



# Influence of H<sub>2</sub>O on the low-temperature NH<sub>3</sub>-SCR of NO over V<sub>2</sub>O<sub>5</sub>/AC catalyst: An experimental and modeling study

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## HIGHLIGHTS

- Influence of H<sub>2</sub>O content on the SCR of NO over V<sub>2</sub>O<sub>5</sub>/AC catalyst was investigated.
- The microscopic reaction mechanism in the presence of H<sub>2</sub>O was identified.
- A 3D mathematical model of monolithic reactor model was established.

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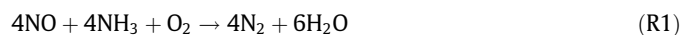
## ABSTRACT

The selective catalytic reduction (SCR) of nitric oxide (NO) by ammonia (NH<sub>3</sub>) at 393–473 K over AC (activated carbon) supported V<sub>2</sub>O<sub>5</sub> (vanadium pentoxide) (V<sub>2</sub>O<sub>5</sub>/AC) catalyst in the presence of H<sub>2</sub>O was investigated. In order to understand the influence of H<sub>2</sub>O on reaction rate and reaction mechanism, the kinetic measurement was performed. Both mechanistic and empirical models were applied to correlate the experimental data. The results showed that the SCR reaction follows the Eley–Rideal mechanism rather than Langmuir–Hinshelwood or Mars–van Krevelen mechanisms whether H<sub>2</sub>O was contained or not. And the pre-exponential factor decreased and activation energy increased with the increasing amount of H<sub>2</sub>O. But at high H<sub>2</sub>O content, the kinetic parameters were almost unchanged with the further increase of H<sub>2</sub>O content. Finally, the intrinsic kinetic models obtained in this work were incorporated into a 3D mathematical model of monolithic reactor. It was found that the Eley–Rideal model was more suitable for describing the SCR of NO by NH<sub>3</sub> in the presence of H<sub>2</sub>O than the empirical models, and thus should be adopted in the actual reactor design and scale-up for controlling the emission of NO<sub>x</sub>.

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## 1. Introduction

The emission of NO<sub>x</sub> must be reduced because it can result in many global environmental problems. As the regulation for NO<sub>x</sub> emission becomes more and more strict, much effort has been focused on the development of efficient NO<sub>x</sub> control (DeNO<sub>x</sub>) technology nowadays [1–4]. One of the most effective technologies is the SCR of NO by NH<sub>3</sub> over various catalysts, and it is generally accepted that under flue gas conditions, i.e. dilute mixtures of NO and NH<sub>3</sub> with O<sub>2</sub> in large excess, the SCR reaction occurs according to the following stoichiometry:



Many metal oxide catalysts [5–7], such as CuO/Al<sub>2</sub>O<sub>3</sub>, V<sub>2</sub>O<sub>5</sub>–WO<sub>3</sub>/TiO<sub>2</sub>, and MoO<sub>3</sub>/TiO<sub>2</sub>, have ever been developed and successfully commercialized for NO removal. However, these catalysts are usually operated at temperatures higher than 623 K so as to avoid

the deactivation by SO<sub>2</sub> and H<sub>2</sub>O which takes place at low temperatures [8], while the flue gas temperature for many burners is in the range of 393–523 K, which will have a great energy consumption if the units for reheating flue gas are added [9]. It is known that the V<sub>2</sub>O<sub>5</sub>/AC catalyst has exhibited quite high activity at low temperatures for NO removal, and SO<sub>2</sub> in the flue gas does not deactivate the V<sub>2</sub>O<sub>5</sub>/AC catalyst but improves the activity in the absence of H<sub>2</sub>O [10]. So the V<sub>2</sub>O<sub>5</sub>/AC catalyst may be an excellent option for SCR of NO with NH<sub>3</sub>. Some researchers go a further step to investigate the kinetics over low-temperature catalysts. By far there have been two kinds of model proposed based on Eley–Rideal mechanism and Langmuir–Hinshelwood mechanism, respectively. Some authors believed that the reaction occurs through an Eley–Rideal type mechanism in which NH<sub>3</sub> is adsorbed on the vanadium-based catalyst in the first step, and then the reaction proceeds with NO from the gas phase [11–14]. Meanwhile, it has also been reported that the Langmuir–Hinshelwood mechanism which considers that NO and NH<sub>3</sub> are both adsorbed on the catalyst surface and then react, is more suitable than Eley–Rideal mechanism. For instance, Valdes-Solis et al. [15] measured the kinetics

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