SCR Deactivation Mechanisms Related to Alkali and Alkaline Earth Elements

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2002 Conference on Selective Catalytic Reduction (SCR) and Selective Non-Catalytic Reduction (SNCR) for NO_x Control
May 15-16, 2002
Pittsburgh, PA

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REI SCR Catalyst Deactivation Program

- DOE-funded program, with EPRI participation to
  - Develop industrially useful slipstream reactor
  - Quantify deactivation by blinding + poisoning
  - Focus on Na and K (poisoning) and Ca (blinding)
  - Develop engineering model for catalyst deactivation useful for industry for fuel switching or blending, fuel selection

- Principal Tasks:
  - o Fundamental analysis of SCR catalyst poisoning and regeneration (BYU)
  - o Multi-catalyst slipstream reactor to be tested at PRB (or PRB-blend) utility boiler for six months (REI, UU)
  - o SCR deactivation model suitable for CFD code (REI)

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Mechanisms for SCR Catalyst Deactivation

- Fouling (surface deposition)
  - Deposition of ash
  - Sulfation of deposit observed with PRB
- Pore condensation (and/or pore blockage)
- Poisoning
  - Vapor-phase As (as As_2O_6) thought to react with active sites in some cases

Literature suggests fouling plays a role in deactivation from both PRB and biomass

Pore condensation could be a factor

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Subtask 1 – Catalyst Deactivation Studies

- Laboratory Investigation at BYU using small catalyst samples
- Effects of Alkali Impurities on Reactivity
- Characterization of catalyst (physical and chemical) before and after lab/field testing
  - Adsorption studies in flow reactor
  - Surface analysis (e.g. XPS), TEM/SEM, XRD, FTIR, TPD
  - No chemical analysis of any commercial catalysts.
- *Current Status:* Literature search completed and laboratory reactor under construction

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Two Primary Analysis Systems

- Catalyst characterization system (CCS)
  - Obtains quantitative activities/deactivation over long exposure times
  - Focuses on kinetic coefficient and mechanistic information
- *In situ* spectroscopy reactor (ISR)
  - Quantifies species adsorbed on surfaces during reaction
  - Provides quantitative indication of acidity and active site mechanisms

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Catalyst Characterization System

- Simulates industrial flows with compositions of: NO, 0.10%; NH_3, 0.1%; SO_2, 0.1%; O_2, 2%; H_2O, 10%; and He, 87.7%
- Custom and commercial catalysts tested as fresh samples and after exposure under both steady and transient conditions:
  – Measure specific intrinsic activity of custom and commercial catalysts impregnated to different contaminant (CaO, Na_2O, and K_2O) levels, plus selected experiments with arsenic.
  – Post-treatment, analyze via XRD, TEM, SEM, and AAS plus pore size distributions and similar analyses.

In Situ Spectroscopy Reactor

- *In situ* transmission FTIR analyses of SO_2, NH_3, and NO_x adsorption and desorption behaviors:
  - Obtain quantitative Brønsted and Lewis acidities on fresh and exposed surfaces based on spectral signatures
- FTIR investigation of coadsorption of NH_3 and NO_x behavior on fresh and exposed catalysts:
  - Determine surface kinetics and active sites
- Temperature programmed desorption (TPD) investigation of NH_3 and NO_x adsorption on both fresh and contaminated catalysts:
  - Quantitative information of acid sites

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Subtask 2 – Field Testing in Slipstream

- Six catalysts evaluated in parallel
  - Four vendors to supply catalyst; one "generic" catalyst from BYU
- Monitor catalyst activity by
  - NO_x measurement
  - Periodic removal of catalyst samples for lab testing at BYU
- Two tests (each ~6 months) planned

Current Status: Discussing field test sites with utilities; obtaining catalyst samples from vendors; Univ. of Utah designing slipstream reactor

Features of Reactor Design

- Multiple catalysts in parallel (plate and honeycomb)
- Catalyst exposed to gas and particulate matter
- Velocity of full-scale SCR
- 1 ½ - 3 foot catalyst samples to avoid favoring end effects
- On-line, continuous NO_x measurement for detailed kinetic information

Multicatalyst SCR Reactor

Flue gas inlet

Catalyst chambers (outer doors have been removed)

Flow control (individual chambers) and sample ports

Flue gas outlet

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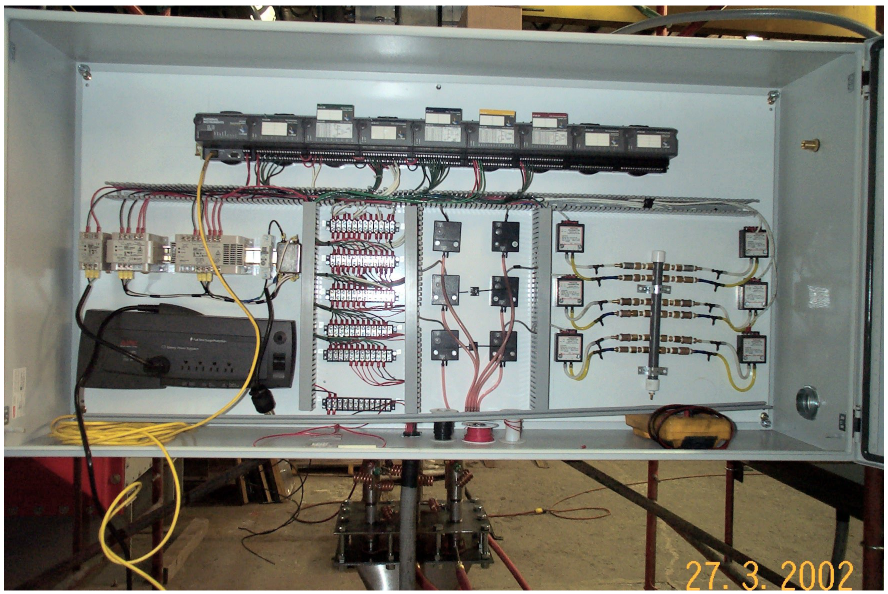
SCR Control Box



- Embedded microcontroller
- Ethernet link to local PC for data logging and communication
- Controlled remotely by REI

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Subtask 3 – Catalyst Regeneration

- Investigate methods for regeneration on
  - Laboratory samples
  - Field-exposed samples

Current Status: Literature search completed

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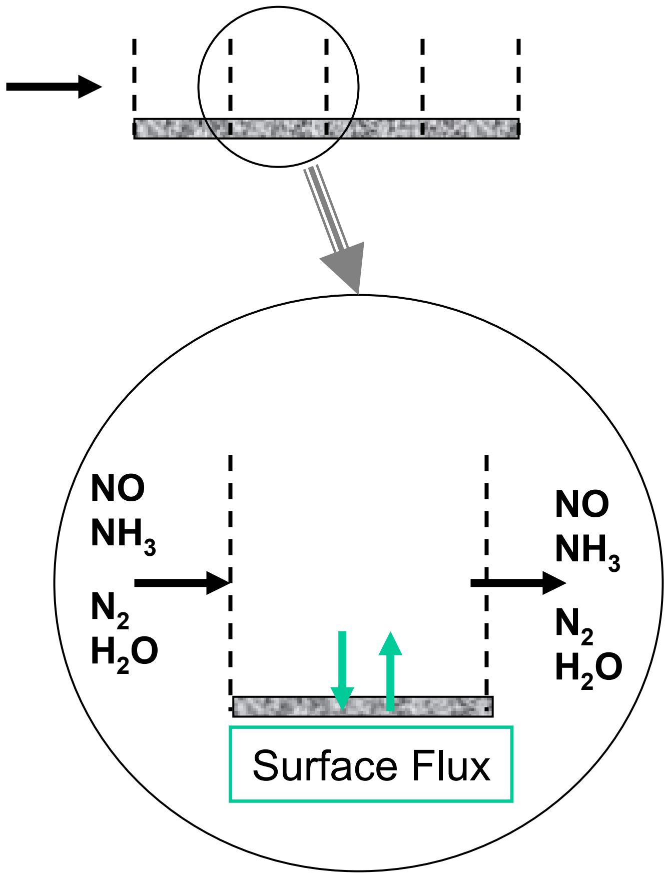
Subtask 4 – Deactivation Model Approach

- Solve gas transport and surface reactions along length of catalyst
- Surface equations are solved
  - Surface species concentrations of specific sites
  - Steady state assumption
  - Solution dependent on local gas species concentration
- Effectiveness factor to compensate for porous diffusion
- Gas species transport equations
  - Rates from surface equation solution



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