catalysts

MDPI

Supplementary Material

NiO, Fe_2O_3, and MoO_3 Supported over SiO_2 Nanocatalysts for Asphaltene Adsorption and Catalytic Decomposition: Optimization through a Simplex–Centroid Mixture Design of Experiments

Daniela Arias-Madrid [1], Oscar E. Medina [1], Jaime Gallego [2], Sócrates Acevedo [3], Alexander A. Correa-Espinal [4], Farid B. Cortés [1,*] and Camilo A. Franco [1,*]

[1] Grupo de Investigación en Fenómenos de Superficie—Michael Polanyi, Facultad de Minas, Universidad Nacional de Colombia, Sede Medellín, Medellín 050034, Colombia; daariasma@unal.edu.co (D.A.-M.), oemedinae@unal.edu.co (O.E.M.)

[2] Química de Recursos Energéticos y Medio Ambiente, Instituto de Química, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín 050010, Colombia; andres.gallego@udea.edu.co

[3] Facultad de Ciencias, Escuela de Química, Universidad Central de Venezuela, Caracas 1040, Venezuela; socrates.acevedo@gmail.com

[4] Departamento Ingeniería de la Organización, Facultad de Minas, Universidad Nacional de Colombia, Sede Medellín, Medellín 050034, Colombia; alcorrea@unal.edu.co

* Correspondence: fbcortes@unal.edu.co (F.B.C); caafrancoar@unal.edu.co (C.A.F.) Tel.: +574-4255137 (F.B.C.); +574-4255000 (44313) (C.A.F.)

* Correspondence: fbcortes@unal.edu.co (F.B.C); caafrancoar@unal.edu.co (C.A.F.)

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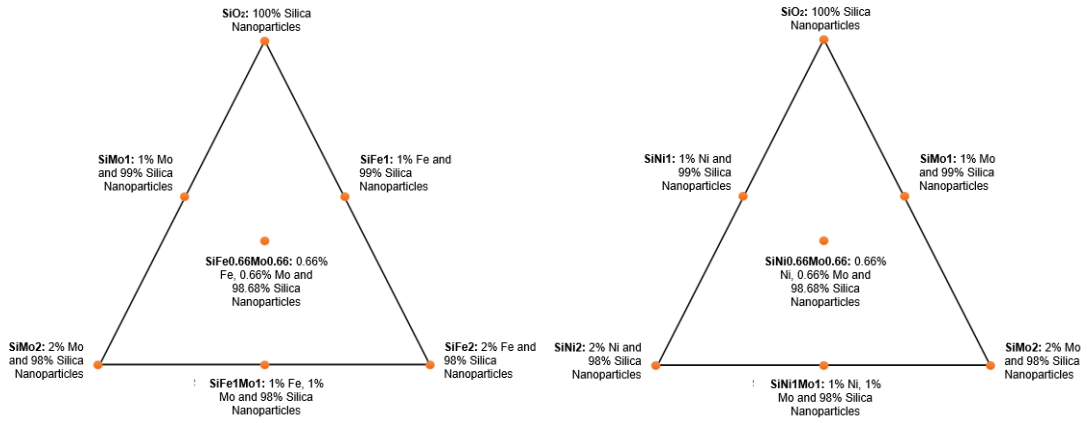


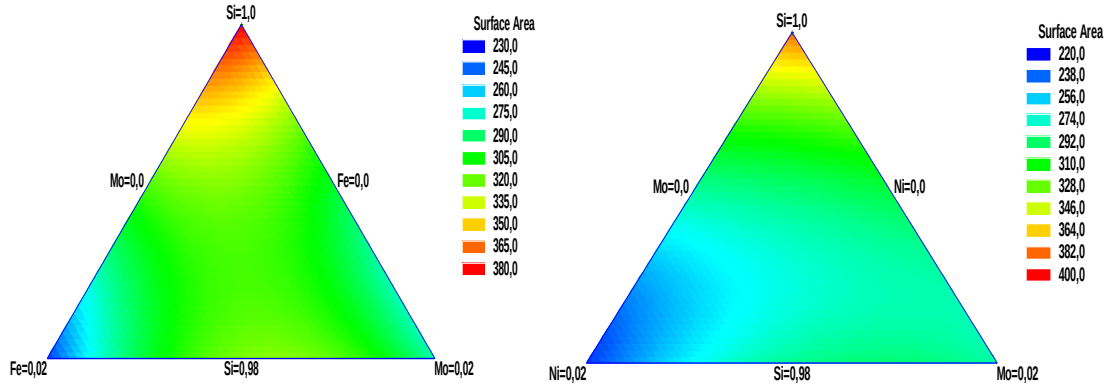
Figure S1. Simplex-centroid mixture design with a) fumed silica (SiO_2), iron oxide (Fe) and molybdenum oxide (Mo); and b) fumed silica (SiO_2), nickel oxide (Ni) and molybdenum oxide (Mo)

Table S1. Parameters of the surface area design for Si-Fe-Mo

β_1	β_2	β_3	β_{12}	β_{13}	β_{23}	β_{123}
380.00	237.61	279.99	14.5	-138.18	253.04	33.77

Table S2. Parameters of the surface area design for Si-Ni-Mo

β_1	β_2	β_3	β_{12}	β_{13}	β_{23}	β_{123}
380.00	228.26	279.99	-102.96	-138.18	116.46	-257.43



a) **b)**

Figure S2. Response surface to surface area of design with a) Si-Fe-Mo and b) Si-Ni-Mo

Table S3. Parameters of the surface area design for Si-Fe-Ni-Mo

β_1	β_2	β_3	β_4	β_{12}	β_{13}	β_{14}	β_{23}	β_{24}
380.15	237.76	228.41	280.14	9.05	-108.40	-143.62	254.25	247.59

β_{34}	β_{123}	β_{124}	β_{134}	β_{234}
111.09	528.76	135.40	-102.34	-587.44

Table S4 Estimated SLE model parameters for SiO_2 and functionalized nanoparticles with elements transition

Material	$K(g \cdot g^{-1}) \pm 0.005$	$H(mg \cdot g^{-1}) \pm 0.01$	$q_m(g \cdot m^{-2}) \pm 0.01$	R^2	*RMS*
SiO_2	0.001	1.08	0.87	0.99	0.54
SiFe1	0.005	1.17	1.06	1.00	0.58
SiFe2	0.004	0.51	0.76	1.00	0.14
SiNi1	5.821	3.58	0.31	1.00	0.81
SiNi2	1.077	1.53	0.66	1.00	0.92
SiMo1	1.374	1.90	0.49	1.00	1.09
SiMo2	0.004	0.68	0.63	1.00	0.48
SiFe1Ni1	3.187	2.48	0.33	1.00	1.33
SiFe1Mo1	0.695	0.73	0.49	0.95	3.98
SiNi1Mo1	2.006	2.38	0.61	1.00	0.91
SiFe0.66Ni0.66	1.729	1.70	0.62	1.00	0.42

SiFe0.66Mo0.66	1.404	1.49	0.50	0.99	1.71
SiNi0.66Mo0.66	2.103	2.04	0.62	1.00	0.15
SiFe0.66Ni0.66Mo0.66	1.098	1.99	0.50	1.00	0.42
SiFe0.33Ni0.33Mo0.33	0.478	1.72	1.04	1.00	0.41

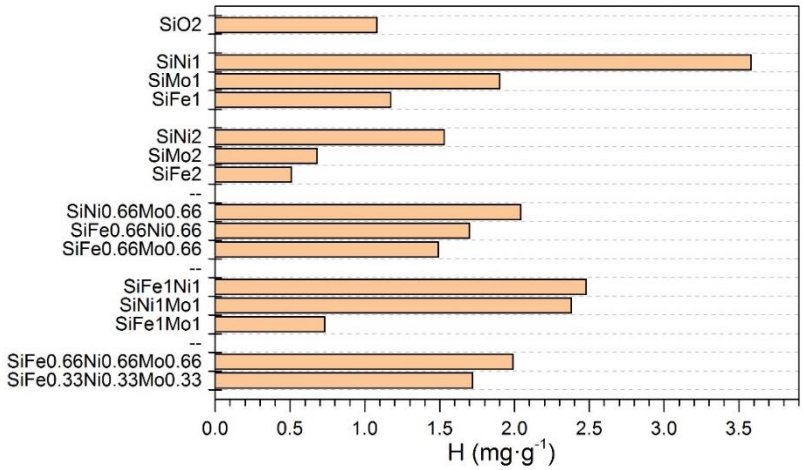


Figure S3. H values from SLE model for silica and functionalized nanoparticles

Table S5. Coefficients to activation energy mixture design for Si-Ni-Mo

β_1	β_2	β_3	β_{12}	β_{13}	β_{23}
124.54	129.41	122.83	9.38	-38.94	-228.72

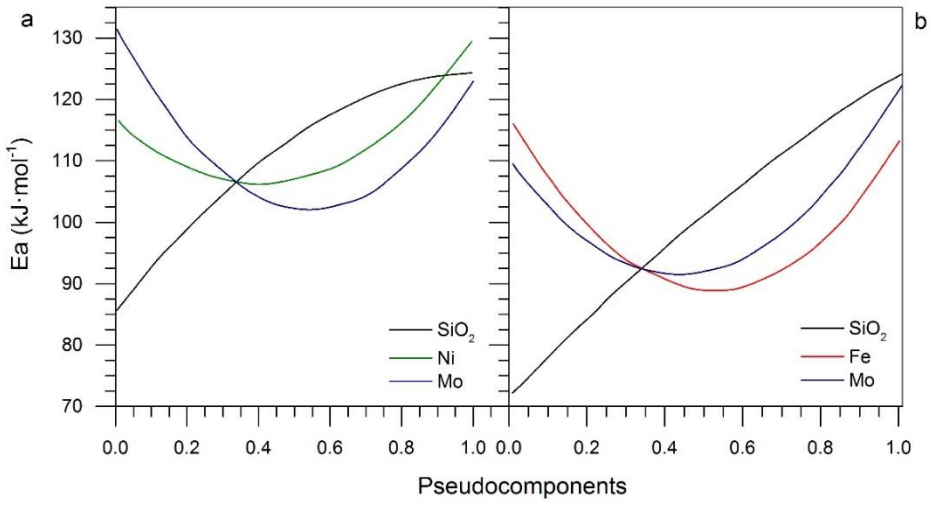


Figure S4. Graphic trace to activation energy for the series a) Si-Ni-Mo and b) Si-Fe-Mo

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53 **Table S6.** Coefficients to activation energy mixture design for Si-Fe-Mo

β_1	β_2	β_3	β_{12}	β_{13}	β_{23}
124.54	112.81	122.83	-46.51	-38.94	-184.16

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55 **Table S7.** Coefficients to activation energy mixture design for Si-Fe-Ni-Mo

β_1	β_2	β_3	β_4	β_{12}	β_{13}	β_{14}
124.54	112.82	122.830	129.41	-46.52	-38.94	9.38
β_{23}	β_{24}	β_{34}	β_{123}	β_{124}	β_{134}	β_{234}
-184.18	-74.06	-162.72	-473.78	-274.18	-624.29	358.71

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