Supporting information

Characterization and activity of N-doped FeCo/ASC catalysts for NOx reduction by CO in a simulated rotary reactor

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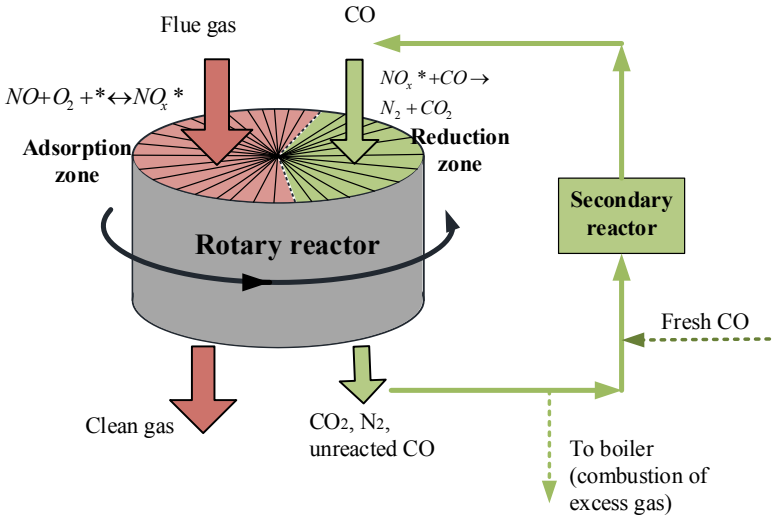
Fig. S1 Schematics of the rotary reactor for NO_x reduction by CO. [1]



S 1.1 Equations of the NO adsorption capacity and NO conversion efficiency

The NO adsorption capacity and NO conversion efficiency were calculated from concentrations of the inlet and outlet flue gases using the equations as follws:

$$q_e = \frac{P \times C_0 \times 10^{-3} \times F \times M_{NO}}{R \times (T + 273)} \times \frac{S}{W_{cat}} \quad (1)$$

where

q_e, the NO adsorption capacity of the catalyst (mg/g);

P, operating pressure (Pa);

C_0, equilibrium NO concentration (ppm);

F, model flue gas flow rate at room temperature (m^3/s);

M_{NO}, molecular weight of NO (30 g/mol);

R, universal gas constant (8.314 J/(mol K));

T_0, ambient temperature (°C);

S, integrated area of the adsorption curve (s);

W_{cat}, catalyst loading (g).

The integrated area, S, of the adsorption curve was calculated by Eq. (2)

$$S = \int_0^{t_{ad}} (1 - \frac{C_{NO_x,out}}{C_0}) dt \quad (2)$$

where

$C_{NO,out}$, the outlet concentration of NO (ppm);

t_{ad}, adsorption time (s).

$$NO\ conversion = \frac{C_{NO,in} - C_{NO,out}}{C_{NO,in}} \times 100\% \quad (3)$$

where

$C_{NO,in}$, the inlet concentration of NO (ppm).

S 1.2 The equations of the parameters used in dynamic NO_x adsorption-reduction experiments

The calculation formulas of the parameters in dynamic experiments are listed as the following equations (4-8):

$$NO_x\ removal = 1 - \int_{t_0}^{t_1} \frac{C_{NO_x,out}}{C_{NO_x,in}} dt \times 100\% \tag{4}$$

$$NO_x\ reduction = 1 - \frac{\int_{t_0}^{t_2} C_{NO_x,out}}{\int_{t_0}^{t_1} C_{NO_x,in}} dt \times 100\% \tag{5}$$

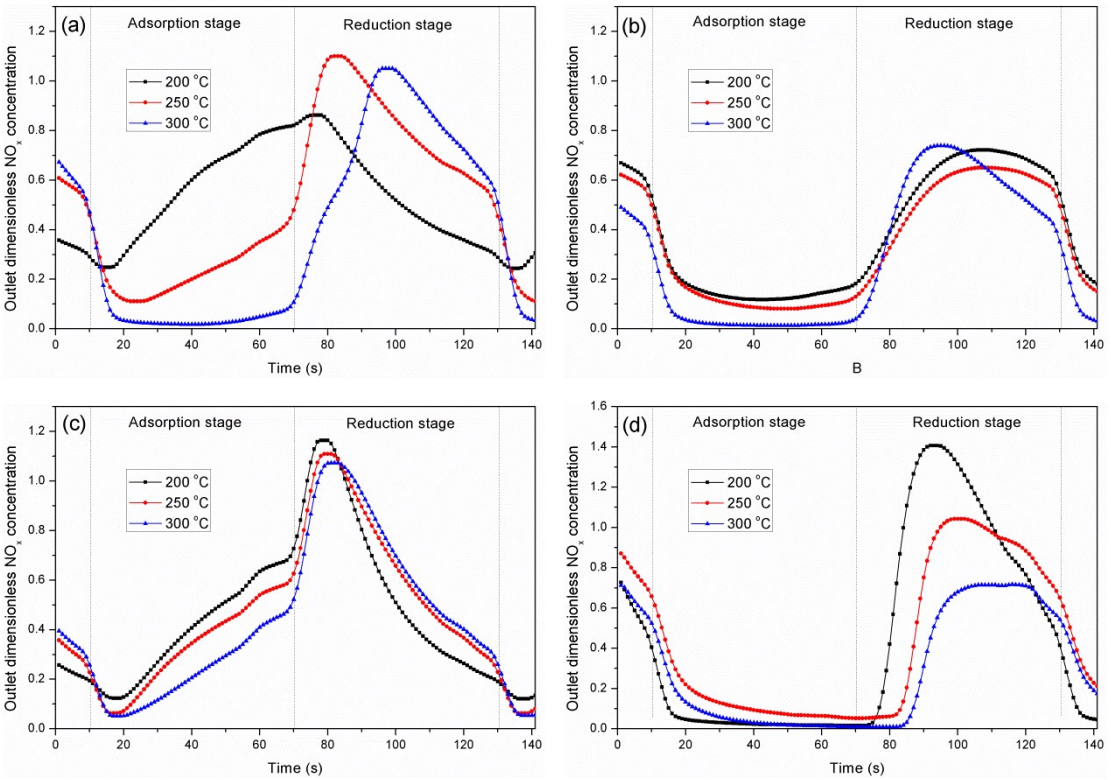
$$NO_x\ slipping = \frac{\int_{t_1}^{t_2} C_{NO_x,out} dt}{\int_{t_0}^{t_1} C_{NO_x,in} dt} \times 100\% \tag{6}$$

$$CO\ oxidation = 1 - \frac{\int_{t_0}^{t_2} C_{CO,out} dt}{\int_{t_1}^{t_2} C_{CO,in} dt} \times 100\% \tag{7}$$

$$CO\ slipping = \frac{\int_{t_0}^{t_1} C_{CO,out} dt}{\int_{t_1}^{t_2} C_{CO,in} dt} \times 100\% \tag{8}$$

t_1, t_2 and t_3 represent the time at the beginning of the adsorption, at the end of the adsorption and at the end of the reduction in an adsorption-desorption process, respectively.

Fig. S2 Outlet dimensionless NO_x concentration profiles at different temperatures of (a) FeCo/ASC, (b) FeCo/N-ASC-1, (c) FeCo/N-ASC-2 and (d) FeCo/N-ASC-3 catalysts. (Reaction conditions: flue gas: GHSV = 10000 h^{-1}, O_2 = 5%, NO = 800 ppm, duration = 60 s; reducing gas: GHSV = 10000 h^{-1}, CO = 1600 ppm, duration = 60 s.)



References

1. X. Cheng, M. Zhang, P. Sun, L. Wang, Z. Wang and C. Ma, *Green Chemistry*, 2016, **18**, 5305-5324.