Electronic supplementary materials *Mendeleev Commun.*, 2023, **33**, 696–698

O_3-assisted NH_3-SCR over FeBEA catalyst at low reaction temperature

Dmitriy A. Bokarev, Ivan V. Paramoshin, Sergey A. Kanaev, Galina O. Bragina and Alexander Yu. Stakheev

Catalyst preparation

The FeBEA catalyst (~1 wt. %Fe) was prepared by ion-exchange of parent BEA (NH_4^+-form, Si/Al=12.5, S_{BET} = 657 m^2/g, "Zeolyst") with an aqueous solution of $Fe(NO_3)_3$ at room temperature for 6 h. After washing and drying, the sample was calcined in air flow at 550°C for 4 h. Fe content according to ICP analysis was found to be 1.0 ± 0.1 wt %. The resulted powder was pressed, crushed and sieved to obtain an appropriate particle size for the catalytic tests (0.2-0.4 mm).

Catalyst characterization

Scanning electron microscopy (SEM-EDS) The surface morphology of catalysts was characterized using SU8000 (Hitachi, Tokyo, Japan) field-emission scanning electron microscope (FE-SEM). Before measurements the samples were mounted on a 25 mm aluminum specimen stub and fixed by conductive graphite adhesive tape. Qualitative and quantitative analysis of catalyst elements were carried out using energy dispersive X-ray spectroscopy (EDS) on Oxford Instruments X-max 80 EDS system with 15 kV accelerating voltage.

X-ray diffraction (XRD). The crystallographic structure of the catalysts was characterized by X-ray powder diffraction (XRD) using a D8 Advance diffractometer (Bruker AXS, Karlsruhe, Germany) with Bragg–Brentano geometry, Ni-filtered CuKα radiation, and LYNXEYE detector. The XRD patterns were recorded in the 2θ range 5–75° (scan rate 1.2°/min). Crystallographic parameters were calculated using the Rietan-FT software, which uses the Rietveld method.

Catalytic tests

Catalytic performance of FeBEA in a conventional NH_3-SCR and NH_3-SCR promoted by O_3 injection (O_3-assisted NH_3-SCR) was studied using fixed-bed flow quartz reactor (id=4mm) operating at atmospheric pressure (Fig S1). Before the experiment, the ozone generator was calibrated for producing the appropriate ozone concentrations of 0, 125, 250 and 400 ppm.

Preliminary experiments on ozone oxidation of nitrogen oxide showed that NO reacts with ozone in a stoichiometry close to one to one. The composition of the feed gas contains 500 ppm NO, 650 ppm NH_3, 0/125/250/400 ppm O_3, 10 vol % O_2, 6 vol % H_2O balanced with N_2. Ozone was obtained using a Medozone YOTA-60-01 ozone generator (Medozone, Russia). Total flow rate was fixed at 500 mL/min (GHSV = 230 000 h^{-1}). The temperature was ranged from 500 to 100°C at a cooling rate of 2°C/min. Ozone content at the inlet and outlet of the reactor was measured by ozone analyzer Medozone 254/5 (Medozone, Russia). Reaction products were analyzed by FTIR gas analyzer "Gasmet'' (Temet Instruments DX-4000). The conversion of NOx was calculated using the follow equation:

$$X_{NOx} = \frac{[NO_x]_{in} - [NO_x]_{out}}{[NO_x]_{in}}$$

where subscripts *in* and *out* are the inlet and outlet concentrations, respectively. It should be noted that $[NO_x]_{out}$ was calculated as $[NO]_{out} + [NO_2]_{out} + 2[N_2O]_{out}$.

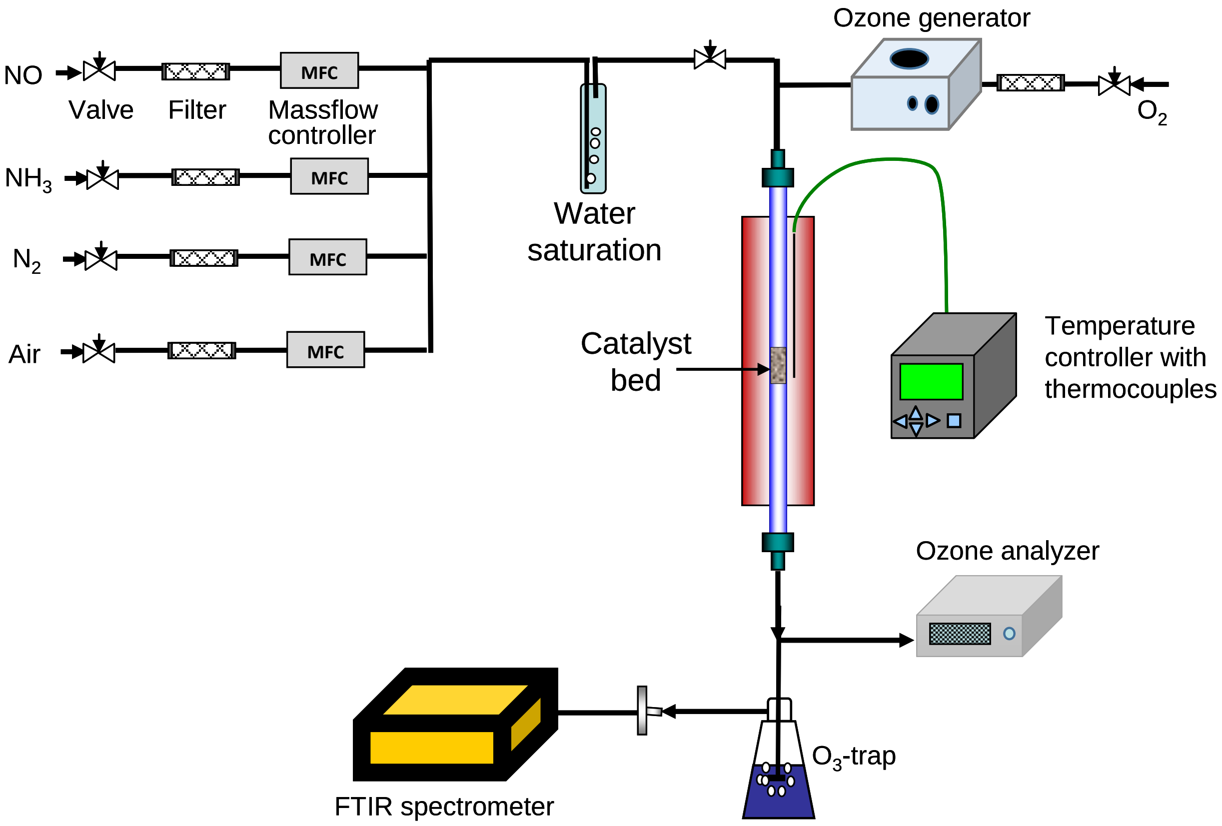

Figure S1 Experimental setup.