Development of a CLEERS Protocol for SCR Catalyst Characterization and Reporting

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Outline

- **The Problem**
- **Objectives of proposed activity**
- **Proposed general approach**
- **Technical issues**
- **Strawman protocol (for SCR and more generally as well)**
- **Feedback/discussion**

The Problem

- **Available kinetics data incomplete; more information needed for model development/ validation/design of engine cell & vehicle tests**
- **Without good models:**
  - **Lab data not predictive for systems (not scalable)**
  - **Hard to consistently compare performance of different catalyst materials**
  - **Large resources spent for performance data on test cells, vehicles**
  - **Separation of system parameter effects from catalyst effects difficult for test cell, vehicle data**
- **Hard to communicate model-related information among suppliers, OEM's, researchers**

Objectives

- **Improve accuracy/value of kinetic information for model development**
- **Streamline lab characterizations to reduce time/cost**
- **Reduce time/cost of test cell, vehicle studies**
- **Improve communication among suppliers, OEM's, research community**

Proposed Approach (General)

- **Develop consensus among stakeholders on minimum requirements for lab-scale testing**
- **Construct protocol for component data in CLEERS database**
- **Determine what available data (if any) meet criteria and add to database**
- **Provide template for future lab testing**
- **Keep CLEERS database updated with important benchmarks for different types of materials (not necessarily exhaustive)**
- **Consider basic set of global rate, capacity parameters derived from standard data for reporting (passing over the fence)**

Technical issues

- **Definition of lab reactor design and operating conditions**
- **Adequate monitoring/control of temperature, species concentrations, flows**
- **Acquisition of both steady-state and transient rate measurements**
- **Separation of mass-transfer, heat-transfer from chemistry**

See presentation by Yezerets, Currier, Mao, and DeWitt from 2nd CLEERS workshop for examples (Oct. 16, 2001)

Strawman Protocol

Collect data from two basic types of lab reactors:

- **Differential reactors**
  - **Small size/well-mixed**
  - **Catalyst often not on monolith (e.g., powder)**
  - **Constant concentrations, temperature**
  - **Reaction rates determined directly from in/out gas speciation**
- **Integral reactors**
  - **Larger size/simple flow (e.g., plug flow)**
  - **Catalyst typically on monolith cores**
  - **Axially varying concentrations, temps may/may not vary**
  - **Reaction rates inferred from in/out speciation and integral models**

Strawman Protocol

Reactor requirements:

- **Simple design, relatively easy to operate (cheaper than engine test cell runs)**
- **If possible, rates should include washcoat/ support effects**
- **Thermal response, mass-transfer, surface capacity similar to application**
- **Characterization/estimation of gas-phase diffusion effects (ΔC between bulk and surface)**
- **Design/operation/measurement that provides surface temperatures to within 10 deg C**
- **Both steady-state and transient operation**

Strawman Protocol

Measurement requirements:

- **Steady state**
  - **Slow response ok (e.g., 1 min)**
  - **In/out gas NO/NO2, N2O, reductant, O2/H2O/CO2, temperature**
- **Transient**
  - **Fast response needed (e.g., 1 s or less)**
  - **In/out gas NO/NO2, N2O, reductant, O2/H2O/CO2, temperature**
  - **N2 balance using inert gas carrier**

Note: Some techniques for surface measurement now possible (e.g., drift)

Strawman Protocol

Experimental condition requirements:

- Atmospheric pressure
- Typical exhaust temperatures (e.g., 150-600 deg C)
- Both pure NO and NO2 inlet as well as mixes typical of exhaust between 100 and 1000 ppm
- Include H2O, CO2 typical of exhaust
- SV between 10,000 and 100,000 1/hr
- Reductant levels between 0 and 110% stoichiometric
- Add reductant as gas (NH3) to avoid vaporization/ thermolysis complications
- Use pure compounds for reductants as opposed to realistic but complex species (e.g., diesel fuel)
- Change one parameter at a time
- Simple transients (e.g., step inputs) with well-defined IC

Strawman Protocol

Background and reporting requirements:

- **Unambiguous identification of material (enough for documentation, future replication by source)**
- **Documentation of material configuration (e.g., monolith core parameters) and preparation (e.g., degreening procedure)**
- **Documentation of initial conditions for transient measurements**
- **Sufficient instrumentation and equipment details for replication**
- **Quantitative summary of measurements in simple text or Excel format**
- **Definition of models or procedures used to derive kinetics from raw measurements (if applicable)**

Levels of kinetics

- **Elementary steps (micro-kinetics)**
- **Global kinetics**
- **Laboratory data at well-defined conditions**

Note: The last includes the previous two

Questions for Discussion

- **Are previous strawman requirements realistic?**
- **Are there important components missing?**
- **Can we identify candidate materials that would not be too proprietary and still useful for benchmarking?**
- **Do such data already exist? Are you willing to make a donation?**
- **Can we agree on a standard set of data/ kinetic parameters that could be 'passed over the fence'?**
- **Do we need to have additional specific requirements for characterization of different catalyst materials (e.g., HC SCR, urea SCR, LNT, etc.)? If so, how should we go about setting these requirements?**