catalysts

MDPI

Supplementary Materials

Transfer hydrogenation of biomass-like phenolic compounds and 2-PrOH over Ni-based catalysts prepared using supercritical antisolvent coprecipitation

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The XRD data of the synthesized catalysts are provided in **Figure S1** and **Table S1**. The phases of Ni^0 and NiO are presented. The mean crystallite size of Ni^0 does not exceed 6.5 nm, at the same time, NiO crystallites are smaller than 3 nm. The TEM microphotographs show that the nanosized particles are aggregated in the bigger ones **Figure S2**. In case of NiCu-SiO_2 the lattice parameter of Ni^0 phase is higher compared to the Cu-free catalysts. This fact can show that Cu^0 is included in the Ni^0 lattice. This suggestion agrees with EDX data (**Figure S2** (A3,B3)) showing the even distribution of copper over the catalysts.

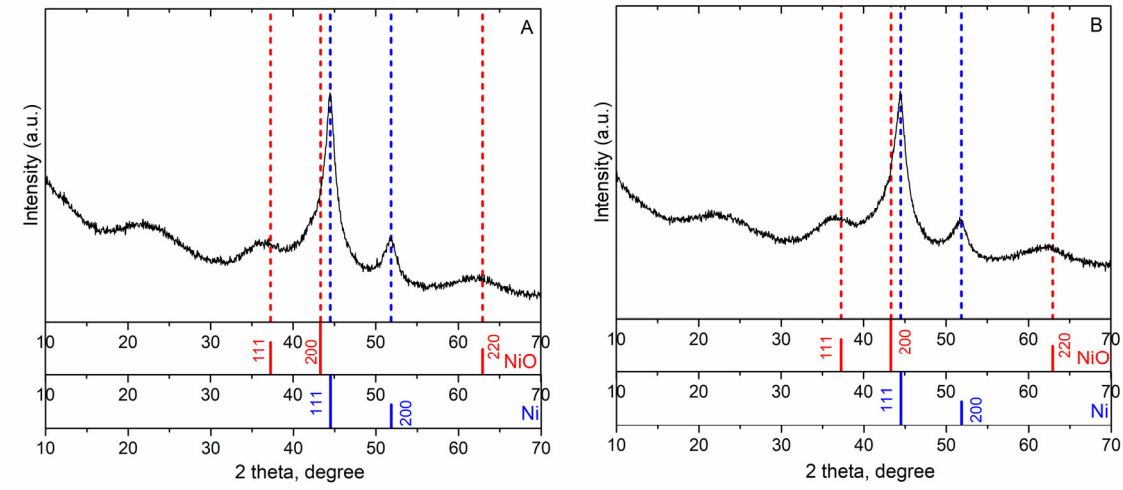

Figure S1. XRD data obtained for the catalysts after activation in H_2. A – Ni-SiO_2, B – NiCu-SiO_2.

Table S1. Content of Ni and Cu in the Ni-Cu catalysts measured by XRF. D – mean crystallite size, a – lattice parameter, measured by XRD, S_{CO} – surface area, measured by CO adsorption.

Sample	Ni, wt.%	Cu, wt.%	D(Ni^0), nm	a(Ni^0), Å	S_{co}, m^2/g
Ni-SiO_2	36.4	-	6.0	3.524	35
NiCu-SiO_2	40.7	4.0	6.5	3.553	32

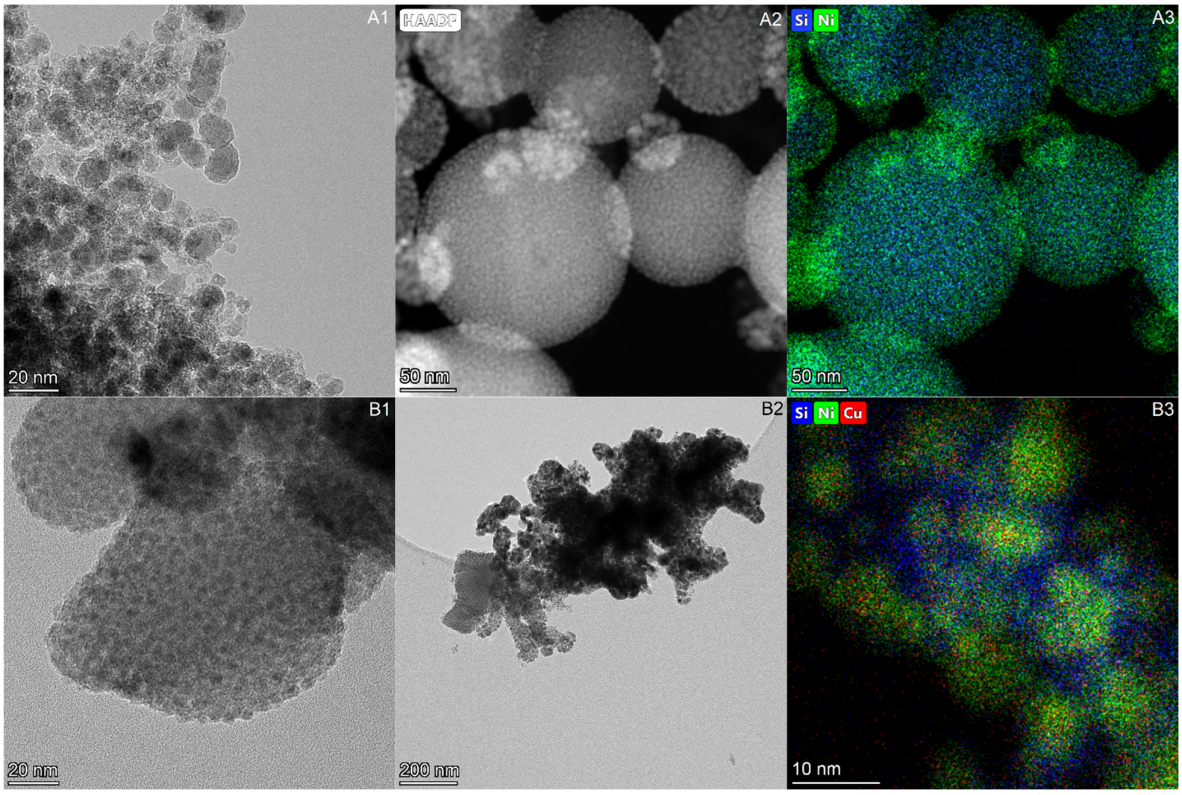

Figure S2. TEM and EDX-mapping pictures obtained for A – Ni-SiO_2, B – NiCu-SiO_2.

The kinetic constants of phenolic compound consumption were calculated using **Equation 3** (see the main text). The calculated constants (k), constants of acetone quasi-equilibium between the solution and the catalyst surface are given in **Figures S3**–**S6**. The coefficient of determination is provided as well.

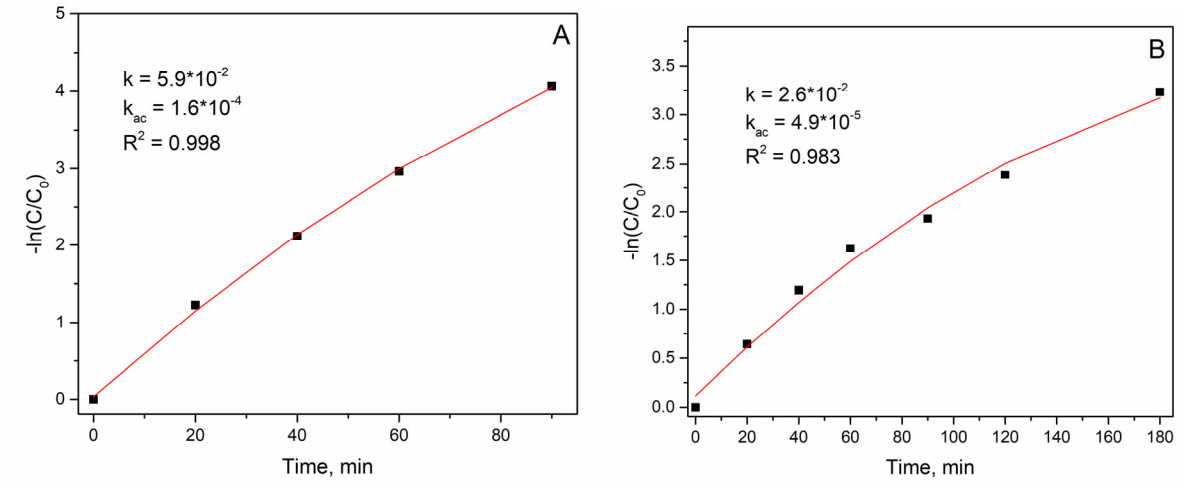

Figure S3. Kinetic data for the experiments with guaiacol over A – Ni-SiO_2 and NiCu-SiO_2. The first order kinetic model was used, the dots – experimental data, the lines – calculated using **Equation 3**.

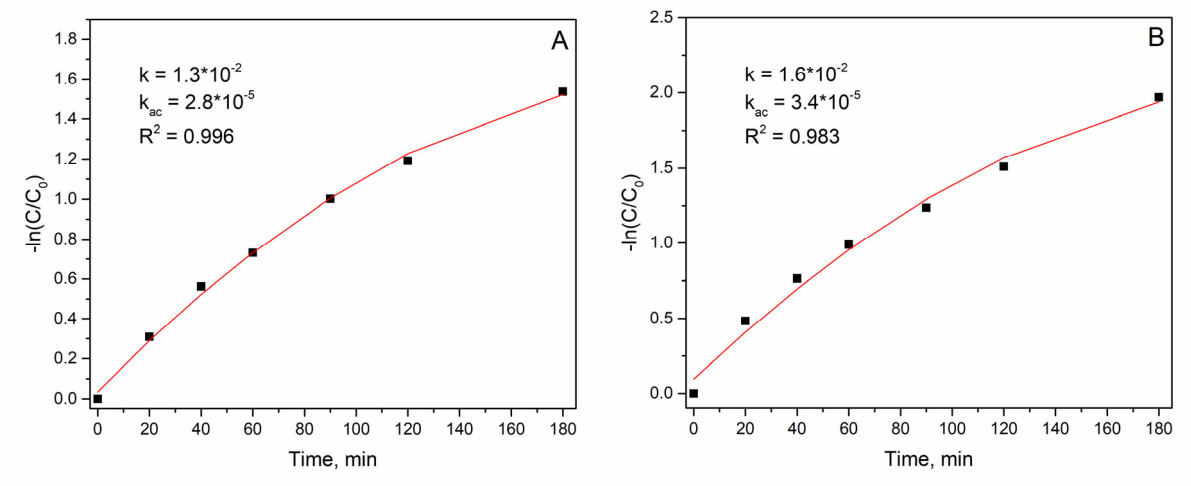

Figure S4. Kinetic data for the experiments with 1,2-DMB over A – Ni-SiO_2 and NiCu-SiO_2. The first order kinetic model was used, the dots – experimental data, the lines – calculated using **Equation 3**.

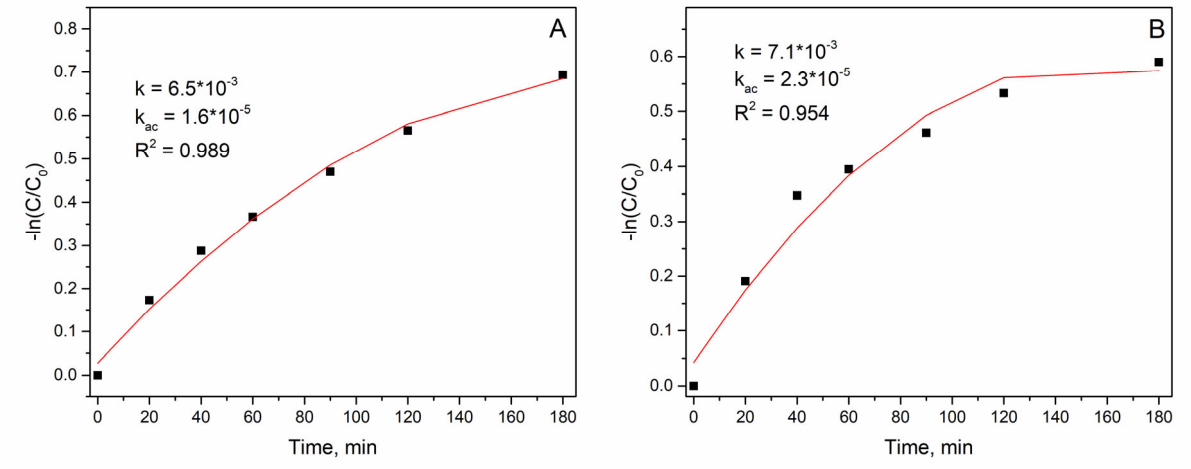

Figure S5. Kinetic data for the experiments with 1,3-DMB over A – Ni-SiO_2 and NiCu-SiO_2. The first order kinetic model was used, the dots – experimental data, the lines – calculated using **Equation 3**.

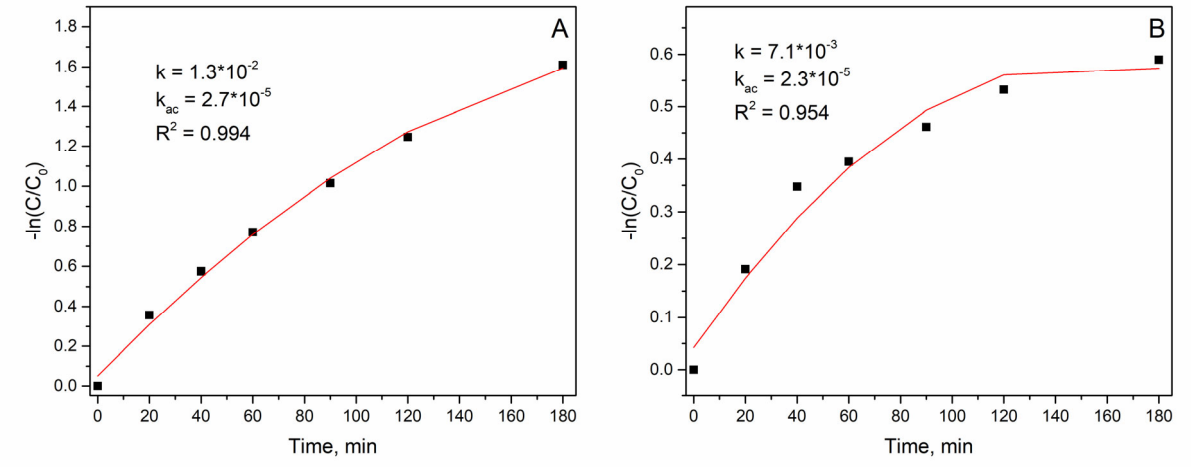

Figure S6. Kinetic data for the experiments with 1,4-DMB over A – Ni-SiO_2 and NiCu-SiO_2. The first order kinetic model was used, the dots – experimental data, the lines – calculated using **Equation 3**.