



Application of Various Flow-Reactor Capabilities to the Aftreatment Research

*2nd CLEERS Workshop
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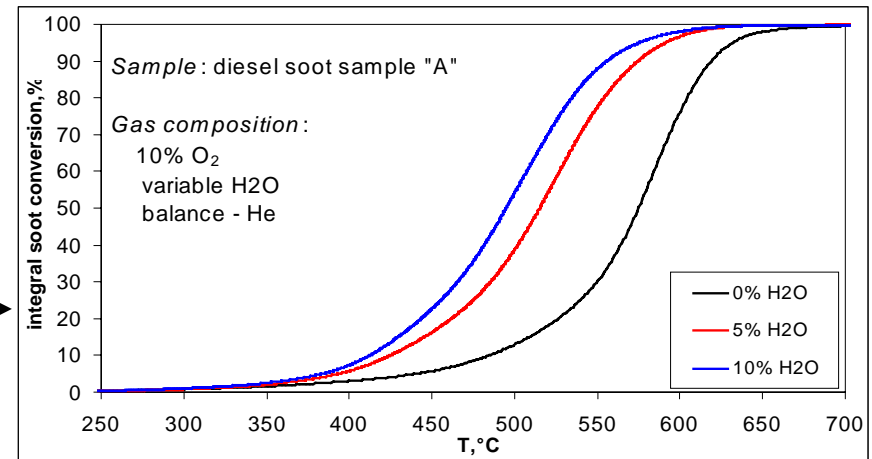
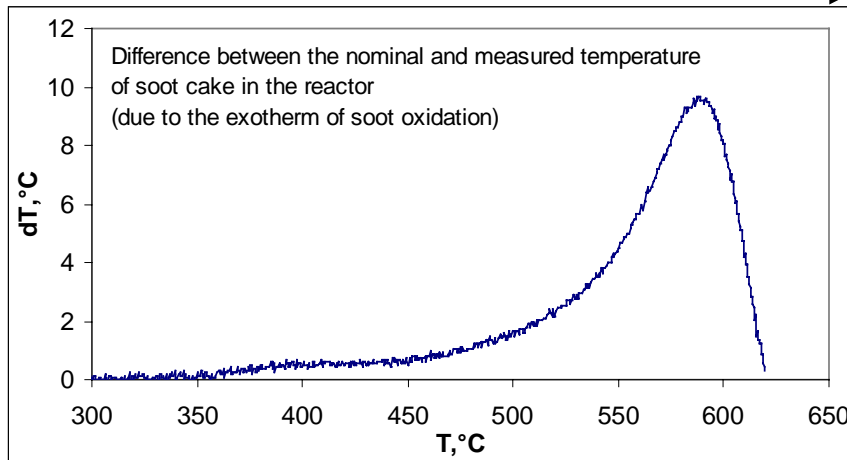
Alex Yezerets, Neal Currier, Frank F. Mao, Matthew J. DeWitt

Support to the Modeling:

- identify major elementary steps vs. conditions
- determine related quantitative parameters

Common features of the reaction systems:

- **Independent** control of the parameters
 - Example: Effect of H₂O on soot oxidation rate.



- **Accurate** control of the parameters
 - *gas composition and temperature measurements.*

Different Reaction Systems



Adapting to the application:

- **Analytical capabilities:**
 - Steady-state vs. fast transient

- **Material balance:**
 - N_2 balance capabilities

Chemistry vs. Engineering:

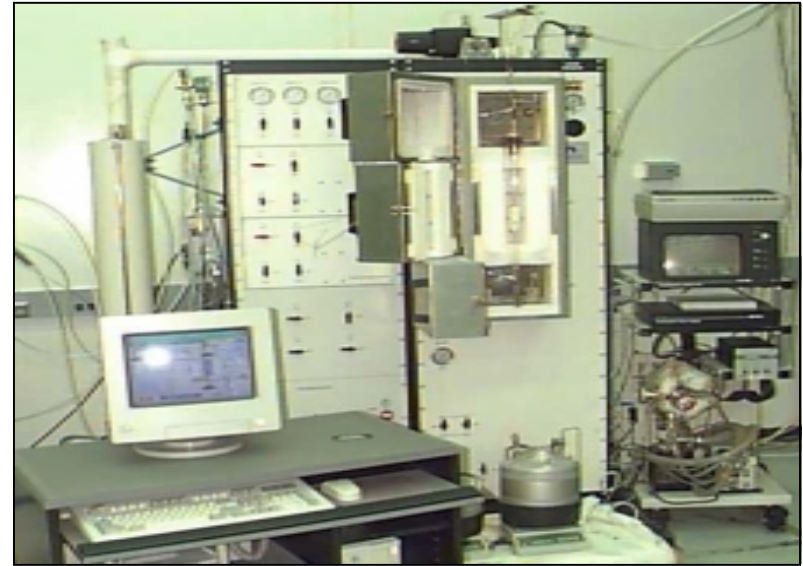
- **Scale (sample type):**
 - “Micro”- and “Pilot”- reaction systems

I. Analytical capabilities:

A. Steady-State:

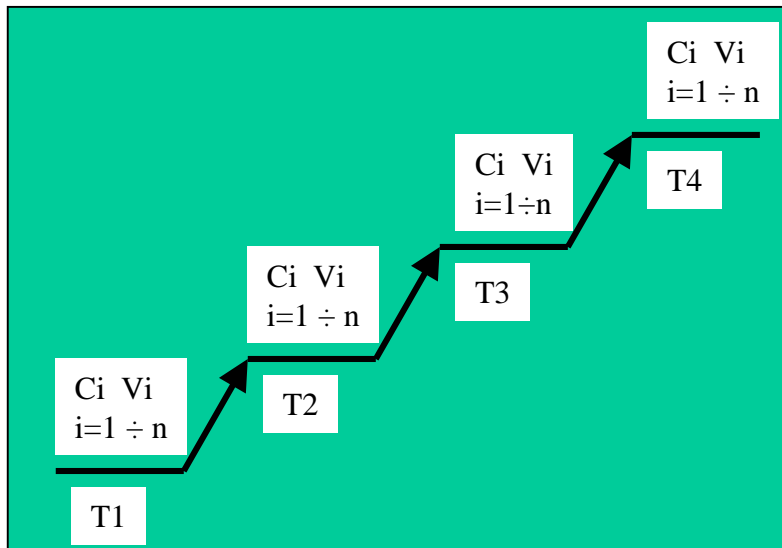
Examples of possible applications:

- Lean NO_x catalysis
- Urea-SCR
- SO_x traps



The *AMI-2000* reaction system at Cummins

Current application: steady state studies of **sulfur trap** catalytic kinetics, mass transfer, catalyst aging, and regeneration processes

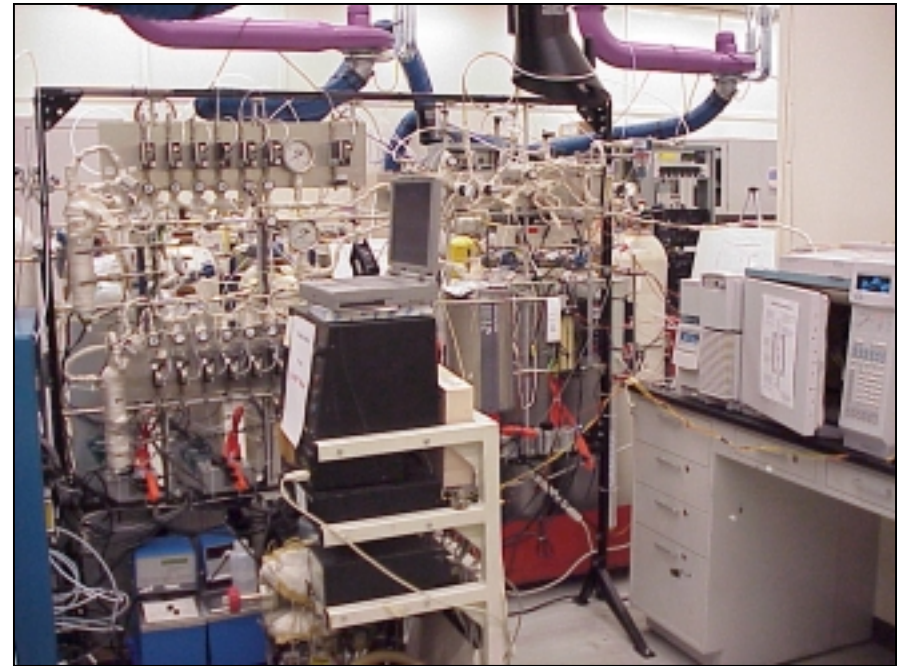


I. Analytical capabilities:

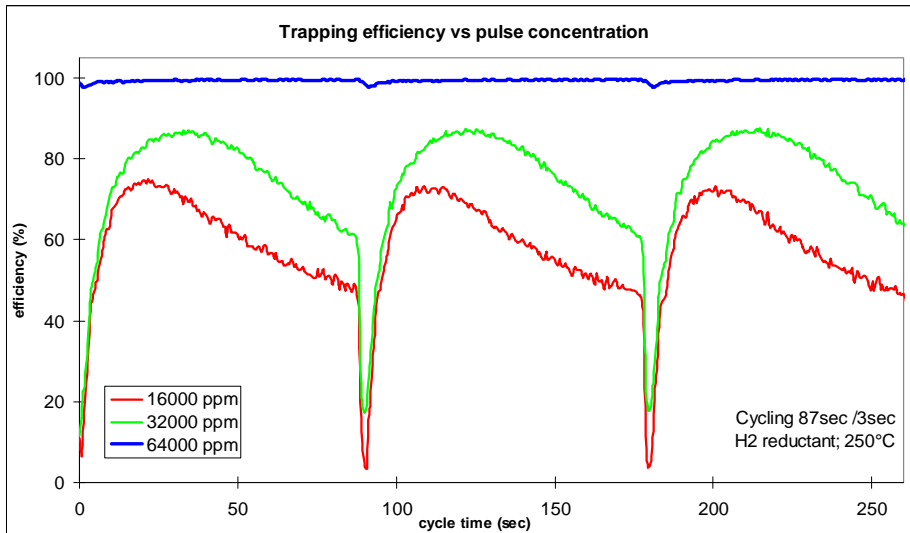
B. Fast-Response:

Example of possible application:

- NO_x adsorbers
- Also, provides advantages for other studies (e.g. soot combustion)



The fast-response Micro-reaction system recently created at Cummins



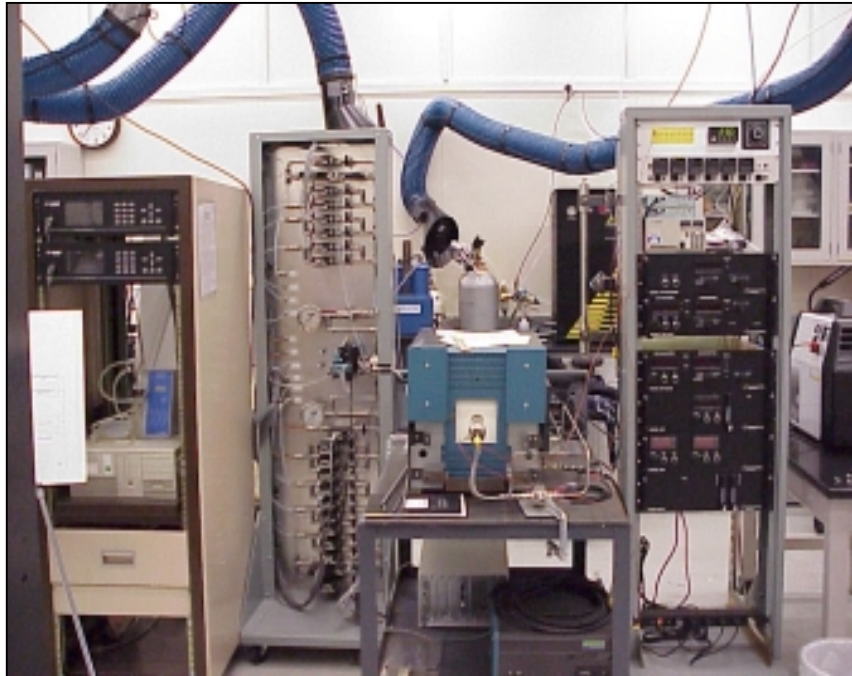
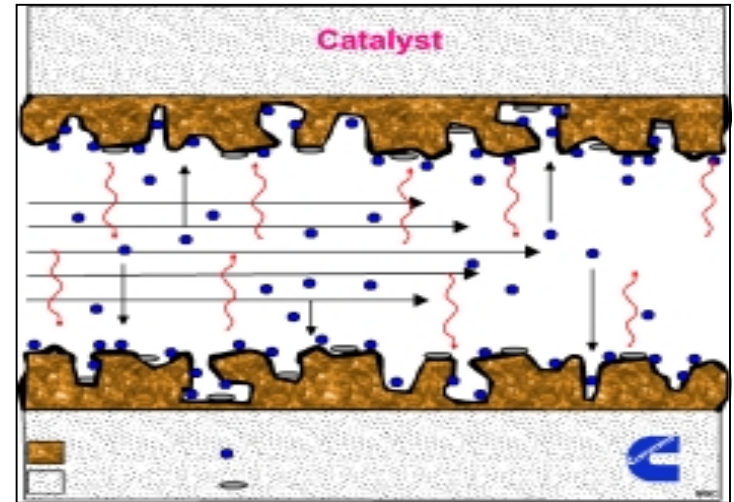
Example: NO_x adsorber regeneration data, obtained by **Shell/Equilon** using their reaction system

II. Scale

A. “Micro”-reaction systems:

Focus: chemical kinetics

Samples: powder (or a single channel of monolith)



B. “Pilot”-reaction systems:

Focus: chemical kinetics + heat and mass transfer effects

Samples: monolith cores

The fast-response Pilot-reaction system created at Cummins

III. Material balancing capabilities

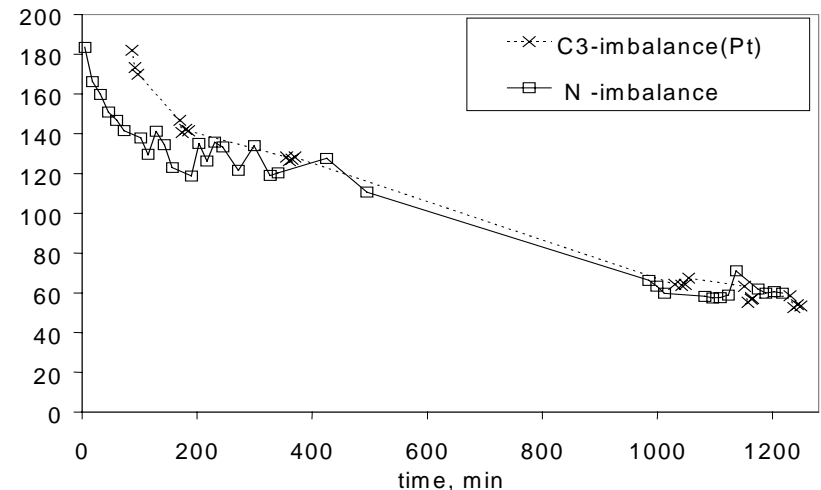
Nitrogen balance:

$$\frac{(\text{NO}_{x(\text{out})} + \text{N}_2(\text{produced}) + \text{N}_2\text{O}(\text{produced}) + \dots) + \text{NO}_{x(\text{“stored”})}}{\text{NO}_{x(\text{in})}}$$

- N₂ could not be used as a carrier gas (He, Ar, etc.)
- Heat- and mass-transfer may be affected by the nature the carrier gas focus on the “micro” systems (kinetics)
- Capabilities: Micro-reaction system at Cummins is equipped for N-balance studies.

Example^[1]:

Data on NO_x imbalance vs. time-on-stream for plasma-assisted NO_x catalysis revealed significant storage of NO_x (might have been wrongfully interpreted as NO_x abatement otherwise).



[1] G.B. Fisher, C.L. DiMaggio, A.Yezerets, M.C. Kung, H. H. Kung, S.Baskaran, J.Frye, M.R.Smith, D.R.Herling W.J. LaBarge and J.Y.Yan. " *Mechanistic Studies of the Catalytic Chemistry of NO_x in Laboratory Plasma-Catalyst Reactors*". SAE paper 2000-01-2965.

Conclusions



- Flow reaction systems represent essential tool for developing knowledge required for *predictive* models.
- Different reaction capabilities (sometimes physically incompatible in one system) may be required for different *applications* and *levels* of understanding.
- Advanced reaction systems developed by Cummins (and also available to us from our partners - EmeraChem, Shell/Equilon) can cover any major aftertreatment technology at various phenomenological levels.