

Supporting Information

RESEARCH ARTICLE

HDS of dibenzothiophenes and hydrogenation of tetralin over a SiO₂ supported Ni-Mo-S catalyst

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Abstract A one-step synthesized Ni-Mo-S catalyst supported on SiO₂ was prepared and used for hydrodesulphurization (HDS) of dibenzothiophene (DBT), and 4,6-dimethyl-dibenzothiophene (4,6-DMDBT), and for hydrogenation of tetralin. The catalyst showed relatively high HDS activity with complete conversion of DBT and 4,6-DMDBT at temperature of 280 °C and a constant pressure of 435 psi. The HDS conversions of DBT and 4,6-DMDBT increased with increasing temperature and pressure, and decreasing liquid hourly space velocity (LHSV). The HDS of DBT proceeded mostly through the direct desulphurization (DDS) pathway whereas that of 4,6-DMDBT occurred mainly through the hydrogenation-desulphurization (HYD) pathway. Although the catalyst showed up to 24% hydrogenation/dehydrogenation conversion of tetralin, it had low conversion and selectivity for ring opening and contraction due to the competitive adsorption of DBT and 4,6-DMDBT and insufficient acidic sites on the catalyst surface.

Keywords hydrodesulphurization (HDS), hydrogenation, dibenzothiophene (DBT), 4,6-dimethyldibenzothiophene (4,6-DMDBT), tetralin

Table S1 Operating conditions for the bench scale experiments

Run No.	Reaction temperature /°C	Operating pressure /psi	H ₂ /oil ratio /NL·L ⁻¹	LHSV /h ⁻¹	Oil feed rate /g·h ⁻¹ (mL·h ⁻¹)	Gas rate /NL·h ⁻¹
R01	320	725	600	1.5	7.5 (9.0)	5.4
R02	310	725	600	1.5	7.5(9.0)	5.4
R03	330	725	600	1.5	7.5(9.0)	5.4
R04	340	725	600	1.5	7.5(9.0)	5.4

R05	320	725	600	1.5	7.5(9.0)	5.4
R06	320	435	600	1.5	7.5(9.0)	5.4
R07	300	435	600	1.5	7.5(9.0)	5.4
R08	200	435	600	1.5	7.5(9.0)	5.4
R09	260	435	600	1.5	7.5(9.0)	5.4
R10	280	435	600	1.5	7.5(9.0)	5.4
R11	220	435	600	1.5	7.5(9.0)	5.4
R12	240	435	600	1.5	7.5(9.0)	5.4
R13	240	300	600	1.5	7.5(9.0)	5.4
R14	240	735	600	1.5	7.5(9.0)	5.4
R15	240	435	600	1	5(6.0)	3.6
R16	240	435	600	2	10.1(12.0)	7.2
R17	240	435	600	1.5	7.5(9.0)	5.4
R19	240	300	600	1.5	7.5(9.0)	5.4
R19	260	435	600	1.5	7.5(9.0)	5.4

Table S2 Operating conditions for GC×GC-FID/SCD analysis

Item	Descriptions/conditions
1 st column	Varian Factor 4 VF5-HT, 30 m × 0.32 mm DF:0.1
Main oven program	50–340 °C; 5 °C·min ⁻¹
2 nd column	Varian Factor 4 VF17-MS, 1.5 m × 0.1 DF:0.2
Secondary oven program	40 °C offset from main oven
Inlet temperature	350 °C
Injection size	0.2 µL
Split ratio	40 : 1
Carrier gas	He, constant flow, 1.5 mL·min ⁻¹
Modulator temperature	55 °C offset from main oven
Detector	FID and SCD, 350 °C
Acquisition rate	100 Hz
Modulation period	8 s