

Electronic Supplementary Information

Number and intrinsic activity of cobalt surface sites in platinum promoted zeolite catalysts for carbon monoxide hydrogenation

Alexandre Carvalho^{a,b}, Vitaly V. Ordomsky^a, Nilson R. Marcilio^b and Andrei Y. Khodakov^a

Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ.Artois, UMR 8181 – UCCS – Unité de Catalyse et Chimie du Solide, F-59000 Lille, France.

Department of Chemical Engineering, Federal University of Rio Grande do Sul, Porto Alegre, 90040-040, Brazil

Determination of Turnover Frequency of SSITKA (TOF_{SSITKA}):

$$TOF_{SSITKA} = \frac{\text{Fractional coverage}}{\text{Surface residence time of } CHx} \quad Eq.1$$

$$\text{Fractional coverage} = \frac{\text{Number of } CHx \text{ sites}}{\text{Total number of active sites}} \quad Eq.2$$

Determination of the number of adsorbed species (N_{CO} and N_{CHx}):

The amount of adsorbed species was calculated from SSITKA using the formula described by Efstathiou¹ and Dijk²:

$$N_{CO} \left(\frac{\text{mol}}{\text{g}} \right) = \frac{F_{CO}}{W_{cat}} \left(\int_0^{\infty} [nCO(t) - nNe(t)] dt \right) \quad Eq. 3$$

Where F_{CO} : carbon monoxide outlet molar flowrate in mol/s

W_{cat} : catalyst loading in g

$nCO(t)$ and $Ne(t)$: CO and Ne normalized MS data obtained during SSITKA switches.

In order to correct the chromatographic effect, the following formula applied by Biloen et al.³ was applied to determine the number of intermediates:

$$N_{CHx} \left(\frac{mol}{g} \right) = \frac{F_{CH4}}{W_{cat}} \left(\int_0^{\infty} [nCH4(t) - 0.5(nCO(t) - nNe(t))] dt \right) \quad Eq. 4$$

Where F_{CH4} : CH₄ outlet molar flowrate in mol/s

$nCH4(t)$: normalized MS data obtained during SSITKA for CH₄

¹ Kalamaras, C.M.; Gonzalez, I.D.; Navarro, R.M.; Jose Luis G. Fierro, J.L.G.; Efstathiou, A.M. *J.Phys.Chem C* **2011**, *115*, 11595–11610.

² Van Dijk, H.A.J.; Hoebink, J.H.B.J.; Schouten, J.C. *Chem. Eng. Sci.* **2011**, *56*, 1211-1219.

³ Biloen, P.; J. N. Helle, F; G. A. van den Berg; Sachtler, W.M.H. *J. Catal.* **1983**, *81*, 450-463.

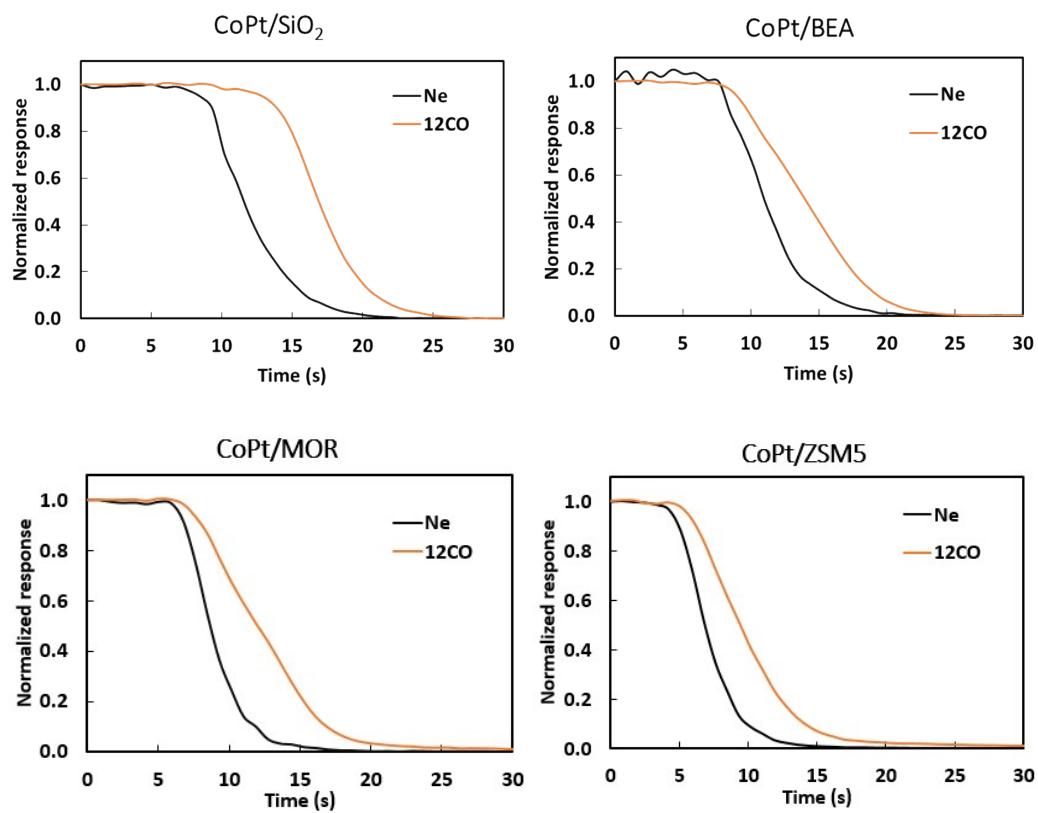


Figure S1. Transient curves of CO and inert (Ne) during CO adsorption at 100 °C over cobalt catalysts supported on SiO₂, BEA, MOR and ZSM-5. Experimental error in the number of active sites equal to 6%.

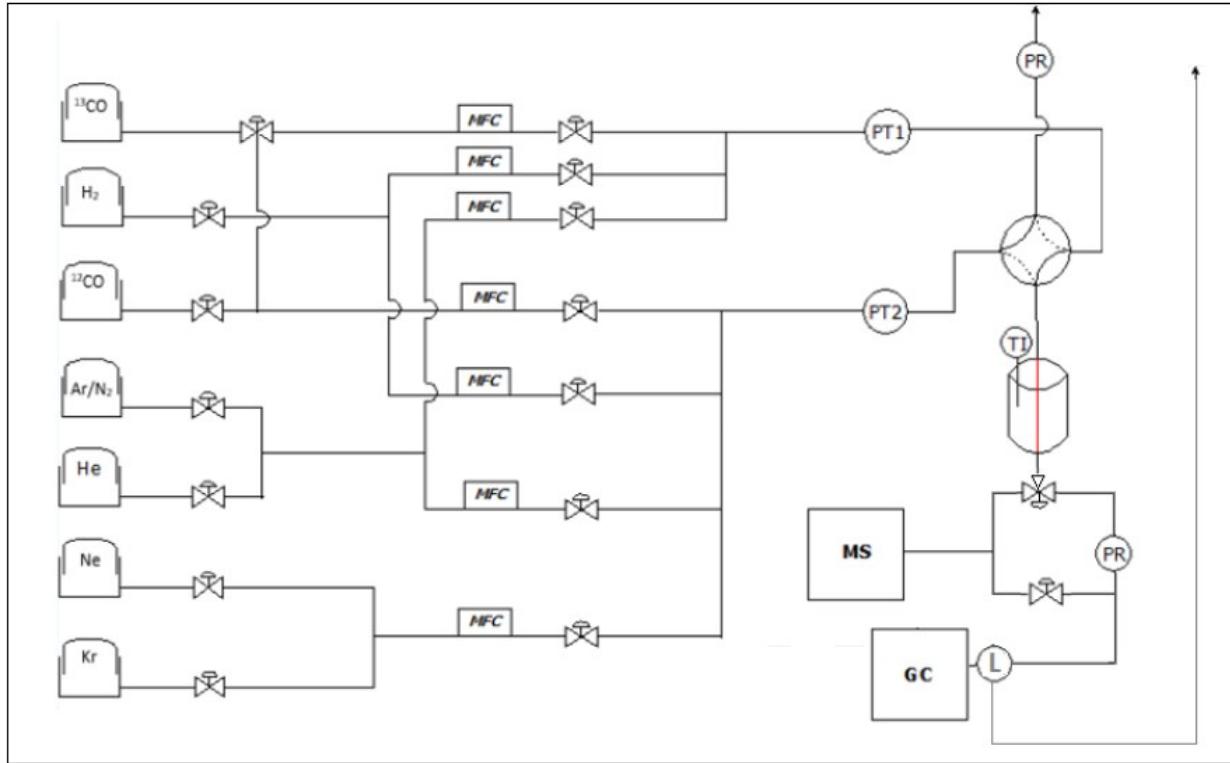


Figure S2. Schematic representation of the SSITKA setup. (MFC = flow controller; PT = pressure transducer; PR = pressure regulator ; TI = temperature indicator; MS = mass spectrometer; GC = gas chromatograph; L = GC loop).