Supplementary Information

CFD simulations, experimental validation and parametric studies for the catalytic reduction of NO by hydrogen in a fixed bed reactor

Maria Mihet[a], Vasile–Mircea Cristea[b*], Paul–Serban Agachi[b], Ana–Maria Cormos[b], Mihaela D. Lazar[a*]

[a]*National Institute for Research & Development of Isotopic and Molecular Technologies – INCDTIM, 67-103 Donat Str., 400293 Cluj-Napoca, Romania*
[b]*Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, 11 Arany Janos Street, 400028 Cluj Napoca, Romania*

[*]corresponding authors: diana.lazar@itim-cj.ro, mcristea@chem.ubbcluj.ro

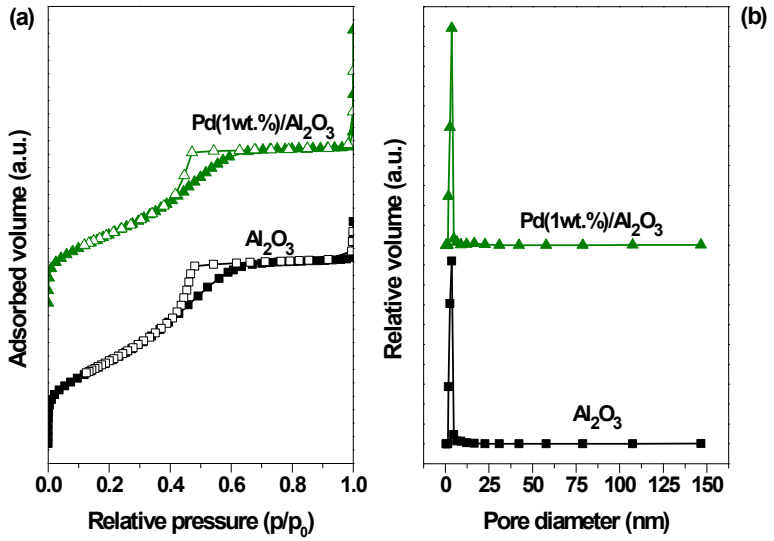


Fig. S1. (a) N_2 adsorption–desorption isotherms, and (b) pore size distribution for Al_2O_3 and Pd(1wt.%)/Al_2O_3.

Table S1. Specific surface area (S_{BET}), pore specific volume (V_p), and average pore radius (R_m) of the support and Pd(1wt.%)/Al_2O_3 catalyst.

Catalyst	S_{BET} (m^2/g cat)	V_p (cm^3/g)	R_m (nm)
Al_2O_3	245	0.22	1.74
Pd(1wt.%)/Al_2O_3	220.6	0.19	1.73

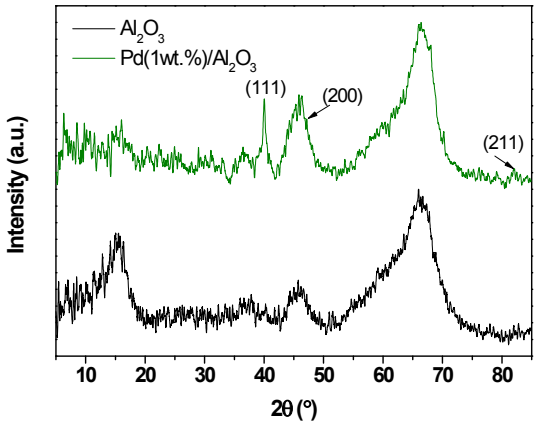


Fig. S2. XRD patterns of the Pd(1wt.%)/Al_2O_3 catalyst and Al_2O_3 support; Pd(111) diffraction peak situated at 39.9°.

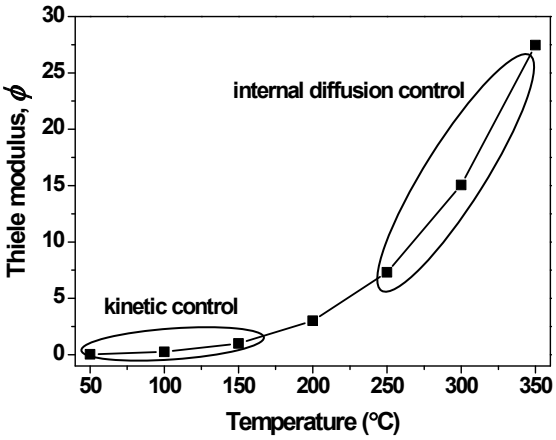
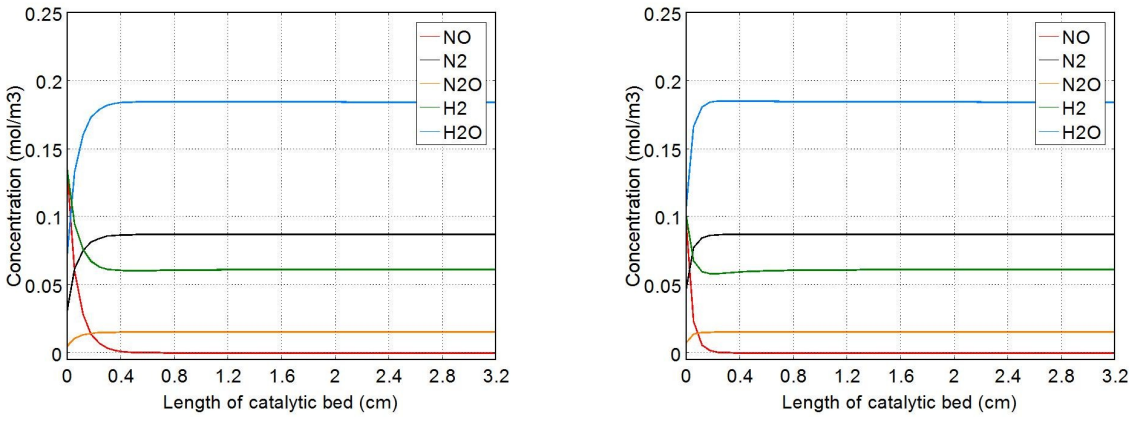


Fig. S3. Temperature dependence of the Thiele modulus, Φ.



(a) (b)

Fig. S4. Concentration profiles of the reactants and products at 200°C – (a) and 250°C – (b) along the catalytic bed ($GHSV$ = 7,200 h^{-1}, NO/H_2 = 1:1.2, C_{NO}^{in} = 0.5 vol.%, L_{bed} = 3.2 cm).

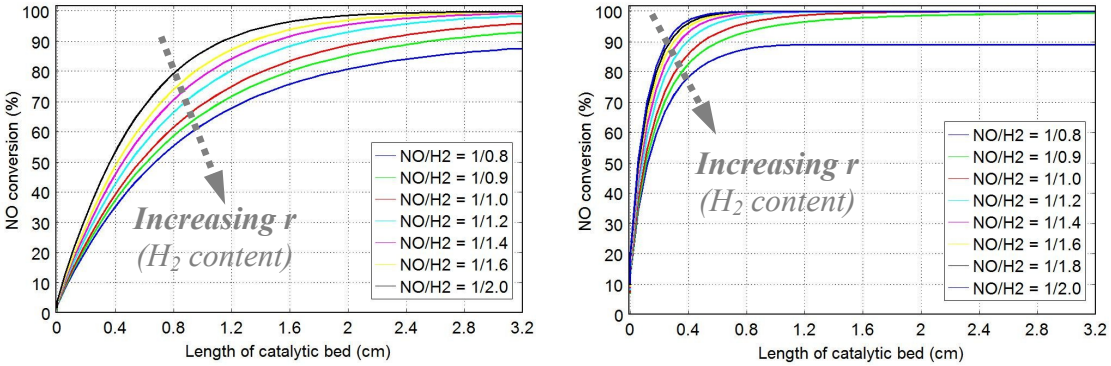


Fig. S5. NO conversion profiles at 100°C – (a) and 150°C – (b) along the catalytic bed at different ratios between the reactants (*GHSV* = 7,200 h^{-1}, C_{NO}^{in} = 0.5 vol.%, L_{bed} = 3.2 cm).

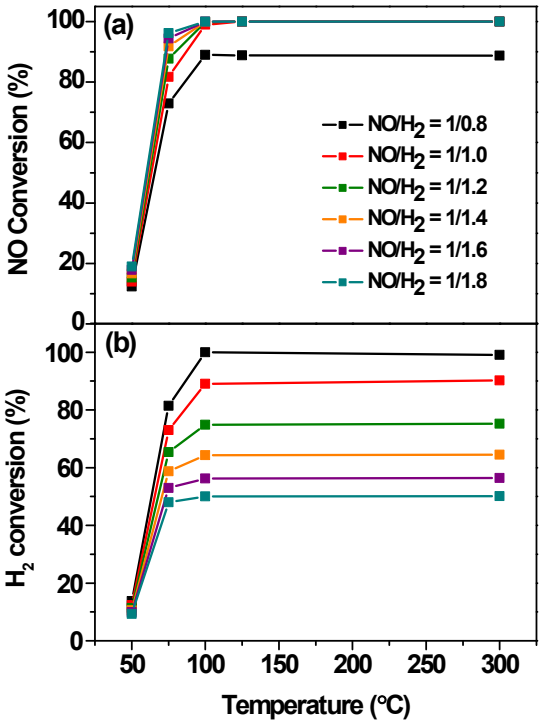


Fig. S6. Influence of reactants ratio (NO/H_2) on the conversion of NO – (a) and H_2 – (b) at different operating temperatures at catalyst bed outlet (*GHSV* = 4,500 h^{-1}, C_{NO}^{in} = 0.5 vol.%, L_{bed} = 3.2 cm).

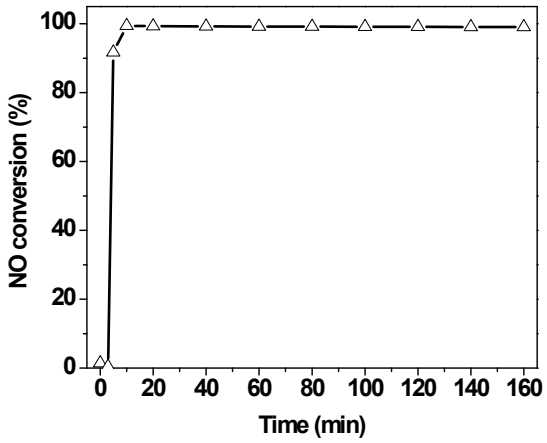


Fig. S7. Effect of time on stream upon the conversion of NO in case of a shorter Pd (1wt.%)/Al_2O_3 catalyst bed (reaction conditions: L_{bed} = 1.6 cm, T = 150°C, $GHSV$ = 9,000 h^{-1}, NO/H_2 = 1:1.3, C_{NO}^{in} = 0.5 vol.%).