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Study of poisoning mechanism of Hg and As on $V_2O_5-WO_3/TiO_2$ SCR de-NO_x catalysts

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ABSTRACT

$V_2O_5-WO_3/TiO_2$ catalysts are used as the most mature and extensive techniques, which are applied to de-NO_x in the coal-fired flue gas at present. And yet, the deactivation of catalysts is caused by the complex flue gas compositions under the work environment restriction. Heavy metals, such as mercury and arsenic that play increasingly prominent roles in the toxicity of catalysts, have attracted increasing attention in recent years. Accordingly, the catalysts poisoning of Hg and As also has been a hot research area. This paper has discussed the poisoning mechanism of Hg and As by simulating flue gas. On the basis of the impacts of Hg and As on pore structure, acid sites, and surface functional group, the behaviors of Hg and As have been revealed with DFT molecular calculations. Meanwhile, the proposed catalysts poisoning mechanism of Hg and As provides the theoretical foundation to solve the catalysts poisoning and deactivation of Hg and As.

KEYWORDS: $V_2O_5-WO_3/TiO_2$ catalysts, mercury, arsenic, poisoning mechanism