NO REMOVAL FROM FLUE GAS BY NH₃ RADICAL SHOWER – ESTIMATIONS
BASED ON A WELL MIXED REACTOR MODEL

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Abstract

The effectiveness of NO removal from the flue gas in an NH₃ radical shower system is estimated based on a well mixed reactor model. The rate of NO removal as dependent on the NO concentration in the flue gas, the flue gas flow rate and the initial concentration and rate of radical injection into the discharge is calculated.

Adoption of a corona radical shower is a promising way of removing NOₓ from flue gases [1,2]. It allows one to effectively produce radicals in the corona discharge active zone without undue activation of the bulk of the flue gas. This contribution is concerned with estimations of the effectiveness of NO removal in an NH₃ radical shower system.

It is assumed that a corona discharge occurs between a row of hollow electrodes, through which ammonia is injected, and a grounded plate. The row is located in the centre plane of a reactor through which the flue gas at atmospheric pressure flows. A well mixed reactor model is adopted for the calculations. Use of that model is supported by recent LIF measurements of NO abatement in a streamer corona discharge [3], which suggest that electrohydrodynamic flow phenomena enhance the mixing of the gas in the plasma reactor.

The plasma chemistry in the corona radical shower is fairly complex. Apart from the production in the flue gas of various chemically active species, such as O, OH, N, O₃ or HO₂, the NH₂ and NH radicals are produced among others directly by the dissociative excitation of NH₃ [4]. A detailed analysis of all those processes is still to be done. Up to now the attention of those that have analyzed the processes in the NH₃ corona radical shower [5,1,2] has been turned mainly to the neutral chemistry. It was ascertained that the main processes leading to a fast elimination of NO in the presence of NH₃ are those of reduction with NH₂ and NH:

\[
\begin{align*}
\text{NO} + \text{NH}_2 & \rightarrow \text{N}_2 + \text{H}_2\text{O} & k_1 = 2.1 \times 10^{-17} \text{ m}^3 \text{ s}^{-1} \\
\text{NO} + \text{NH} & \rightarrow \text{N}_2 + \text{OH} & k_2 = 4.7 \times 10^{-17} \text{ m}^3 \text{ s}^{-1}
\end{align*}
\]

(1) (2)

It follows from data presented in [5,6] that for production of the NH₂ and NH radicals by neutral chemistry the reactions of NH₃ with O and NH₂ with O, respectively, are mainly responsible, their rate coefficients being of the same order. As a result an inequality \( n_{\text{NH}} < < n_{\text{NH}_2} \) should be satisfied for the number densities of these radicals. It is therefore acceptable to omit, as a first approximation, reaction (2) and calculate the rate of NO removal in an NH₃ corona radical...
shower as resulting from reaction (1) only. In doing so one neglects also various reactions of NH$_2$ with other species [6,7], which reduce the number density of that radical.

We assume that the flue gas containing NO with a number density equal to $n_{\text{NO}}$ flows across the reactor at a flow rate $v_f$. The NH$_2$ radicals are produced by the corona radical shower system at a rate equivalent to injecting them into the reactor with a number density of $n_{\text{NH}_2}$ at a flow rate $v_{\text{NH}_2}$. Normally, the radicals are produced from NH$_3$ entering the discharge in a mixture with a carrier gas (e.g., Ar, possibly diluted with air [2]). One would have to take that into account, if the content of NH$_3$ were calculated based on the electron and neutral kinetics in the discharge. In our calculations $n_{\text{NH}_2}$ and $v_{\text{NH}_2}$ will be regarded as given.

Based on the considerations presented above the following equations governing the reduction of NO may be written

$$\frac{d n_{\text{NO}}}{dt} = -k_1 n_{\text{NO}} n_{\text{NH}_2} + R_{\text{NO}}$$  \hspace{1cm} (3)

$$\frac{d n_{\text{NH}_2}}{dt} = -k_1 n_{\text{NO}} n_{\text{NH}_2} + R_{\text{NH}_2}$$  \hspace{1cm} (4)

where $R_{\text{NO}}$ and $R_{\text{NH}_2}$ are the net rates of flow of NO and NH$_2$, respectively, into the reactor. For a stationary state the left hand sides become 0 and a very simple set of algebraic equations is obtained. This is solved for various flow rates and initial concentrations of NO and NH$_2$, to give a rough estimate of the radical shower effectiveness. The problems to be considered next are the inclusion of reaction (2) and of the self-recombination of NH$_2$. The resulting set of nonlinear algebraic equations describing the stationary state shall be solved using the Newton-Raphson algorithm. A routine newt [8] shall be used for that purpose. Given the vector of initial values $x_0$, the routine seeks by iteration for the values of the solution vector $x$. This work is in progress.

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References