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ScienceDirect
Energy Procedia 75 (2015) 2345 – 2350
Energy Procedia

The 7th International Conference on Applied Energy – ICAE2015

Investigation of Dual Layered SCR Systems for NOx Control

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Abstract

Nitrogen Oxides (NOx) emissions are one of the major pollutants emanating from industrial plants as well as automobiles. Due to their harmful effect on human health and the environment, strict regulations on the acceptable amount of NOx that can be released from stationary plants have been enacted. Selective Catalytic Reduction (SCR) is an established technology for achieving high NOx reduction from stationary plants. However, due to progressively stringent emissions regulations, the SCR systems need to undergo continuous modifications. Their performance can be improved by gaining better understanding of the various processes that occur within these complex systems. Computational Fluid Dynamics (CFD) provides a cost effective means of achieving this understanding that can be used as a guide for the design of future systems for better NOx conversion from the SCR system. The SCR systems are typically made up of multiple layers of catalyst. While a lot of computational work has been done on the system, most of these previous works were 1-dimensional and 2-dimensional. The present study uses a 3-dimensional model to study the behavior of the SCR system; this will give a more realistic behavior of the SCR system. Furthermore, most work has concentrated on the interactions within a single catalysed channel. This work however, tries to study the influence of a second catalysed layer on the overall performance of an SCR system. The results show that the second catalyst layer plays a vital role in the reduction of NOx as well as ammonia. Hence, the second layer is found to enhance the performance of the system.

Peer-review under responsibility of Applied Energy Innovation Institute

Keywords: NOx; SCR; Computational Fluid Dynamics (CFD)

1. Introduction

Emission reduction from stationary plants is one of the major concerns in today's world. With the ever growing demand to meet the needs of the products and services provided by these plants, there is an

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Peer-review under responsibility of Applied Energy Innovation Institute
doi:10.1016/j.egypro.2015.07.484

increase in the number of plants. Consequently, there is an increase in harmful emissions. Among these harmful gases are NOx: oxides of nitrogen which include NO and NO_2. They are usually formed in the combustion process by the oxidation of nitrogen containing compounds in fuels in automobile engines and stationary plants or by the oxidation of nitrogen in the combusting air. The emission of NOx from stationary sources is estimated to account for about half of the total NOx emitted into the atmosphere from anthropogenic processes [1]. For instance, typically from a stationary coal fired plant, the annual NOx generated can reach up to 10200 tones [2]. The main stationary sources of NOx emissions include power generation plants, stationary engines, industrial boilers, process heaters and gas turbines [3]. To combat the emission of NOx, progressively stricter emission regulations have been passed in different parts of the world [4]. Thus efforts to meet these emission levels have received serious attention. Selective catalytic reduction (SCR) of NOx is one of the most promising technologies for the reduction of NOx [5]. Some of the advantages of the SCR system are the high efficiency, selectivity and economics of the systems [6]. The SCR process involves the reduction of NOx by the chemical reaction between the exhaust gases and a reductant such as urea or ammonia in the presence of a catalyst. This reduction reaction usually takes place within multiple layers of catalysts walls. Industrial SCR process has the capability of NOx reduction of 60-90% and can be effective at low temperature, resulting in great energy savings [7]. However, further improvement in the SCR system is still being pursued to meet the progressively stringent NOx emission regulations. To achieve the target set out by the various emissions regulations, higher NOx conversion efficiencies are desired as well as minimal ammonia slip. This would require that the processes that occur within the systems are thoroughly understood so as to provide guidance for future improvement of the system design. Mathematical models have proven to be a cost effective and efficient means for carrying out such investigations. Effects of key parameters such as space velocity, size of channels, shapes of the channels, feed rates, and species ratio on different systems ranging from 1D to 3D have been investigated using various mathematical models. Most of the modelling was done for single channel shapes of the SCR for simplifications [8-10].

The current study attempts to investigate the effect of various channel lengths on the performance of the SCR system composed of square channels of monolith honeycomb structured catalysts for stationary plants applications. In this work, the two major NOx reduction reactions described below are considered [11]. Most work on the single monolith channels considered only the reaction between NO and the reductant ammonia for stationary plants, this model also takes into consideration the NO_2 reaction on the overall performance of the system. Studies by [11] showed that for stationary applications it is also a very important reaction in the SCR. In addition, only a few 3D CFD analyses have been carried out on the subject. A novel computation study was carried out using Ansys Fluent, which investigates the interactions within the dual layer catalyst systems and their results compared with having a single long catalysed layer. The objective was to see the influence of the second catalyst layer on the overall performance of the systems for a dual layer system. No past work has carried out this analysis according to the authors' knowledge.

2. Mathematical Formulation

Figure 1 shows the schematic of the SCR system for a stationary application [11]. The governing equations for the conservation of mass, conservation of species as well as the conservation of momentum and energy were applied. These are shown below: Where *i* represents the species in the reactions.

Continuity equation: $\nabla \cdot (\rho \mathbf{u}) = 0$

Momentum balance equation: $\nabla \cdot (\rho \mathbf{u} \times \mathbf{u}) = -\nabla P + \nabla \cdot (\mu(\nabla \mathbf{u} + (\nabla \boldsymbol{u})^T)$

Energy balance equation: $\nabla \cdot \left(\rho c_g \mathbf{u} T\right) = \nabla \cdot (\lambda_g \nabla T) + (\sum_k (-\Delta H_{k,j}\, r_{k,j})) \times F_j$

Mass balance equation for the species: $\nabla \cdot (\rho \mathbf{u} w_i) = \nabla \cdot \left(\rho D_{i,N_2} \nabla w_i\right) + \left(\sum_k \left(v_{i,j,k} M_{i,j} r_{k,j}\right) \times F_j\right.$

The SCR reaction involves the reaction between the exhaust gas and NH_3 on a catalyzed surface of the monolith. The equations for the reactions considered in this modeling work 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 representative single channel of the SCR with geometry similar to the geometry used by [5]. Further work was carried out using a dual layer square-shaped channel of the system. The dimension of the dual-layer single channel is shown in Figure 2. In the dual layer system studied, the two layers were modeled as catalyzed walls with the space between both layers left un-catalyzed. In order to capture the reactions correctly, various governing equations were solved. The conservation equations for the process in the gas phase such as mass, momentum and energy conservation were considered as shown in the equation below [5].

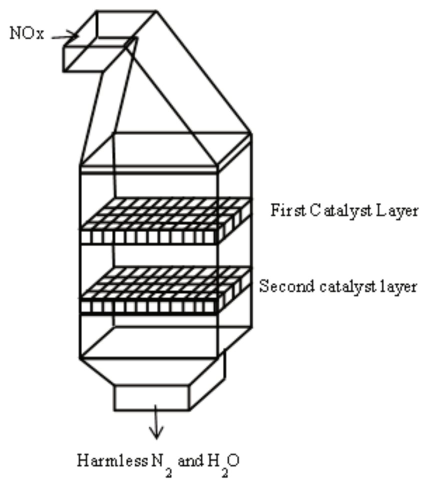

Figure 1. SCR system schematic [11]

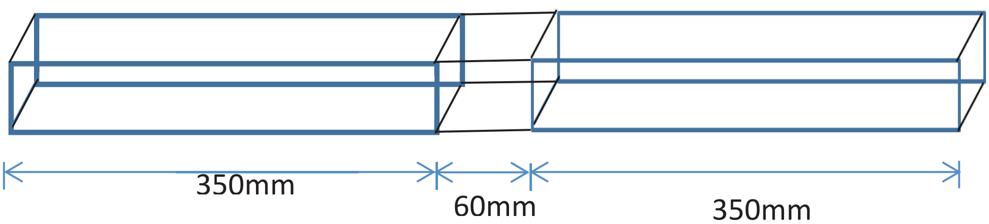

Figure 2 Dual layer SCR channel

3. Results and Discussions

Model validations were carried out by comparing the results to other studies. Figures 3 below shows the pressure drop obtained from the present model compared with experimental and simulation results carried out by [5]. The figure shows that there is an excellent agreement (within 3%) between the current results and the results from [5]. Thus the study was in excellent agreement with the results compared with. Further validation was carried out by comparing the NO conversion prediction of the present study with the experimental results by [5] and simulation results carried out by [4] and is shown in Figure 4. The figure shows that there is an excellent agreement between the results obtained from the present study and those by [4]. There is a very slight variation between the results obtained from the present study and those obtained by [5].

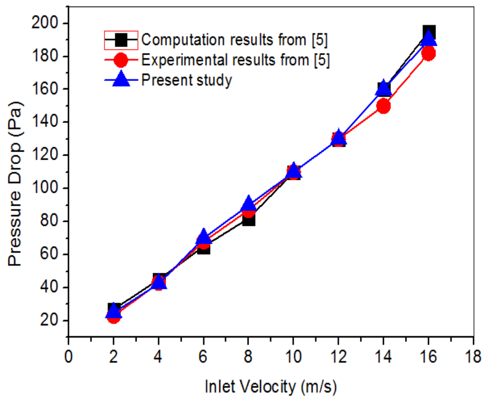

Figure 3: Model validation: prediction of pressure drop

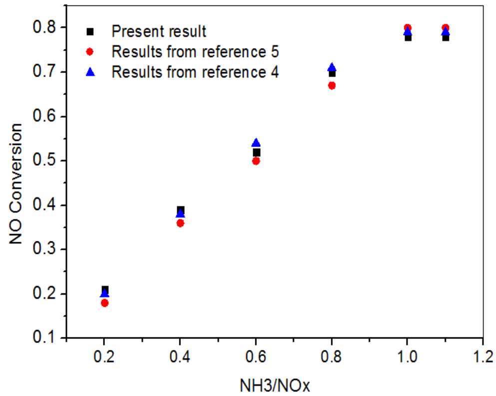

Figure 4: Model validation: prediction of NO conversion

After the model was validated, it was employed to investigate the effect of catalyst layer lengths. Catalyst lengths ranging from 150mm to 700mm were considered. Figure 5 shows the NOx conversion obtained for each catalyst length for different NH3/NOx ratios. The result shows as expected, that the NOx conversion increases as the length of catalyst layers is increased. The influence of the catalyst length on the NOx reduction increases significantly at higher NH3/NOx ratios. Furthermore, the difference in the NOx reduction between the system of 150mm and 350mm is more significant than the difference between the NOx conversion for the 350mm and 500mm catalyst system. This suggests that NOx reduction is more sensitive to the catalyst length for shorter catalysts.

The present study also investigates the NOx conversion efficiencies for a dual layer SCR system as shown in Figure 2. Figure 6 shows the NOx conversion efficiencies for the dual layer SCR system for different inlet exhaust gas temperatures and different NH3/NOx ratios. The figure shows that the at all temperatures, the NOx conversion efficiencies increase as the NH3/NOx ratios are increased. However, after NH3/NOx ratios of 0.6, there is a very minimal increase in the NOx conversion efficiencies at the three temperatures of inlet exhaust gases investigated.

To investigate the effect of dual layer, simulations were carried for a single layer SCR system with the same catalyst channel length. Figure 7 shows the comparison between the NOx conversion efficiencies for the single and dual catalyst layers of the same lengths at different temperatures (ranging from 350K to 650K) and NH3/NOx ratios. The figure shows that the NOx conversion is slightly better for the dual layer SCR system. However the difference between the NOx conversions for the two systems is remarkably higher at NH3/NOx ratios of 0.6 at all the temperature that were investigated. This is due to the fact that the NOx conversion at the NH3/NOx of 0.6 ratio gets close to the peak values for the dual layer while the

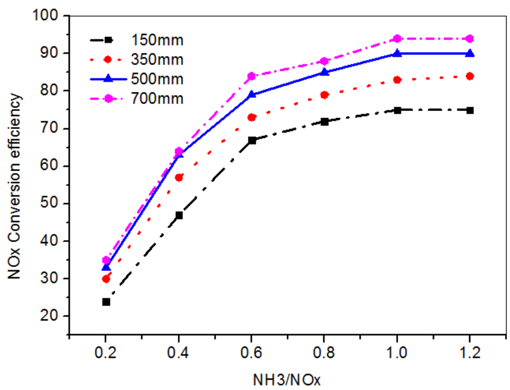

Figure 5: NOx reduction for different catalyst lengths

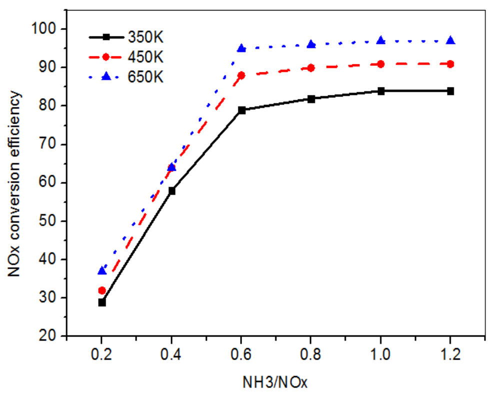

Figure 6: NOx conversion for dual layer SCR

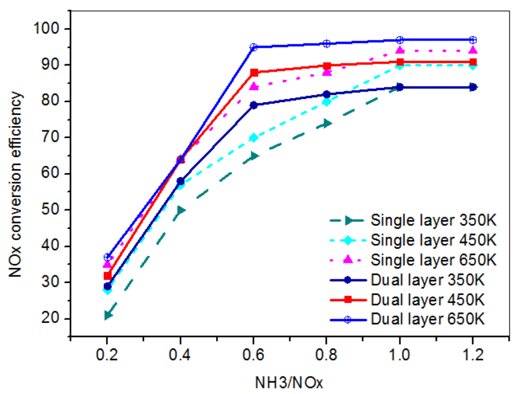

Figure 7: Comparison between NOx conversion for dual and single layer

conversion reaches peak values at NH3/NOx ratios of 1.0. This difference as well as the higher NOx conversion for the dual layer SCR system means that the use of dual layer may lead to cost savings as less ammonia is required to achieve high NOx conversion.

4. Conclusions

SCR systems are a promising technology for the efficient reduction of NOx from stationary sources. These systems can achieve NOx reduction of up to 95 percent efficiency. In the present study, the NOx reductions for different catalyst lengths were studied. From the study, it was discovered that the NOx reduction efficiencies increased as the catalysts lengths were increased. However, the difference between the NOx reduction efficiency waned with continued increments in the catalyst lengths after 350mm. This showed that it is not economical to continually increase the catalyst lengths beyond certain limits for the space velocities of operation investigated. A model study of the NOx reduction within the dual layer SCR system was also carried out. The results obtained showed that the dual layer SCR of similar catalyst length to a single SCR system performed better than the single layer SCR system. The NOx conversion efficiencies of the dual layer SCR system also peaked at values of NH3/NOx of 0.6 as against a value of

1.0 for the single layer SCR. This shows that it is more advantageous to have a dual layer SCR system than a single layer of similar catalyst length.

Acknowledgement

This research was supported by the Government of Abu Dhabi to help fulfil the vision of the late President Sheikh Zayed Bin Sultan Al Nayhan for sustainable development and empowerment of the UAE and humankind

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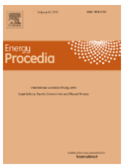

Biography

Oghare Ogidiama is a PhD student at Masdar Institute of Science and Technology, Abu Dhabi, UAE. He works with Professor Tariq Shamim on pollutants abatement. The above work was part of his research work during his master's degree.