Analytical Management of SCR Catalyst Lifetimes and Multipollutant Performance

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Utility SCRs Contain Diverse Layers With Much Different Ages

N81

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
45																			
46	***SCR Operating Conditions***																		
47		SCR Inlet Conditions																	
48			NH_3/NO		Molar Ratio														
49			Inlet NO		ppmv or		ppmv dry												
50			Inlet SO_3		ppmv or		ppmv dry												
51			Inlet Hg^{2+}		% Total Hg														
52		Gross Size																	
53			GHSV		1/hr@32F														
54			No. Layers	5															
55		Calculation Sequence:			Detailed catalyst properties required for Design Simulations and only SCR shape specs required for a Global Reactivity Analysis.														
56			Design Simulation			Y or N ?		Global Reactivity Analysis				Y or N ?							
57		Layer Specifications:																	
58			For Layer 1:																
59			Length		m				Wall	Thickness		mm			F_{Hg}		Adjustment to Hg oxidation rate		
60			T_{IN}		°C					V_2O_5		wt. %			F_{NO}		Adjustment to NO reduction rate		
61			T_{OUT}		°C					WO_3		wt. %			F_{HCl}		Adjustment to HCl adsorption rate		
62			Monolith		Honeycomb or Plate ?					MoO_3		wt. %			F_{NH3}		Adjustment to NH_3 adsorption rate		
63			Pitch		mm					TiO_2		wt. %		Conv.	Tolerance				
64			Shape		Circular, Square, Rectang, or Triang					$^{Macro}d_{Pore}$		Angstroms							
65			Make		COR, ARG, KWH, HAT, or HIT					$^{Macro}EPS$		Fractional MacroVoidage							
66			k_D/k_0		Deactivation Ratio					$^{Micro}d_{Pore}$		Angstroms							
67										$^{Micro}EPS$		Fractional MicroVoidage							
68									Default	Reactivity	N	Y or N ?							
69											A-Fac	Ea							
70									Hg Oxid.	by Cl									
71										by Br									
72										NO Red.									
73										SO2 Oxid.									
74										HCl Ads.									
75										NH3 Ads.									
76										HBr Ads.									
77									Conv.	Tolerances									

Full-Scale SCR | Lab-Scale Catalyst | Sheet1

Ready 130%

Estimate An Activity Ratio for Any SCR Age

$$\frac{k_d}{k_0} = \frac{\frac{k_t}{k_0} - 1}{t_t} t + 1 \qquad {}^{I}X_{NO,d} = \alpha\left[1 - \left(1 - \frac{{}^{I}X_{NO,0}}{\alpha}\right)^{\frac{k_d}{k_0}}\right]$$

- 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

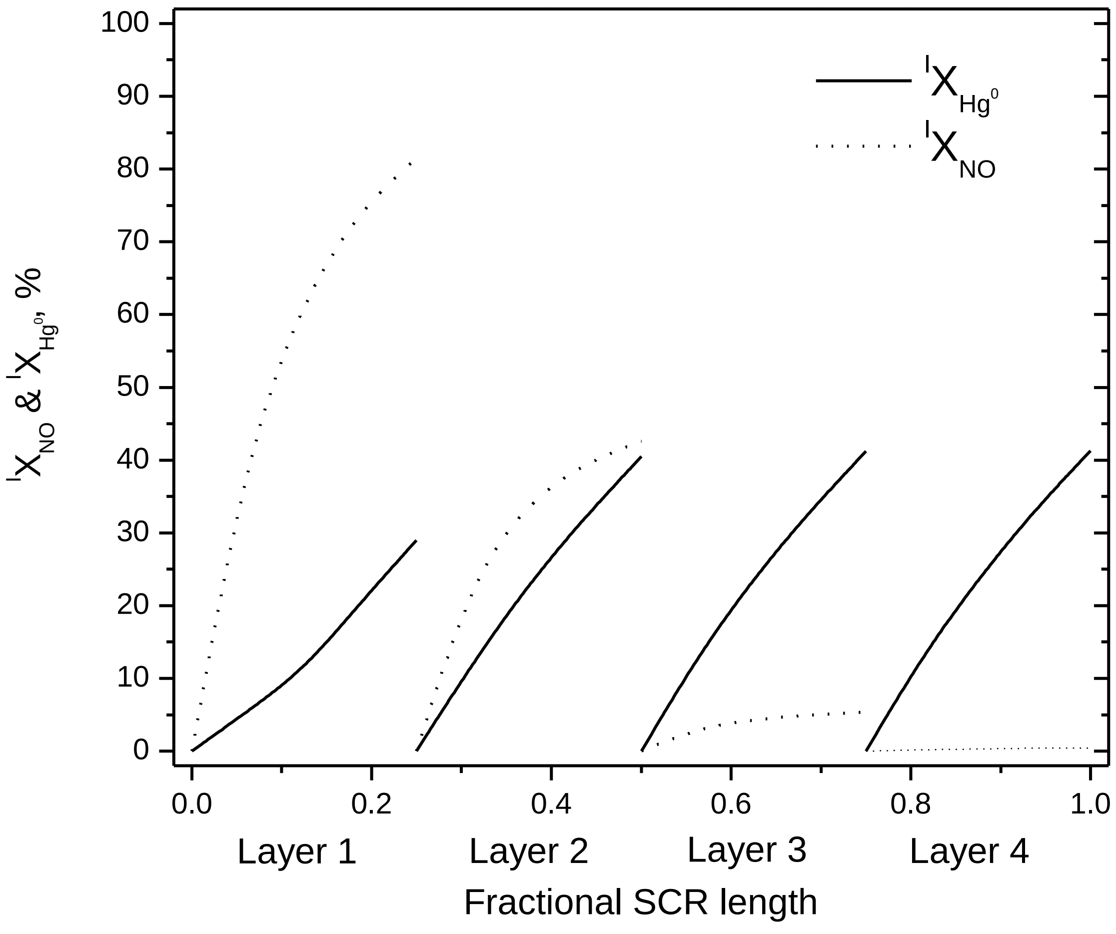
- *16 full-scale SCRs.*
- *Wide ranges of fuel quality, HCl, T, and GHSV.*
- *Different vendors & monolith types.*
- *2, 3, or 4 layers.*
- *Up to tens of thousands of operating hours per layer.*
- *Activity ratios from 0.4 to 0.99+.*

Extent of Hg^0 Oxidation

$$ {}^{SCR}X_{Hg^0} = 100\frac{{}^{IN}C_{Hg^0} - {}^{OUT}C_{Hg^0}}{{}^{IN}C_{Hg^0}} $$

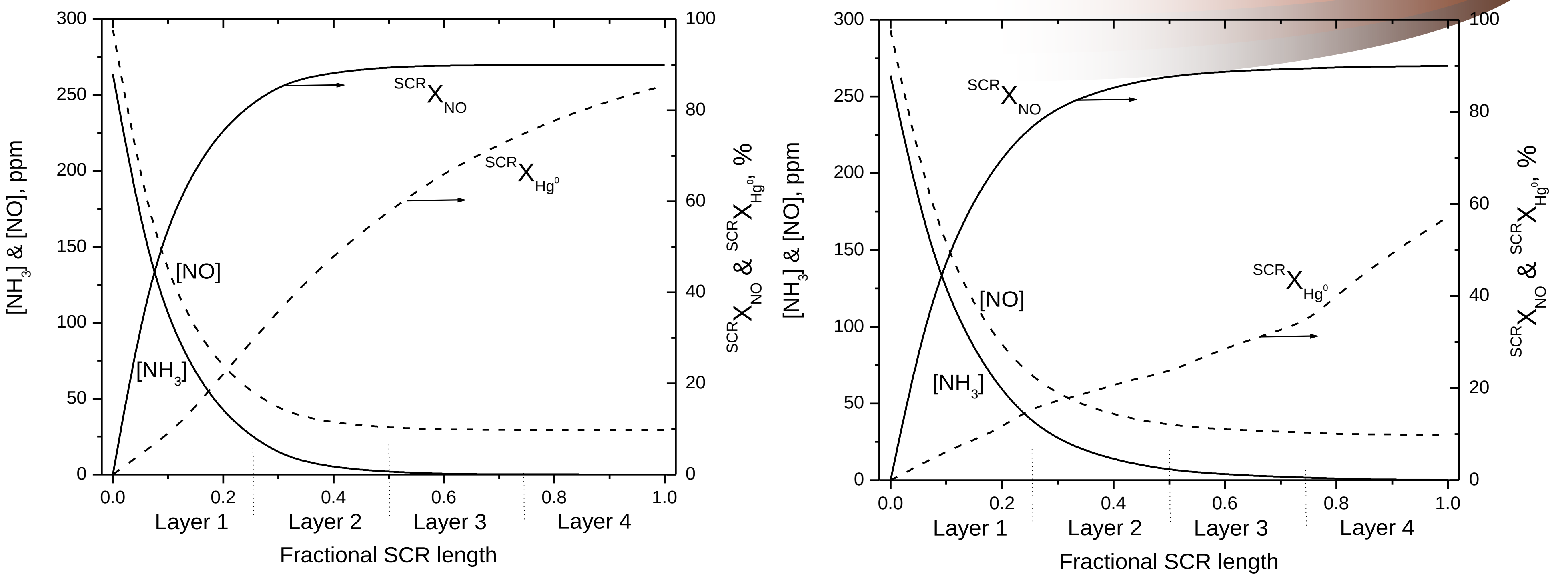
- *Unaffected by variations in Hg^{2+} at the SCR inlet.*

NH_3 Inhibition of Hg^0 Oxidation Is Always Significant



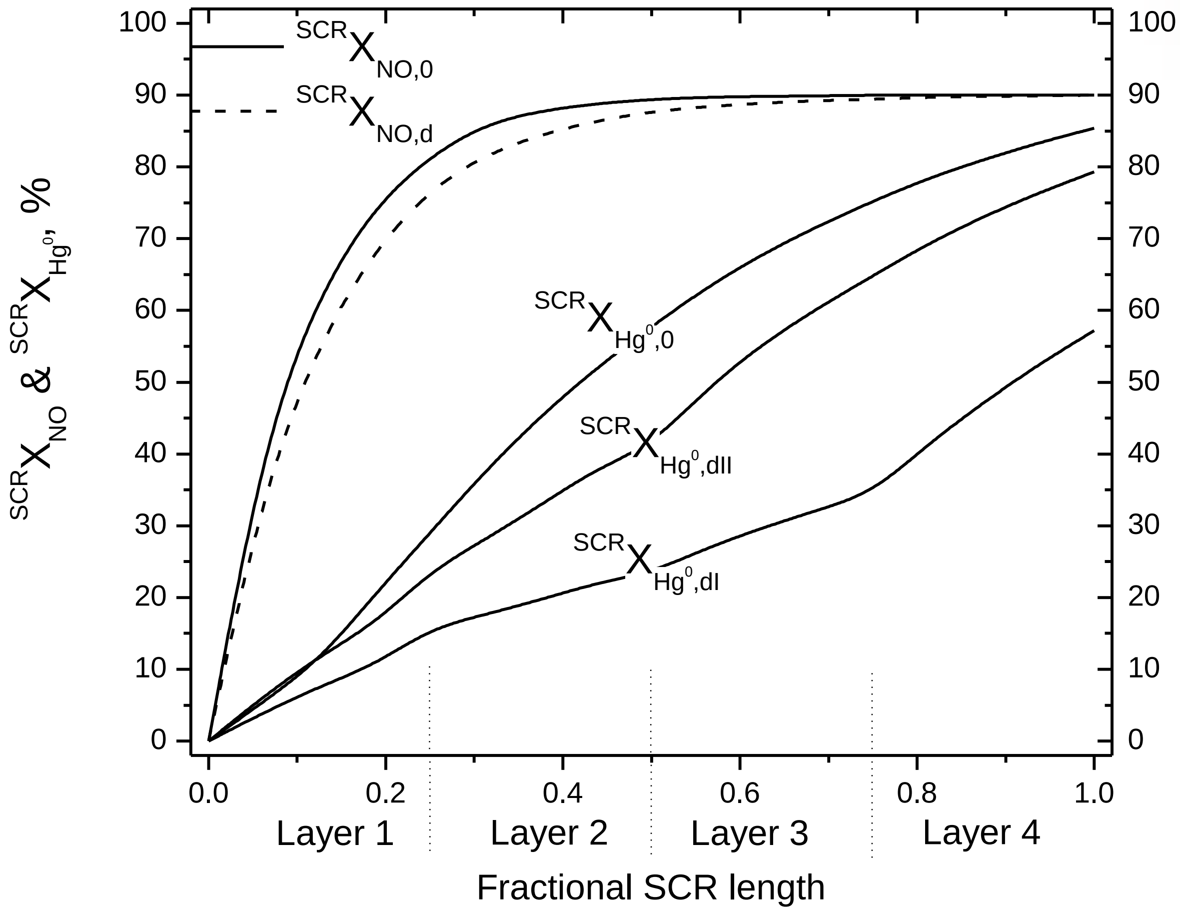
- *Early layers have highest NH_3 concentrations.*
- *Most Hg^0 oxidizes on the trailing layers.*

Catalyst Deactivation Enables Deeper NH_3 Penetration Into the Trailing Layers

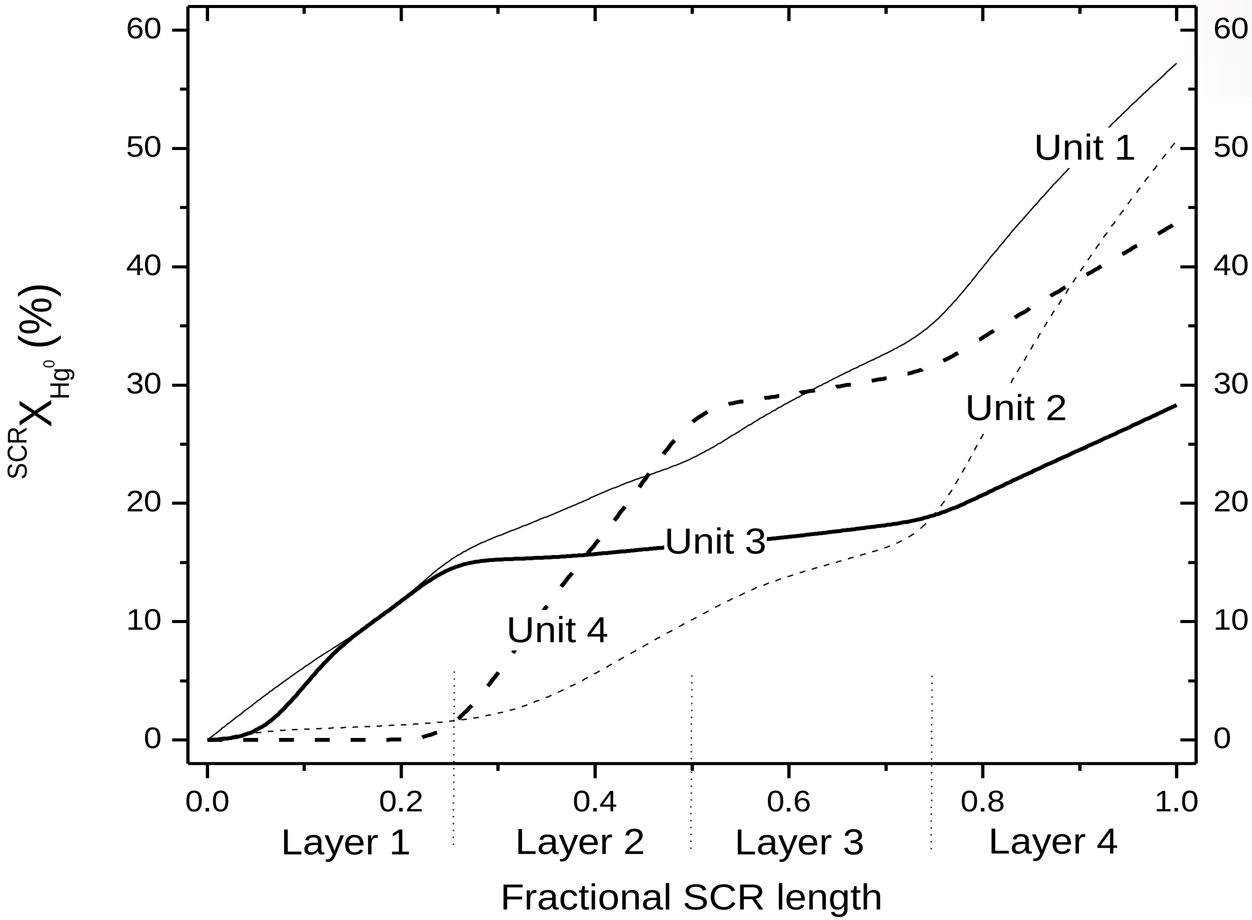


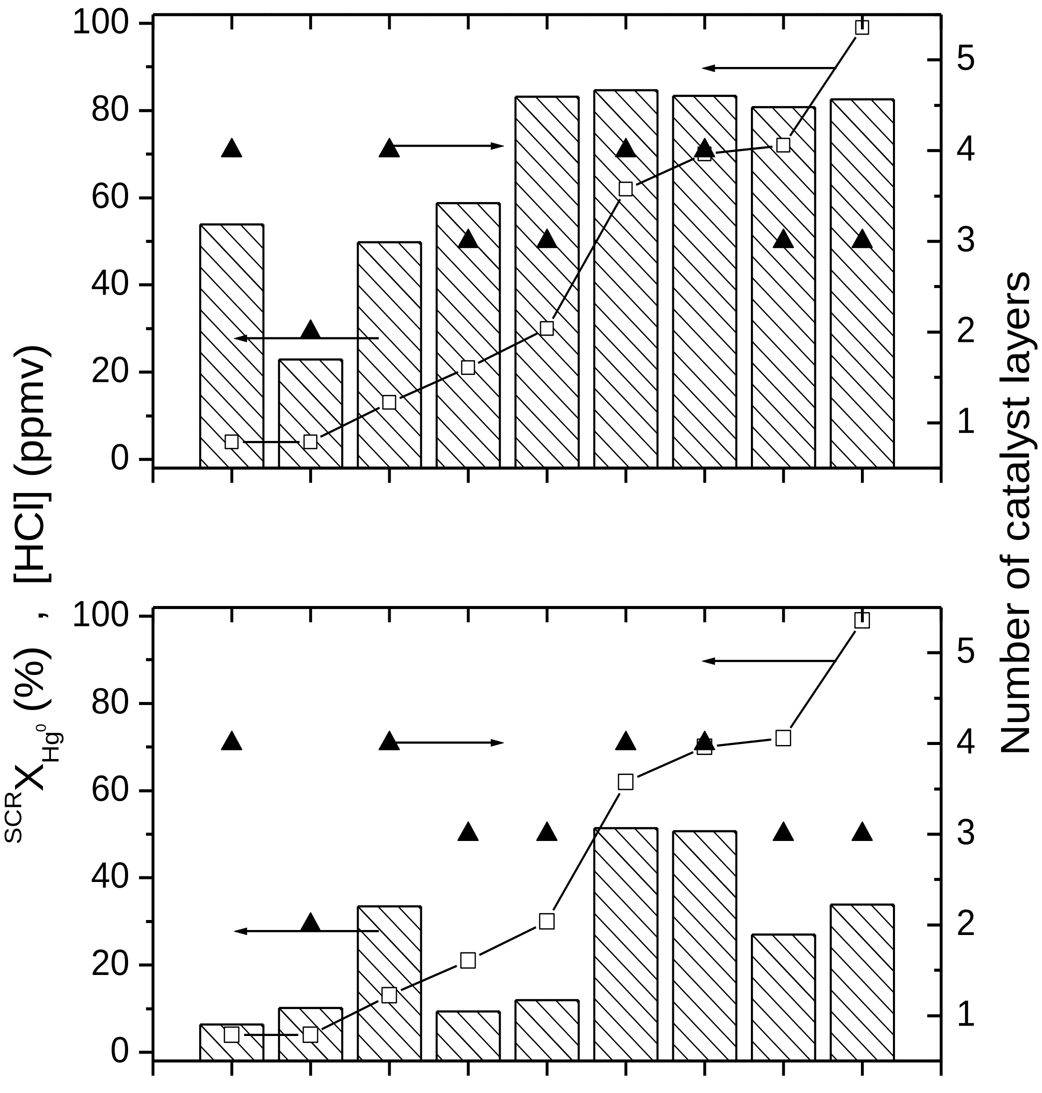
- *All deactivated catalysts met the NH_3 slip regulation in our simulations.*

Substantially Less 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.*

Acknowledgement

This study was sponsored by Southern Company Services, Inc. and reflects their generous cooperation in providing detailed gas cleaning conditions for their SCR fleet.

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.*