Effect of Cu addition on the selectivity of Ni-based catalysts for methylcyclohexane dehydrogenation

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Supplementary information

Table 1: Crystallite size estimation by the Scherrer equation for reduced catalysts.

Catalyst	Reflection	2θ (°)	FWHM (°)	Crystallite Size (nm)
Ni 12% / Al_2O_3	Ni (111)	44.77	Overlap	Overlap
	Ni (200)	52.18	1.12	7.90
	Ni (220)	76.92	0.78	13.01
Ni 12.8% Cu 3.2% / Al_2O_3	Ni (111)	44.50	0.39	22.01
	Ni (200)	52.00	0.52	17.00
	Ni (220)	76.00	0.78	12.92
Ni 12.8% Cu 7.2% / Al_2O_3	Ni (111)	44.50	0.34	25.25
	Ni (200)	52.10	0.37	23.90
	Ni (220)	76.40	0.64	15.80
	Cu (111)	43.30	0.41	20.85
	Cu (200)	50.40	0.32	27.44
Cu 20.0% / Al_2O_3	Cu (111)	43.27	0.27	31.65
	Cu (200)	50.40	0.31	28.32
	Cu (220)	74.05	0.37	26.89

Notes: Crystallite sizes calculated using the Scherrer equation: $D = \frac{K\lambda}{\beta \cos\theta}$, with $K = 0.9$, $\lambda = 1.5406$ Å (Cu Kα radiation), β (FWHM)

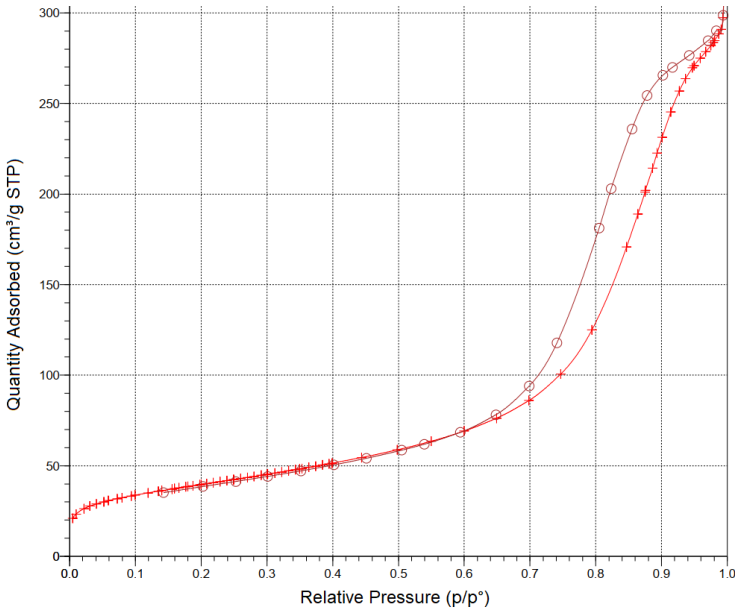

Fig. 1: BET isotherm calcined Al_2O_3

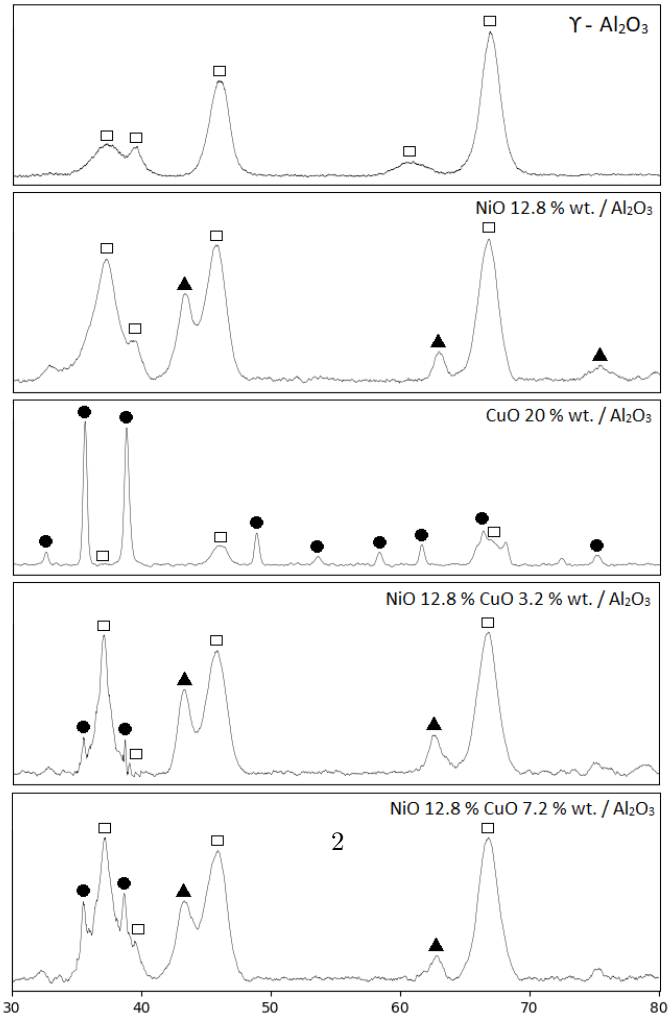

Fig. 2: XRD of the catalysts before reduction: γ-Al_2O_3 (□), CuO (•), NiO (▲) peak positions as per CIF reference: NiO (36.92, 42.90, 62.28, 74.66, 78.60) CuO (32, 35.5, 38.5, 48.5, 53.5, 58, 62, 66, 75)

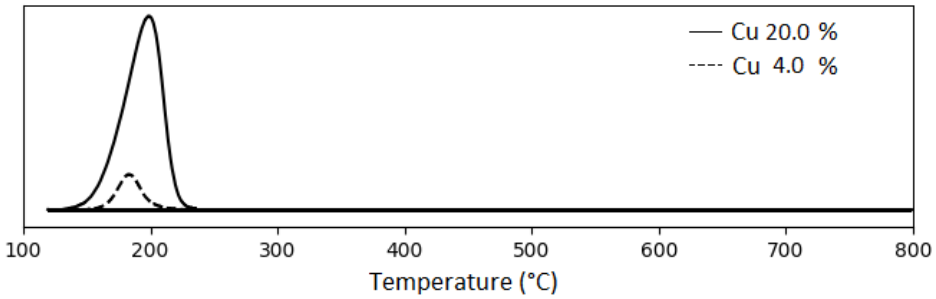

Fig. 3: H_2-Temperature programmed reduction of Cu/Al_2O_3 with increasing loading

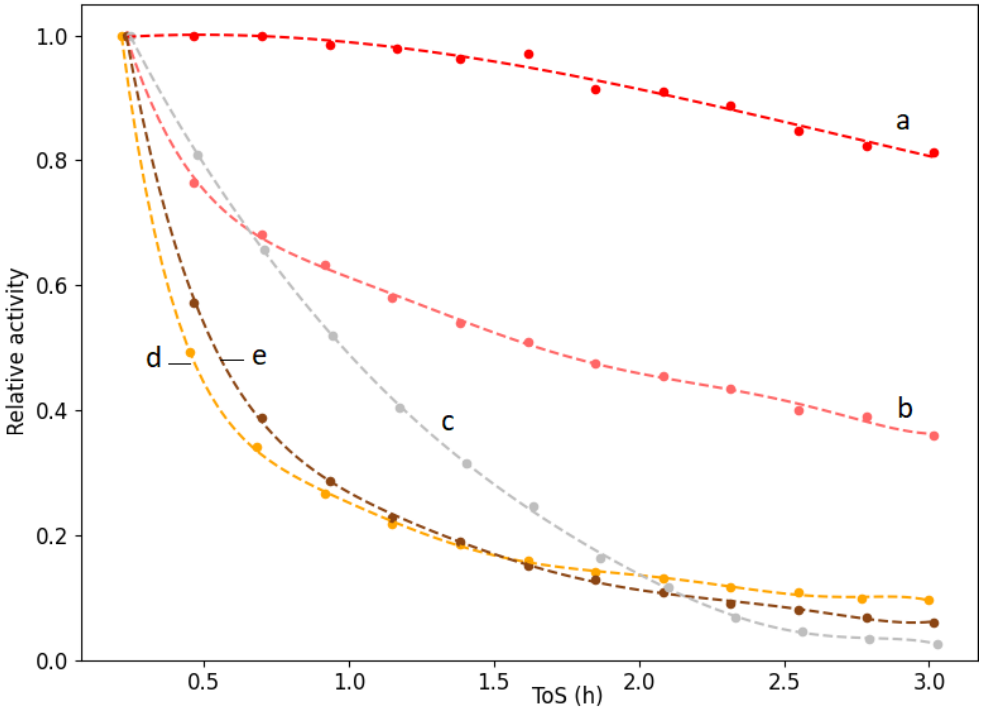

Fig. 4: Deactivation: Line fit for data visualization, Relative activity as eq. 3
a) Ni 20.0 wt.%, b) Ni 12.8 wt.%, c) Pt, d) Cu:Ni = 0.25, e) Cu:Ni = 0.56

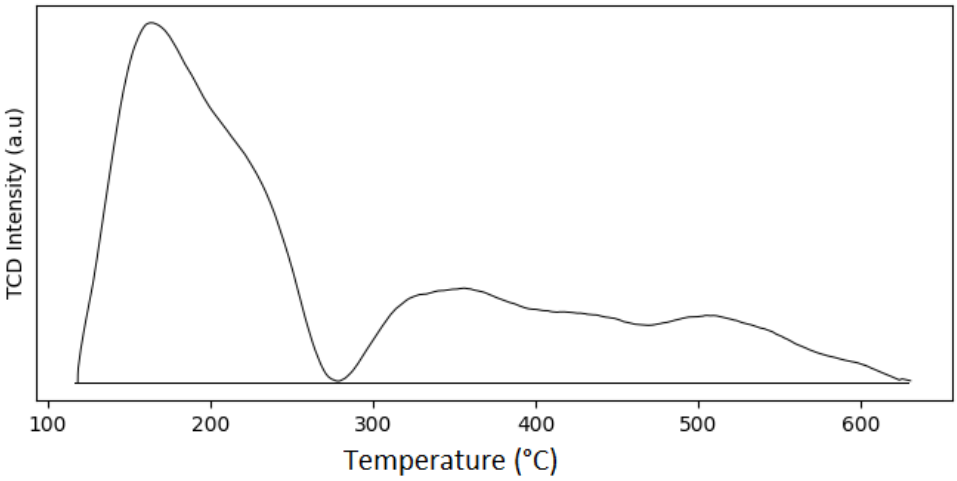

Fig. 5: Temperature programmed oxidation-TCD signal - Ni 12.8 wt.% Cu 7.2 wt.%/Al_2O_3