catalysts

MDPI

Supplementary Materials

Co-Processing of Jatropha-Derived Bio-Oil with Petroleum Distillates over Mesoporous CoMo and NiMo Sulfide Catalysts

Shih-Yuan Chen [1,*] Masayasu Nishi [1], Takehisa Mochizuki [1], Hideyuki Takagi [1], Akira Takatsuki [1], Wuttichai Roschat [2,3], Makoto Toba [1] and Yuji Yoshimura [4]

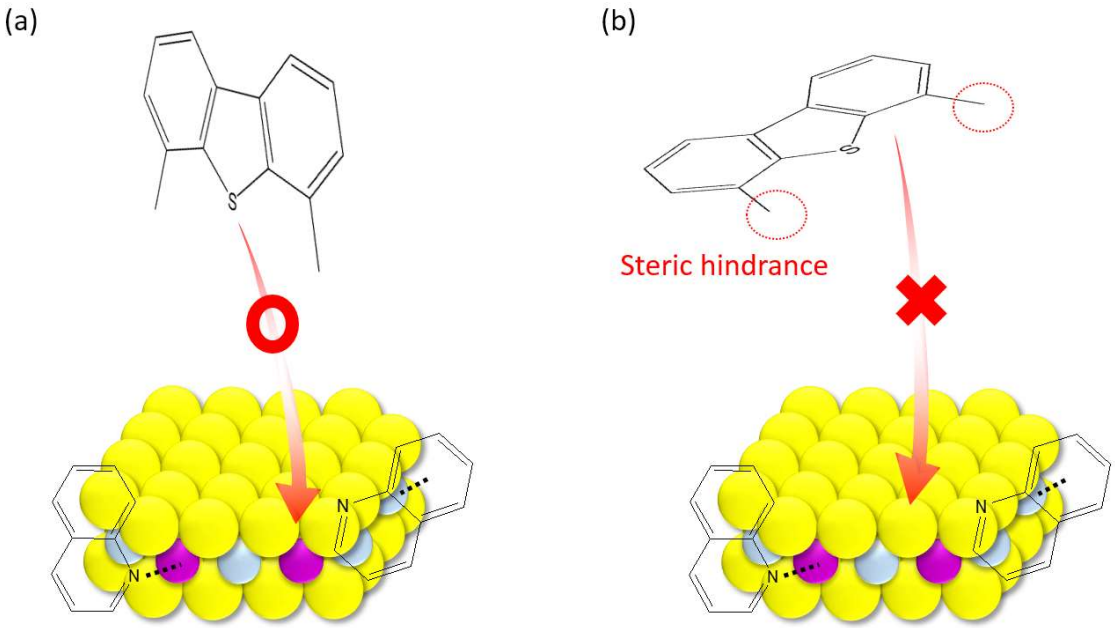
[1] Research Institute of Energy Frontier (RIEF), Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology (AIST), 16-1 Onogawa, Tsukuba, Ibaraki 305-8569, Japan; m.nishi@aist.go.jp (M.N.); t.mochizuki@aist.go.jp (T.M.); hide-takagi@aist.go.jp (H.T.); akira-takatsuki@aist.go.jp (A.T.); m.toba@aist.go.jp (M.T.)

[2] Program of Chemistry, Faculty of Science and Technology, Sakon Nakhon Rajabhat University, 680 Nittayo Rd., Mueang District, Sakon Nakhon 47000, Thailand; roschat1@gmail.com

[3] Center of Excellence on Alternative Energy, Research and Development Institute, Sakon Nakhon Rajabhat University, 680 Nittayo Rd., Mueang District, Sakon Nakhon 47000, Thailand

[4] Materials for Energy Research Unit, National Metal and Materials Technology Center (MTEC), Pahonyothin Rd. Klong 1, Klong Luang Pathumtani 12120, Thailand; y.yoshimura@aist.go.jp

* Correspondence: sy-chen@aist.go.jp; Tel: +81-29-861-2680; Fax: +81-29-861-4532



Scheme S1. Possible reaction pathways for the HDS of DMDBT on the Co- or Ni-incorporated MoS_2-like slabs via (a) σ adsorption and (b) π adsorption.

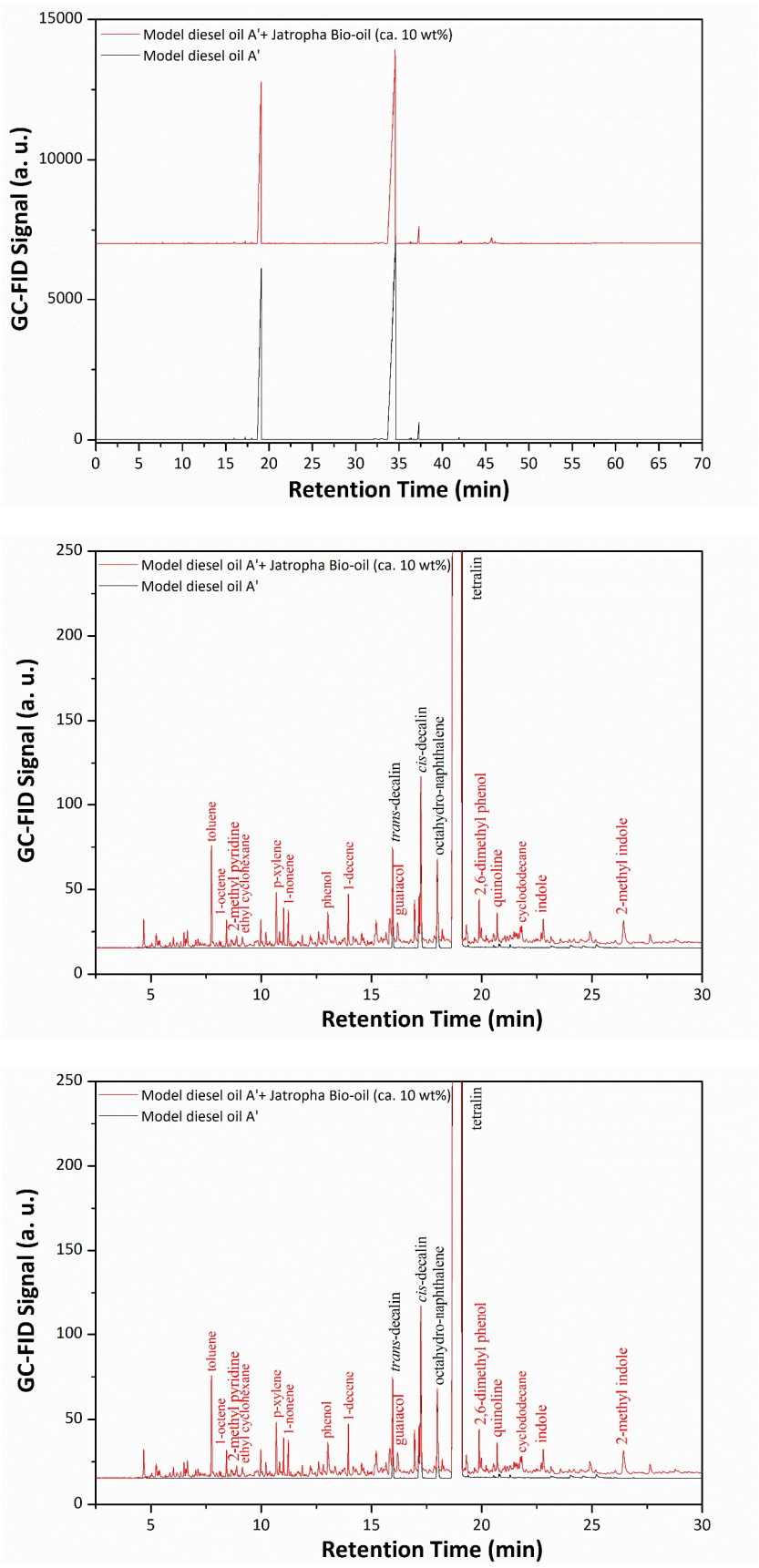


Figure S1. GC-FID patterns of the model diesel oil A′ and the low-grade feedstock, which is a mixture of Jatropha bio-oil (ca. 10 wt%) and model diesel oil A′ (ca. 90 wt%).

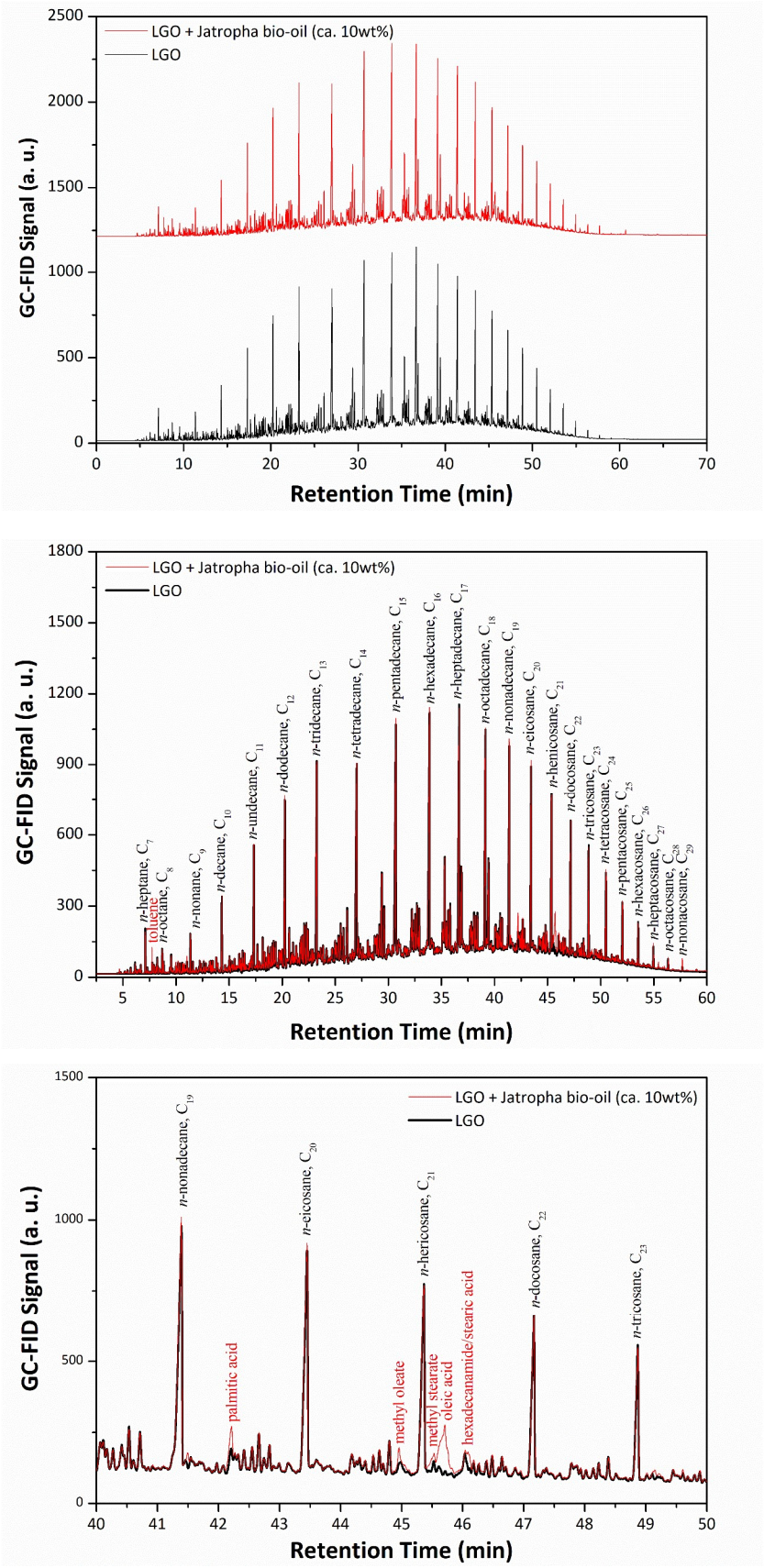


Figure S2. GC-FID patterns of LGO and the low-grade feedstock, which is mixture of Jatropha bio-oil (ca. 10 wt%) and LGO (ca. 90 wt%).

Table S1. The model diesel oils A-D with sulfur-, nitrogen- and oxygen-containing compounds.

Model diesel oils[a]	Sulfur[b] (ppm)[b]	Nitrogen[c] (ppm)[b]	Oxygen[d] (wt%)[c]
A	3500	0	0
B	3500	0	1.5
C	3500	3500	0
D	3500	3500	1.5

[a] The model diesel oil comprises 70 wt% of *n*-hexadecane and 30 wt% of tetralin; [b] Dibenzothiophene (50 wt%) and 4,6-dimethyldibenzothiophene (50%) as sulfur-containing model compounds; [c] Quinoline as nitrogen-containing model compound; [d] Stearic acid as oxygen-containing model compound.

Table S2. The activity of mesoporous sulfide catalysts in the upgrading of model diesel oils A-D at 330 °C and 5 MPa of H_2 for 1 h.

Mesoporous Sulfide Catalysts	Feedstocks	Hydrotreating Activity (mmol g·cat^{-1} h^{-1})[a]	Conversions (mol%)				
			DBT	DMDBT	Tetralin	Quinoline	Stearic Acid
CoMo/γ-Al_2O_3[a]	A	1.1	98	98	28	-	
	B	1.0	84	93	14	-	> 99
	C	0.49	77	2.4	2.1	76	
	D	0.30	73	0.7	1.5	75	~ 98
NiMo/γ-Al_2O_3[b]	A	1.1	97	94	47	-	
	B	1.0	95	88	41	-	> 99
	C	0.58	93	1.9	2.7	77	
	D	0.51	90	1.1	2.2	75	> 99

[a] The hydrotreating activity is calculated by dividing the molar faction of oil desulfurized by the catalyst amount at the first 1 min of the reaction.

Table S3. The selectivity of mesoporous sulfide catalysts in the upgrading of model diesel oils A-D at 330 °C and 5 MPa of H_2 for 1 h.

Mesoporous Sulfide Catalysts	Feedstocks	DDS of DBT[a] (%)	DDS of DMDBT[a] (%)	*cis*-decalin[b] (%)	DDN[c] (%)	C_{17}[d] (%)
CoMo/γ-Al_2O_3[a]	A	52	3.7	57	-	-
	B	42	6.6	60	-	50
	C	64	49	50	4.0	-
	D	44	23	55	5.7	46
NiMo/γ-Al_2O_3[b]	A	26	17	39	-	-
	B	29	20	39	-	67
	C	73	32	37	3.0	-
	D	61	27	40	3.9	50

[a] The molar faction of biphenyl divided by the molar faction of DBT desulfurized. The molar faction of 3,3'-dimethylbiphenyl divided by the molar faction of DMDBT desulfurized; [b] The molar faction of *cis*-decalin divided by the molar faction of tetralin hydrogenated; [c] The molar faction of propylbenzene divided by the molar faction of quinoline denitrogenated; [d] The molar faction of heptadecane divided by the molar faction of stearic acid deoxygenated.