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Performance analysis of industrial selective catalytic reduction (SCR) systems

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Abstract

Selective catalytic reduction (SCR) is an established technology for post-combustion nitrogen oxide (NOx) emissions control from different power/chemical plants. This approach requires a reducing agent such as ammonia to reduce NOx selectively in the presence of excess oxygen and a suitable catalyst. The ammonia is injected into the exhaust gas stream and is mixed with NOx. This mixture of ammonia and NOx passes through the catalyst bed, where a high percentage of NOx reacts on the catalyst surface, with adsorbed ammonia decomposing into diatomic nitrogen and water molecules, thereby reducing the NOx level in the exhaust gas. In this study, a 3-dimensional computational fluid dynamics (CFD) model of a single monolith honeycomb structure of the SCR system is developed to investigate the effect of various important parameters including the NO_2/NOx ratio, space velocity, shapes and NH3/NOx ratio for stationary SCR applications. The steady state model was developed by considering the conservation of mass, momentum and energy of reacting gases. The results showed that as the NO_2/NOx ratio is increased, the nitrogen dioxide (NO_2) reaction with ammonia becomes more pronounced and results in an overall improvement of the NOx reduction in the SCR system.

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Keywords: NOx emissions; monolith honeycomb; space velocity

1. Introduction

Owing to their environmental impacts, nitrogen oxide (NOx) emissions from power and chemical plants are a major concern. Hence, progressively stricter emission regulations have been enacted in different parts of the world [1]. Efforts to meet these stipulated low NOx levels have received serious attention. Among the technologies for the conversion of NOx, selective catalytic reduction (SCR) of NOx is a very promising method, due to its high efficiency, selectivity and cost [2,3]. Commercial SCR process has the capability of

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NOx reduction of 60-90% and can be effective at low temperature, resulting in great energy savings [4,5]. However, continuous progress in this endeavour is still being pursued to meet the progressively stricter NOx regulations.

The study investigates the effects of various parameters on the performance of various shapes of monolith honeycomb structured catalysts for stationary plants applications. Most work on the single monolith channels considered only the reaction between NO and the reductant ammonia for stationary plants. The present study also includes the effect of NO_2 reaction on the overall performance of the system, which has been found to be an important reaction for the SCR of NOx in automotive applications [6]. Furthermore, there is very limited work on the investigation of 3-dimesnional effects on the SCR performance. Hence, the present study develops a 3-D CFD model using ANSYS FLUENT to analyse and accurately predict the performance of SCR system for stationary applications.

2. Mathematical Formulation

The SCR process involves the reaction between exhaust gas and NH3 on a catalyzed surface on the wash coat of the monolith. The equations for the reactions are as given below:

$$4NH_3 + 4NO + O_2 \longrightarrow 4N_2 + 6H_2O \quad (1)$$

$$4NH_3 + 2NO_2 + O_2 \longrightarrow 3N_2 + 6H_2O \quad (2)$$

The work is based on a 3-D representative single channel of the SCR system similar to the work of [1]. Different channel shapes were considered. In order to capture the reaction correctly, various governing equations were solved. The conservation equations of mass, momentum and energy in the gas phase were considered. The details of the equations may be found elsewhere [1].

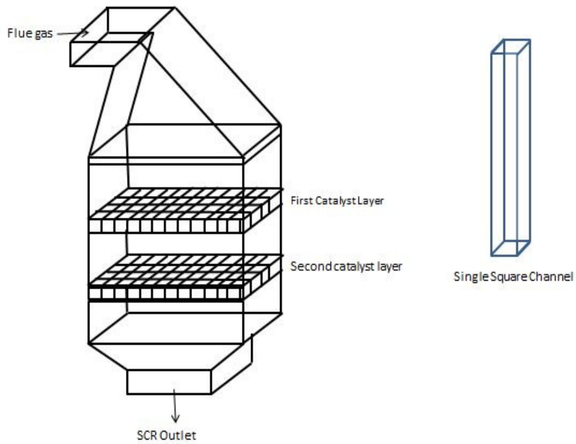

Fig. 1. Schematic of the SCR system

3. Results and Discussions

The model was validated by comparing its results with the work of [1]. Figure 2 shows the comparison between the pressure drop obtained from the present study, and the simulation and experimental results of [1]. The figure shows an excellent agreement among these results for different values of inlet velocity. Figure 3 shows the comparison of the results obtained for the single reaction of NO with ammonia for different values of NH_3/NOx. The result fit in perfectly with the experimental results obtained by Tronconi [7] but varies slightly from the results obtained by [1].

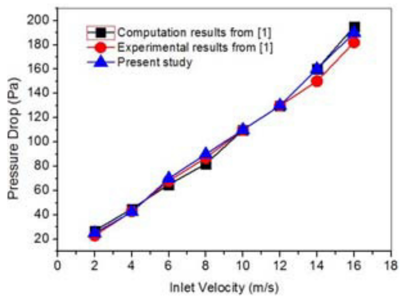

Fig. 2. Model validation: prediction of pressure drop

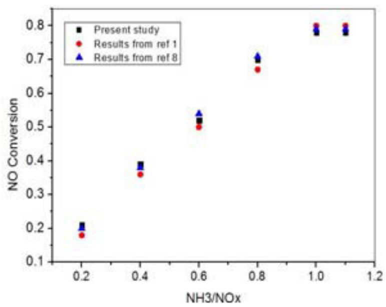

Fig. 3. Model validation: prediction of NO conversion

Figure 4 shows the effect of space velocity for square, circular and triangular channels on the NOx conversion. As expected, the NOx conversion efficiencies decrease as the space velocity is reduced for all channel shapes. The results show that the NOx conversion is generally higher for the square channel and is lowest for the triangular channel. Also, the space velocity effects on pressure drop for the different channel shapes were investigated. The results show that the pressure drop increases as the space velocity increases, with the square channel showing the most stable pressure regime.

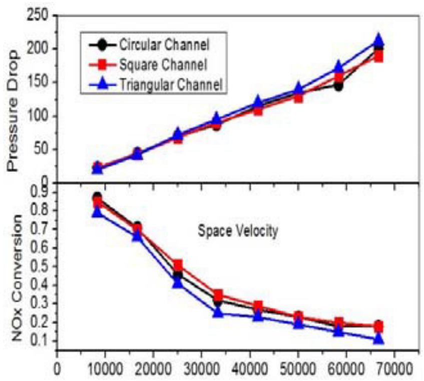

Fig. 4. Effect of SV on NOx conversion and pressure drop

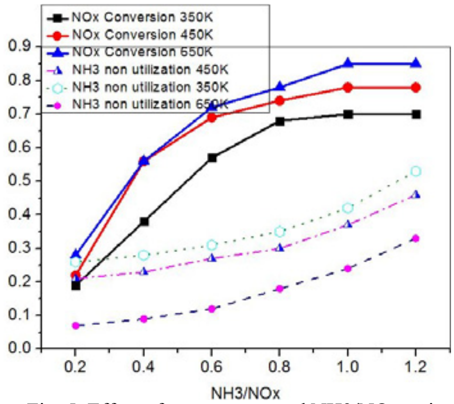

Fig. 5. Effect of temperature and NH3/NOx ratio on NOx conversion and ammonia non-utilization

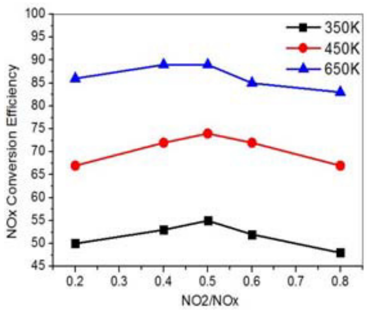

Fig. 6. Effect of NO_2/NOx ratio on the NOx conversion efficiency

Further studies were carried out for the square monolith channel to investigate the optimal conditions for NOx reduction. Figure 5 shows the NOx conversion efficiency for a multiple reaction model of the square shaped channel at different temperature conditions of inlet exhaust gas (350K, 450K, and 650K) and different NH_3/NOx ratio at space velocity of 25000 hr^{-1}. The results show that the NOx conversion efficiency increases as the temperature of the inlet gas is increased and as NH_3/NOx ratio is increased tending to reach the peak value near stoichiometric condition.

Figure 5 also shows the ammonia non-utilization as a function of the different inlet temperatures. The results depict that the ammonia non-utilization is increased with the increase of NH_3/NOx ratio for all inlet temperatures. At higher inlet gas temperatures, the ammonia non-utilization was less than that at lower temperatures; which is desirable.

Figure 6 shows the effect of the NO_2 to NOx ratio in the inlet gas on the NOx conversion efficiency. The result shows that with the increase of NO_2/NOx ratio, the NOx conversion efficiency is increased. This increasing trend continues until NO_2/NOx ratio becomes 0.5 (i.e. when NO_2/NO ratio is 1) after which there was a reduction in the NOx conversion efficiency.

4. Conclusions

In the present study, a NOx model with multiple reactions was examined and the effects of various parameters were investigated. This model takes into account the effect of the NO_2 reaction which has been neglected in many past studies. The objective was to identify the geometrical and operating parameters which yield high performance for SCR system for stationary applications.

The results show that higher space velocities lead to lower NOx conversion efficiencies similar to the case for automotive SCR systems. This is due to lower interaction time between the NOx, the ammonia and the catalyst. The square shaped channel showed better NOx conversion and more stable pressure drop in response to changes in the values of space velocity. The NOx conversion efficiency is also influenced by NH_3/NOx and NO_2/NOx ratios. Considering the ammonia non-utilization and the NOx conversion, the results suggest that the optimal NH_3/NOx ratio should be near stoichiometric. The maximum NOx conversion efficiency is found when the NO_2/NOx ratio is 0.5 (i.e. when the NO and NO_2 values are equal). This suggests incorporation of an oxidation process of the NO since the exhaust NO_2 content is typically low. The above results will contribute to the design improvement of the stationary SCR systems in order to meet the increasingly stringent NOx emissions regulations.

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