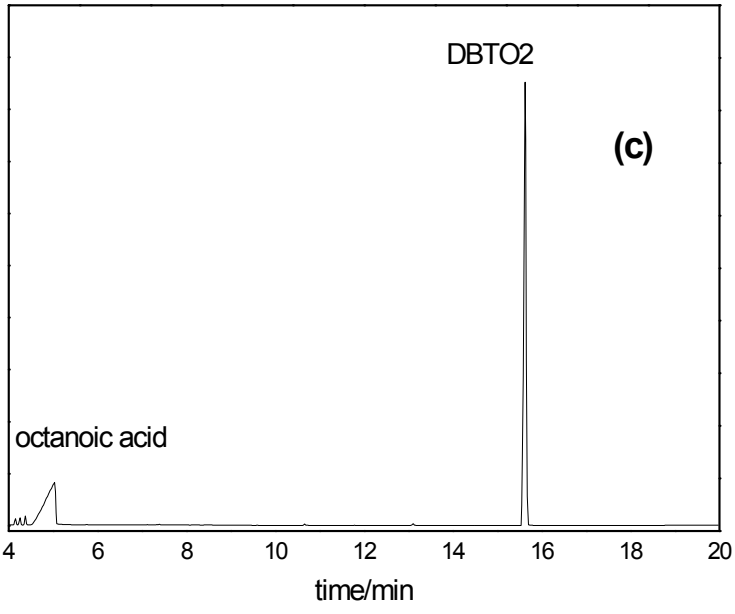
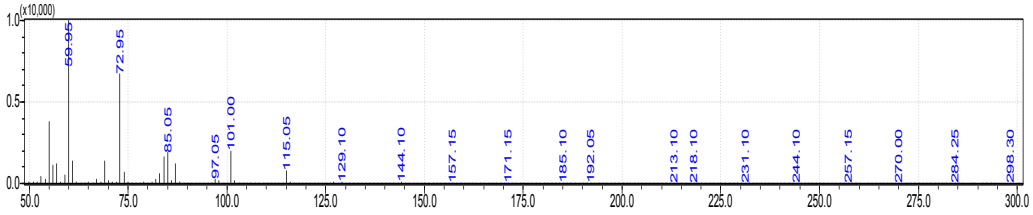
231.00
246.10
259.00
273.00
284.05
296.10


(x10,000)
50.00
63.00
75.00
89.00
104.00
115.00
136.00
144.00
160.00
168.00
187.00
216.00
218.00


DBTO2
(c)
octanoic acid
4
6
8
10
12
14
16
18
20
time/min


(x10,000)
69.95
72.95
85.05
97.05
101.00
115.05
129.10
144.10
157.15
171.15
185.10
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213.10
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244.10
257.15
270.00
284.25
298.30

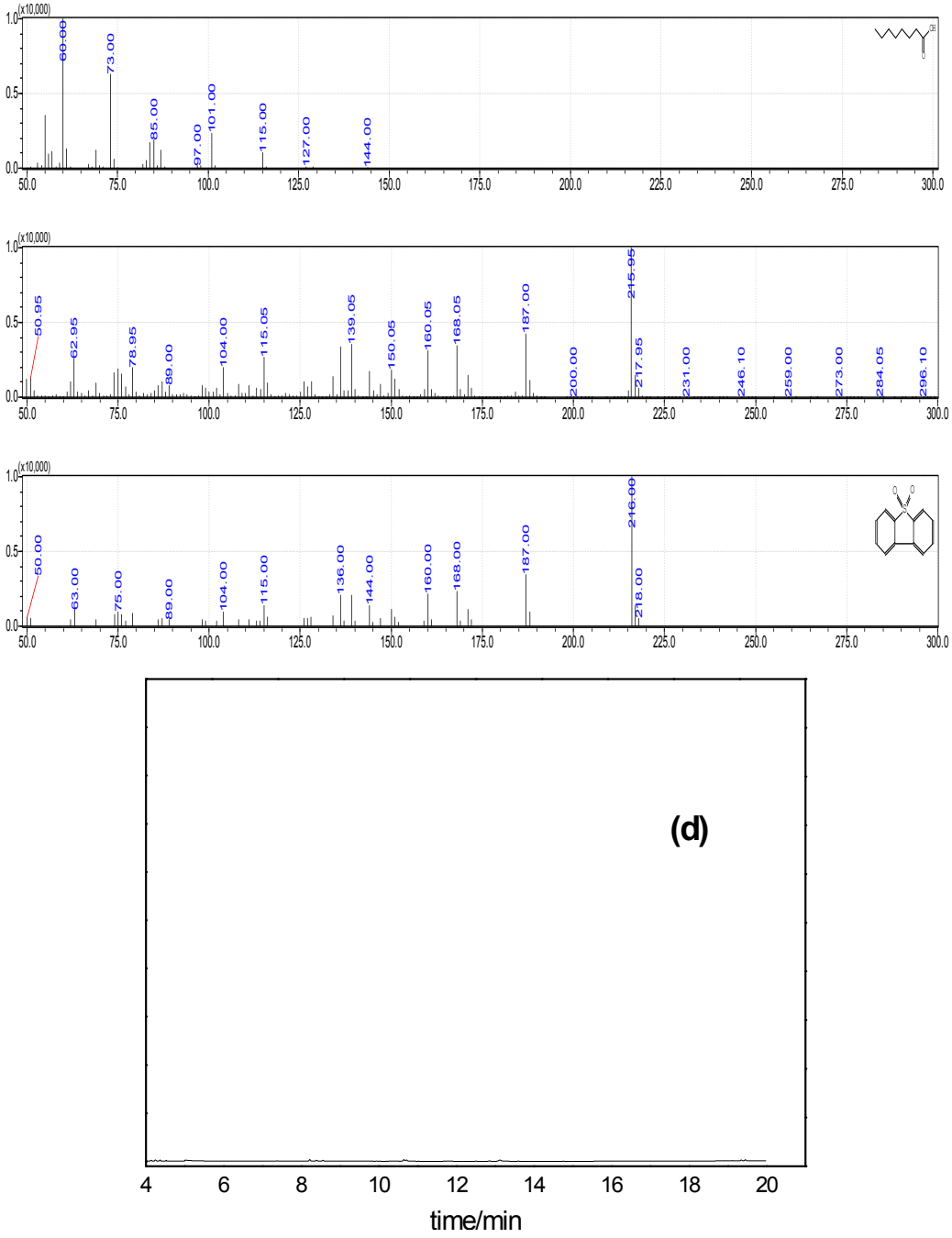

Fig. S2. The GC-MS spectra of the oxidation products ((a) before ODS reaction in the model oil; (b) after ODS reaction in the model oil; (c) after reaction in the eluent of catalyst; (d) after ODS reaction combined with extraction of MeCN in the model oil).

Table S2. The comparison between the different aerobic ODS systems.

catalyst	assistant	Solvent	oxidant	Temperature (°C)	Pressure	Reused times	Sulfur removal (%)	Ref.
$Na_4W_{10}O_{32}\cdot 8H_2O$	--	MeCN	O_2 H_2O_2	25	0.6 MPa	--	99%	S1
$H_8PV_5Mo_7O_{40}$	--	water	O_2	120	20 bar	--	99	S2
$[C_{18}H_{37}N(CH_3)_3]_5[PV_2Mo_{10}O_{40}]$	isobutyl aldehydes	MeCN	O_2	60	Atmospheric pressure	--	100	S3
CNTs	--	--	O_2	150	Atmospheric pressure	5	100	S4
HPW@MOFs	--	MeCN	O_2	90	Atmospheric pressure	--	90	S5
GO	n-octanal	--	air	60	Atmospheric pressure	3	89.21	S6
$K_6P_2W_{18}O_{62}$/GO	n-octanal	--	air	60	Atmospheric pressure	5	96.10	This work
$K_6P_2W_{18}O_{62}$/GO	n-octanal	MeCN	air	60	Atmospheric pressure	5	100	This work

Table S3. The contrast tests for the proposed mechanism of ODS reaction.

System	Final desulfurization ratio/%
1	48.05
2	48.12
3	62.75
4	67.13
5	99.63

Conditions: system 1: the model oil was only treated by extraction of MeCN for 30 min without ODS treatment;

system 2: the model oil was treated by ODS treatment with 200 ml/min air bubbled for 4 h without any catalyst.

system 3: the model oil was treated by ODS treatment with 200 ml/min air bubbled for 4 h with $K_6[\alpha\text{-}P_2W_{18}O_{62}]\cdot 14H_2O$ as catalyst;

system 4: the model oil was treated by ODS treatment with 200 ml/min air bubbled for 4 h with n-octanal as catalyst;

system 5: the model oil was treated by ODS treatment with 200 ml/min air bubbled for 4 h with $K_6[\alpha\text{-}P_2W_{18}O_{62}]\cdot 14H_2O$ and n-octanal as catalysts;

The other conditions were same as described in Figure 3.

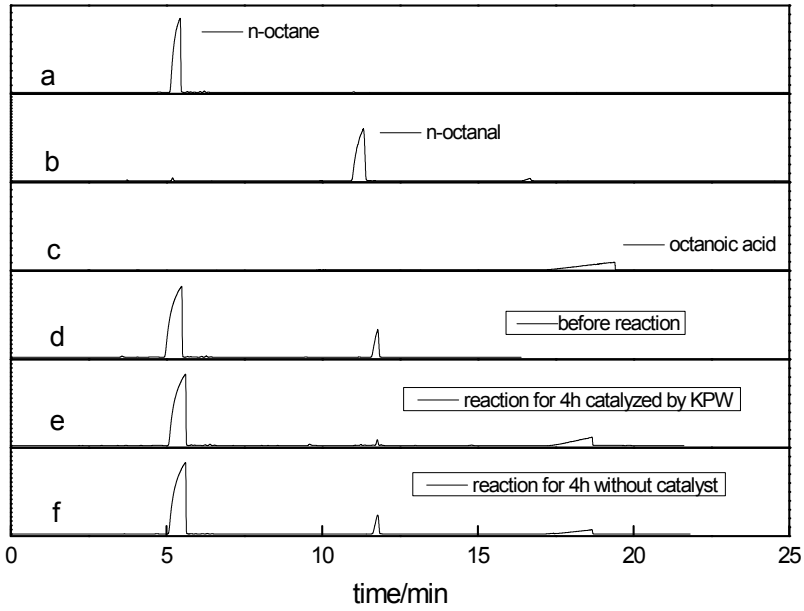

Fig. S3. The GC analysis of the oxidation reaction of n-octanal with molecular oxygen (Condition: T=60 ^{o}C; $w_{cat.}$=0.5%; reaction time is 4 h; the initial n-octanal content is 20 wt%).

REFERENCES

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