Analytical Management of SCR Catalyst Lifetimes and Multipollutant Performance

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Utility SCRs Contain Diverse Layers With Much Different Ages
Estimate An Activity Ratio for Any SCR Age

\[
\frac{k_d}{k_0} = \left(\frac{k_t}{k_0}\right) - 1 \quad t + 1
\]

\[
I X_{NO,d} = \alpha \left[1 - \left(1 - \frac{I X_{NO,0}}{\alpha} \right) \frac{k_d}{k_0}\right]
\]

- \(k_t\) is the reactivity at 16,000 h specified by the manufacturer.
- A value for \(I X_{NO,d}\) determines the rate constant for NO reduction in NEA’s SCR Catalyst Model.
- Consider two deactivation scenarios: (I) Both NO reduction and Hg\(^0\) oxidation are deactivated in direct proportion; and (2) Only NO reduction is directly deactivated.
The SCS SCR Database

- 16 full-scale SCRs.
- Wide ranges of fuel quality, HCl, T, and GHSV.
- Different vendors & monolith types.
- 2, 3, or 4 layers.
- Up to tens of thousands of operating hours per layer.
- Activity ratios from 0.4 to 0.99+. 
Extent of Hg$^0$ Oxidation

\[
SCR \quad X_{Hg^0} = 100 \frac{IN \quad C_{Hg^0} - OUT \quad C_{Hg^0}}{IN \quad C_{Hg^0}}
\]

- Unaffected by variations in Hg$^{2+}$ at the SCR inlet.
**NH₃ Inhibition of Hg⁰ Oxidation Is Always Significant**

- Early layers have highest NH₃ concentrations.
- Most Hg⁰ oxidizes on the trailing layers.
Catalyst Deactivation Enables Deeper NH$_3$ Penetration Into the Trailing Layers

- All deactivated catalysts met the NH$_3$ slip regulation in our simulations.
Substantially Less $\text{Hg}^0$ Oxidation Even With Direct Deactivation of NO Reduction Only (Type II)
Substantial Variations in Hg$^0$ Oxidation Among Different Units at the Same Site (Type I)
Deactivation Distorts the HCl Dependence

- Get the expected saturation curve with fresh catalysts.
- Huge reductions in the extents of Hg\(^0\) oxidation for deactivated layers.
- Number of layers must factor into any performance index.
Summary

• Each simulation took less than 5 s on an ordinary microprocessor.
• NEA’s SCR Catalyst Model obtains converged solutions for any combination of catalyst properties among up to five layers in a commercial SCR.
• Manufacturer’s deactivation histories and reported operating hours for each layer determine a diminished activity ratio, which specified a NO$_x$ conversion across each layer that could be reproduced under two deactivation scenarios for Hg$^0$ oxidation.
• Both types of deactivation slow the rate of NO reduction, which gives deeper NH$_3$ penetration into the monolith, which disrupts Hg$^0$ conversion.
• Both types of deactivation completely disrupt the apparent Cl dependence, so that each SCR behaves as a distinctive reaction system.
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Input Requirements

- The inlet gas concentrations of NO, HCl, HBr (= total Br addition) and SO$_2$.
- The total Hg concentration, in µg/dscm, and the fraction of oxidized Hg at the SCR inlet, based on measured values.
- The molar NH$_3$/NO ratio, which equals the measured NO conversion efficiency.
- The SCR temperature.
- The gas hourly space velocity, GHSV, which is a nominal number of reactor volumes processed per hour, based on the flowrate at the SCR inlet.
- The pitch and channel shape for both honeycomb and plate catalysts.
- The mean sizes in the catalyst pore size distribution, and the associated void fractions in each size class.
- The catalyst manufacturer, to provide a basis for clarifying geometric specifications and for estimating rate parameters.
- Catalyst age and manufacturer’s activity history.