University of Houston and City of Houston: Collaboration to Determine Best Solutions for Diesel Emission Reductions

University of Houston
Dept. of Chemical Engineering

UNIVERSITY OF HOUSTON
Cullen College of Engineering
Department of Chemical Engineering

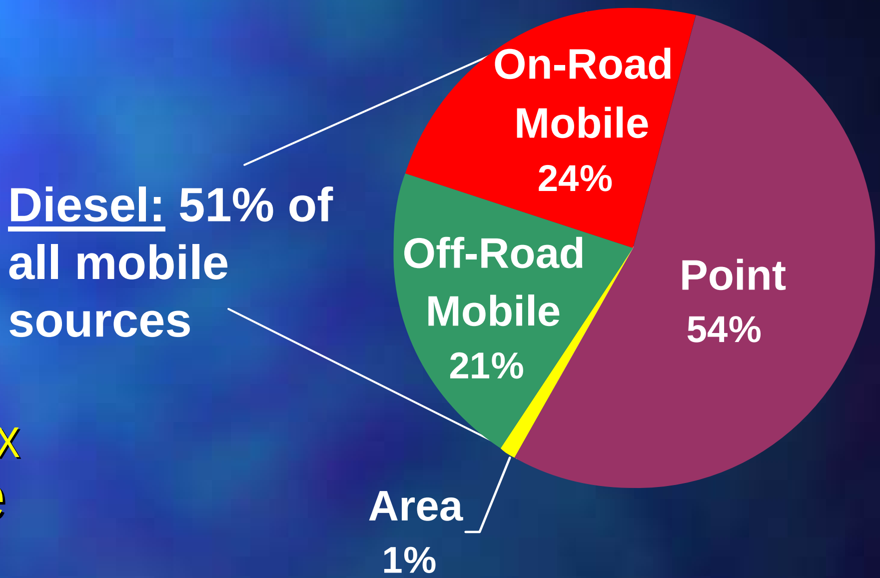
NOx Reduction Challenge

- Diesel Power
  - Large contributor to NOx
  - Increased Durability
  - Improved Fuel Efficiency
  - Lean Combustion
    - Exhaust NO_X –> N_2 difficult
- Challenge: Reduce diesel NO_X emissions* with cost-effective & reliable technology

**EPA Target: 90% reduction in NOx emissions by 2007*

Houston/Galveston Area

NOx Emission Sources**



Total NOx: 417,000 tons/year*

***1996 data; Source: TCEQ Website*

Diesel Emission Technology

Diesel Exhaust → Diesel Oxidation Catalyst → Diesel Particulate Filter → NOx Reduction → Clean Exhaust

	Diesel Oxidation Catalyst	Diesel Particulate Filter	NOx Reduction
Abatement:	VOCs & CO	Soot & Solids	NO & NO_2
Status:	Implemented	In Progress	Under Development

Technology Targets For Development & Testing

- Incremental
  - Fuels: Biodiesel, Fuel additives
  - Exhaust gas recirculation
- Step Change
  - Selective catalytic reduction
  - Lean NOx traps
  - Continuously regenerating soot filters
  - Coupled NOx & soot systems
  - Hybrid systems

UH Testing & Research Capabilities

- Testing
  - 500 HP AC Chassis Dynamometer (Burke Porter)
  - MEXA 7100 Exhaust Gas Analytical System (HORIBA)
  - FTIR spectrometer (MKS)
  - MDLT 1300T Micro Dilution Tunnel (HORIBA)
  - Annubar 485 Exhaust flow meter (Rosemount)
- Research
  - Bench-scale monolith reactor system
    - FTIR (Nicolet)
  - TAP® reactor system
    - UHV to atmospheric pressure
    - High speed reactant pulsing
    - Quadrupole mass spectrometer (UTI)
  - Computational facilities for modeling

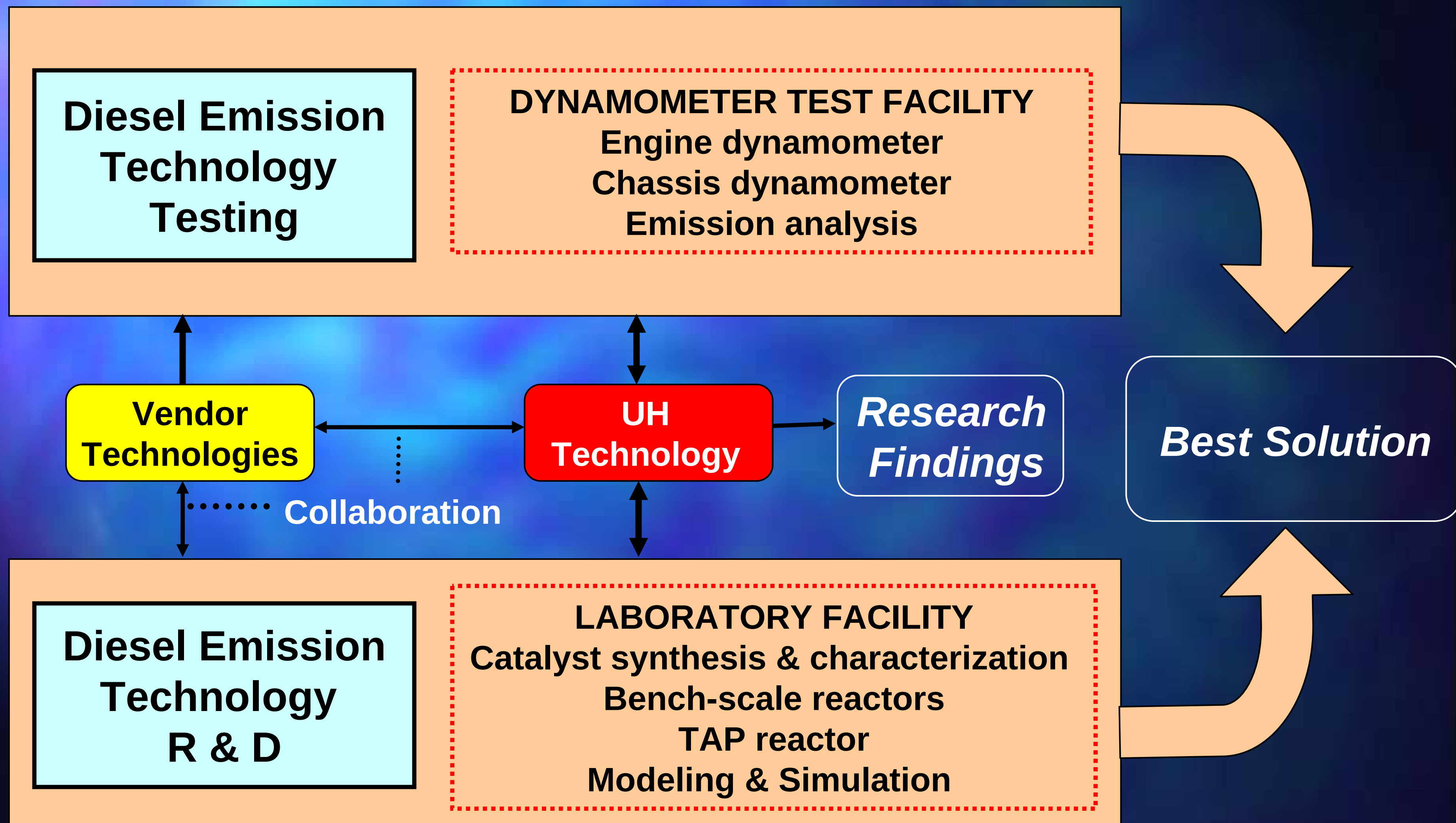
Expanded UH Role: Third-Party Testing and Collaborative Technology Development

- UH to provide unique role:

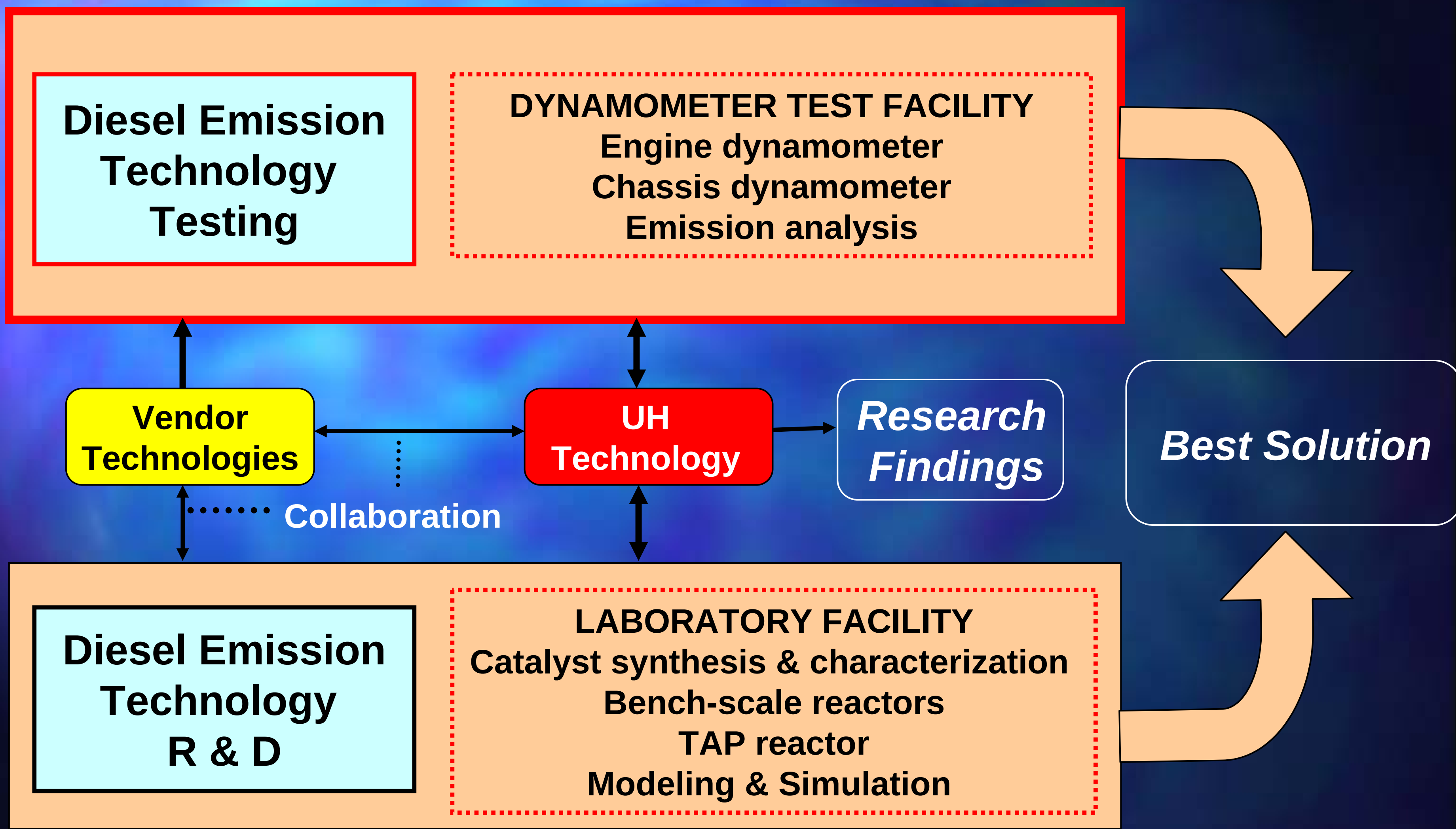
  Research, technology development & testing
  - Fundamental ←→ bench-scale ←→ on-vehicle testing
  - Provide key technology screening role
  - Partner with third parties for technology prototype evaluations, optimization, & retrofit applications
- Win – Win – Win – Win – Win

Win	Win	Win	Win	Win
Federal	State	City	UH	Technology Providers

UH Program: Spans R&D to Testing



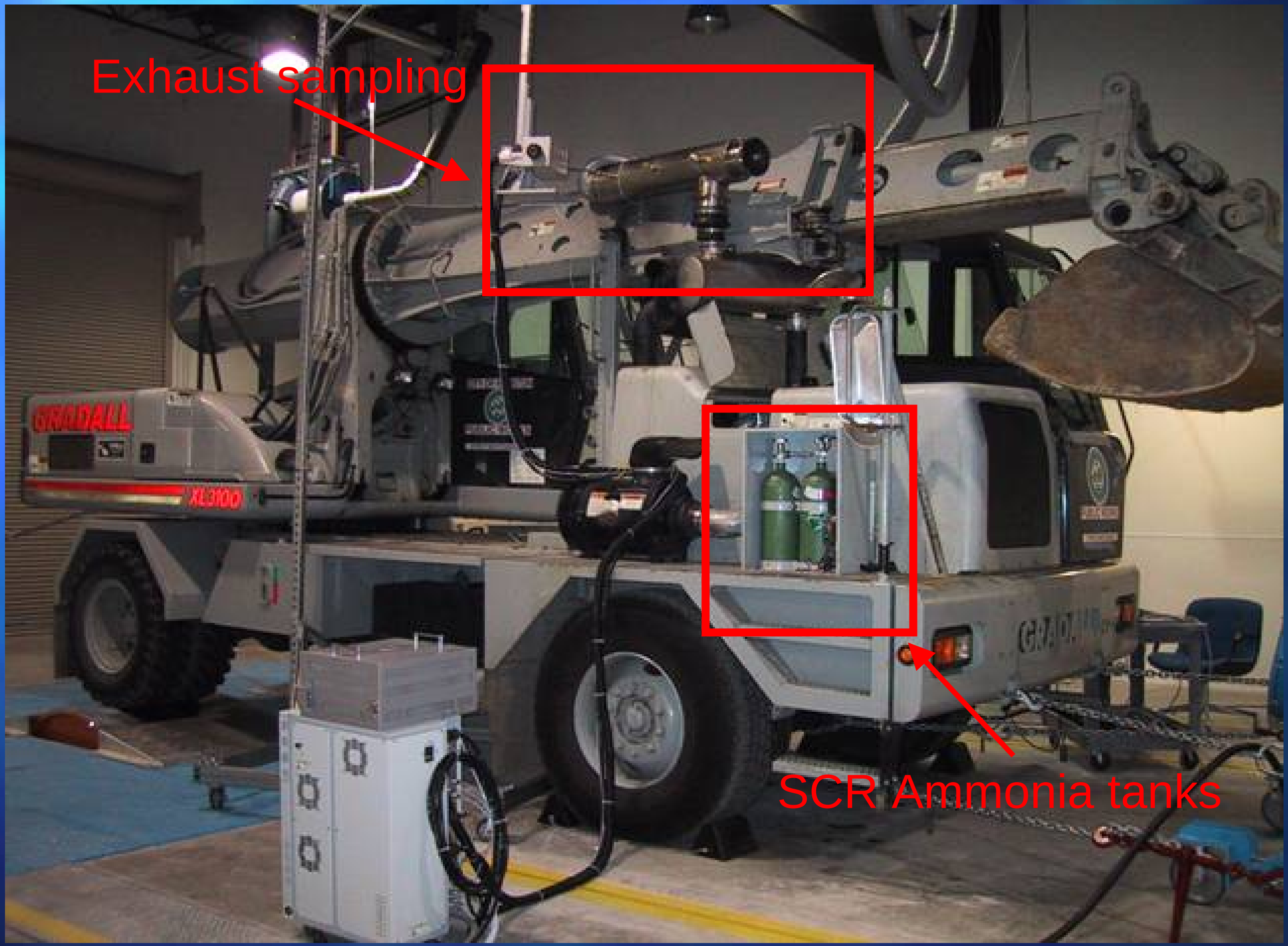
UH Program: Spans R&D to Testing



Testing Facility

- Key measurements
  - Exhaust: NOx, THC, CO, CO_2, O_2, PM, gas flow rate, exhaust temperature
  - Vehicle/engine: Speed, RPM, fuel consumption, boost pressure
  - Ambient pressure, temperature, humidity

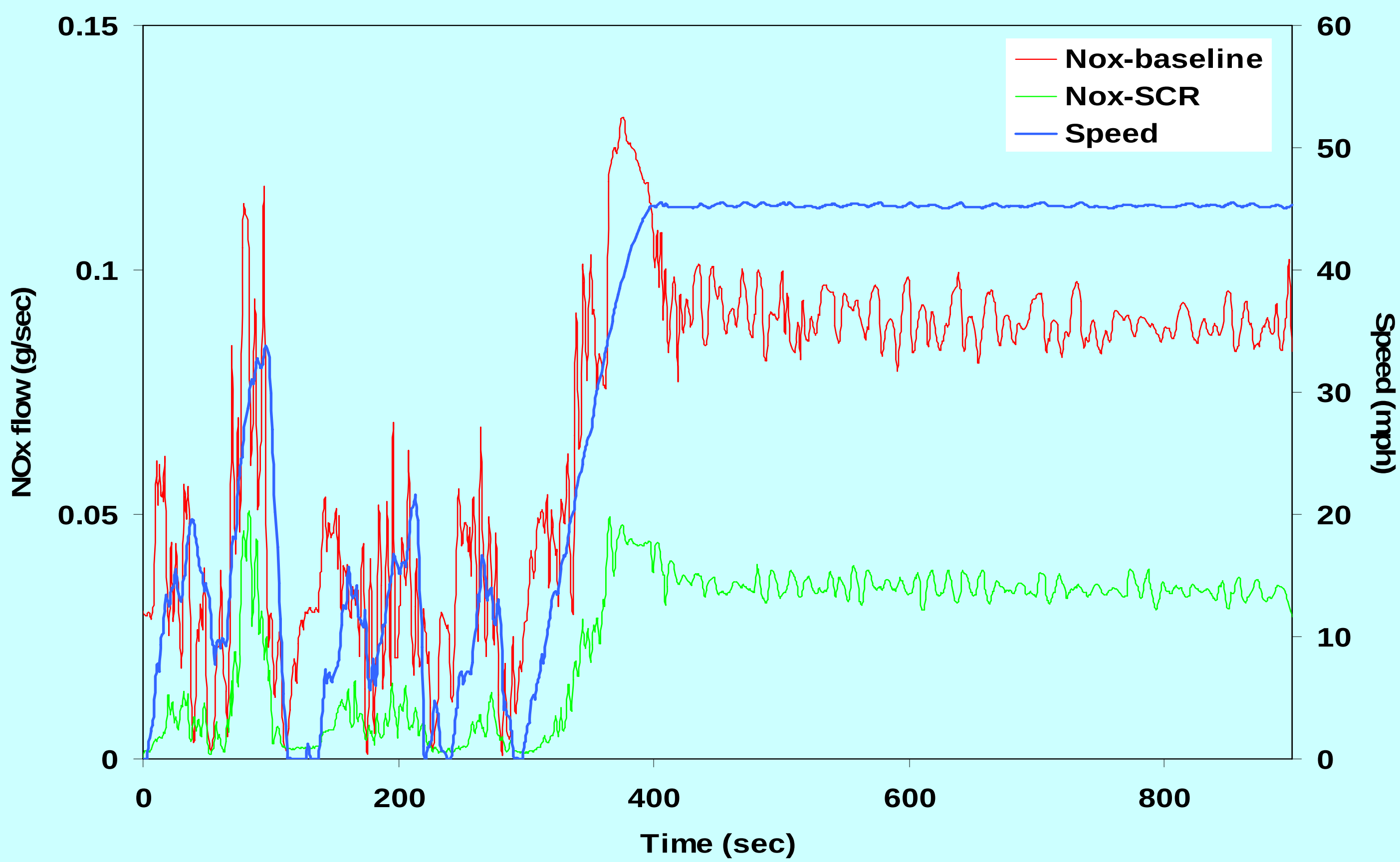
Gradall (Telescoping Boom Excavator)



SCR (Anhydrous NH_3): Typical Results

	% Reduction	g/mile(Baseline)	g/mile(SCR)
NOx	64.90	8.13	2.86

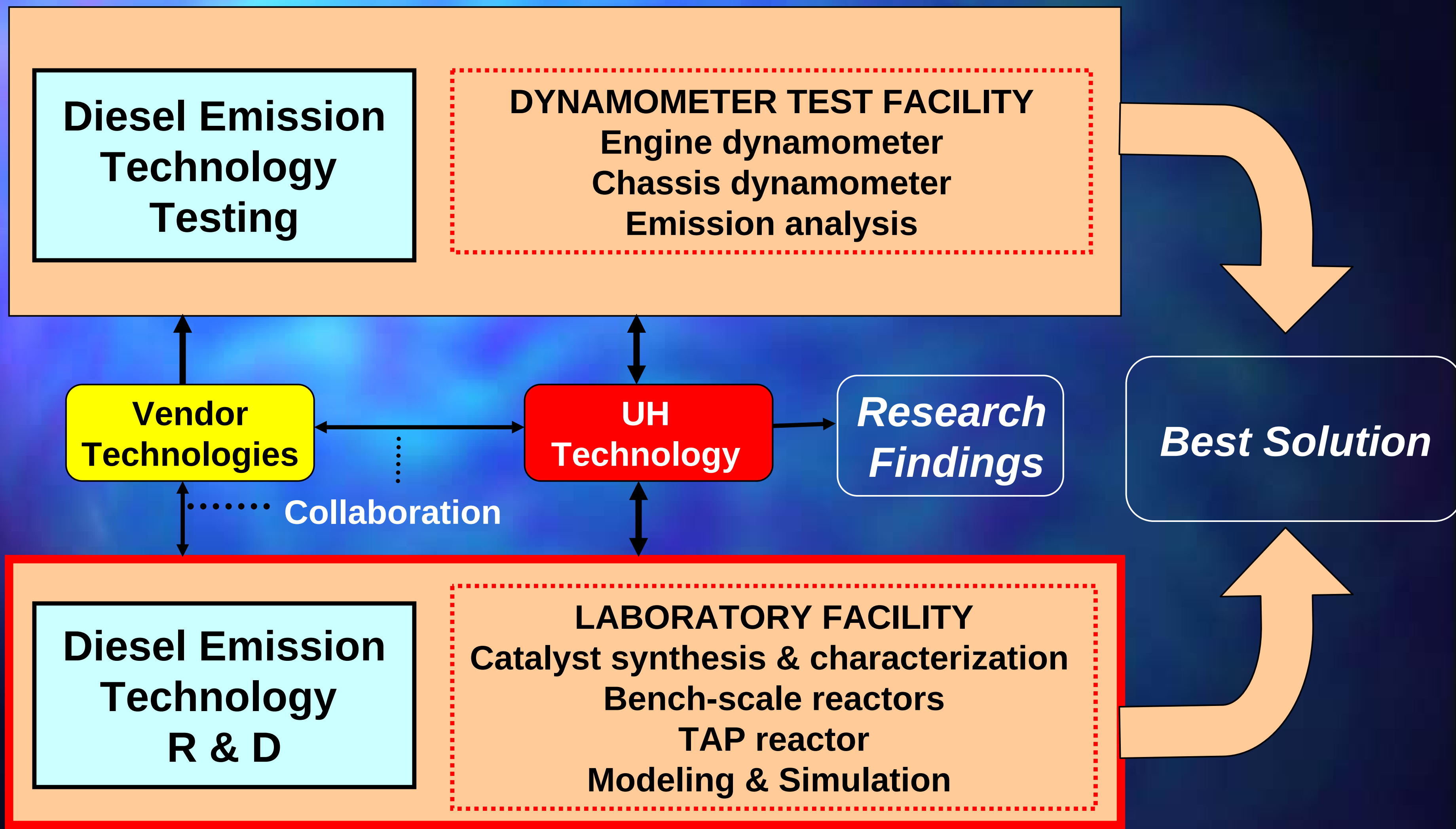
Equipment Type: 1992 Gradall, G3WD
Engine: Cummins 6BT 5.9
Baseline Test Date: 11/22/04
Retrofit Test Date: 11/23/04
Drive Cycle: "Off Road Excavator"



City of Houston Contract

- Expiration in August, 2007
- Fixed-cost contract
- 40 hours per week
- City can designate its time to third party

UH Program: Spans R&D to Testing



UH Program Overview

Objective:

- Understand, develop, and optimize integrated diesel emission system for coupled particulate, NOx and VOC abatement

Approach:

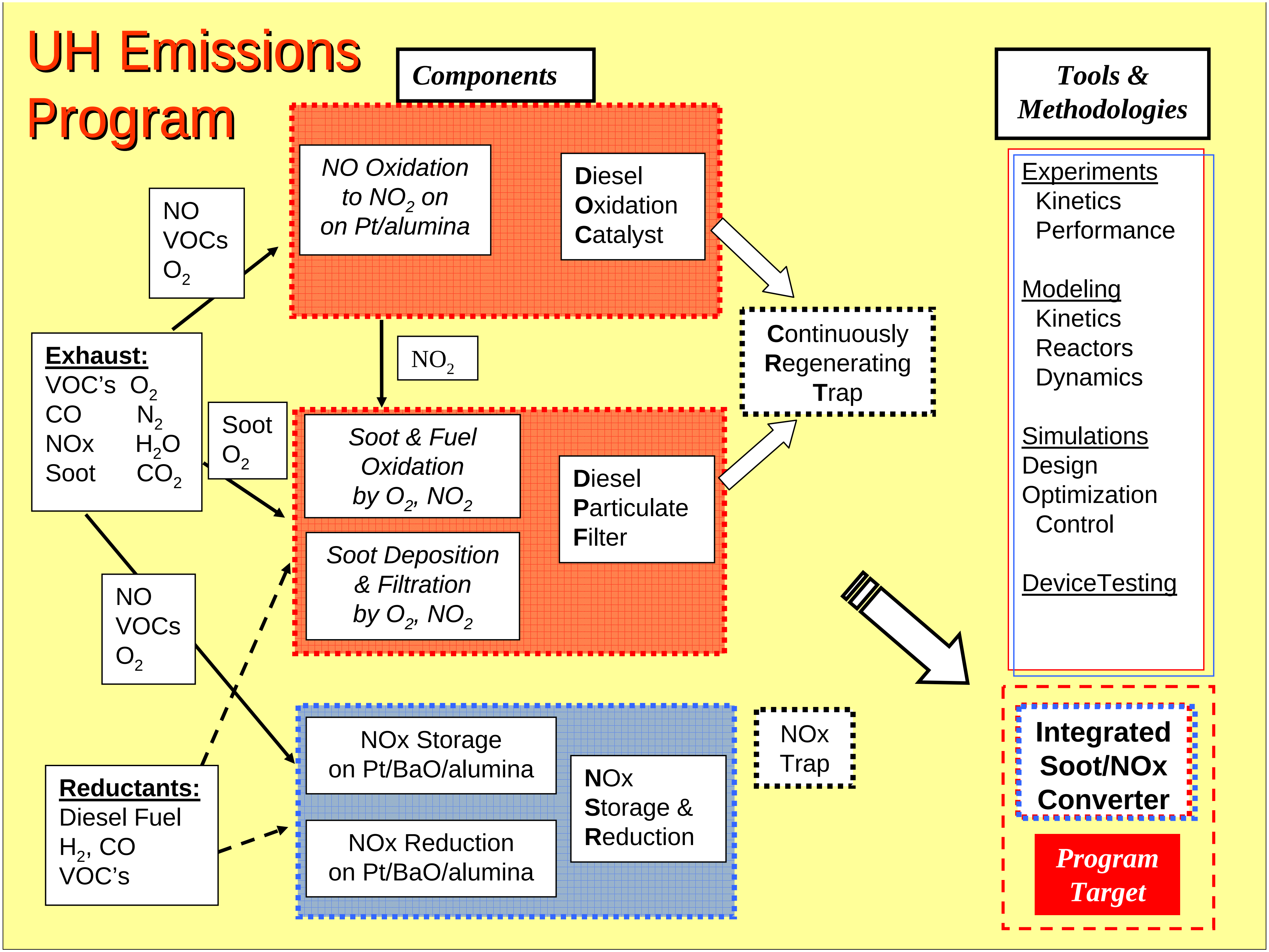
- Application of advanced catalysis and reaction engineering tools spanning fundamental experiments, bench-scale performance studies, first-principles modeling & simulation, and testing

Premise:

- Build R&D expertise and technology know-how in key area of NOx and particulate abatement
- Establish “systems approach” in interdisciplinary effort
- Link program to air quality issues in region

Selected UH R&D Projects

- Reactor studies – NOx trap technology
  - Bench-scale monolith reactor performance
  - Modeling & simulations
- Mechanistic studies – NOx trap technology
  - Temporal Analysis of Products (TAP)
  - Storage and regeneration – microreactor & TGA
  - Microkinetic model development
- Monolith reactor modeling
  - Simulations of light-off, hot spot propagation
  - Evaluation of monolith channel shape
- Integrated NOx reduction & soot oxidation
  - Bench-scale studies
- On-board NH_3 generation for SCR


UH Emissions Program
Components
Tools & Methodologies
NO Oxidation to NO_2 on on Pt/alumina
Diesel Oxidation Catalyst
NO VOCs O_2
Exhaust: VOC's O_2 CO N_2 NOx H_2O Soot CO_2
NO_2
Continuously Regenerating Trap
Soot O_2
Soot & Fuel Oxidation by O_2, NO_2
Soot Deposition & Filtration by O_2, NO_2
Diesel Particulate Filter
NO VOCs O_2
Reductants: Diesel Fuel H_2, CO VOC's
NOx Storage on Pt/BaO/alumina
NOx Reduction on Pt/BaO/alumina
NOx Storage & Reduction
NOx Trap
Experiments
Kinetics
Performance
Modeling
Kinetics
Reactors
Dynamics
Simulations
Design
Optimization
Control
DeviceTesting
Integrated Soot/NOx Converter
Program Target

Diesel Emission Technology

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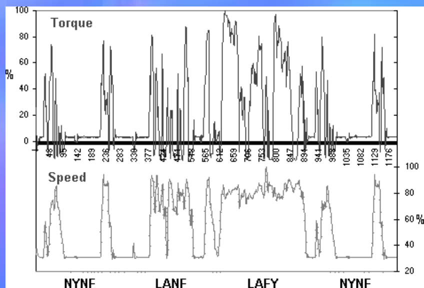
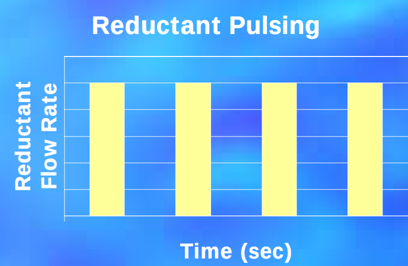
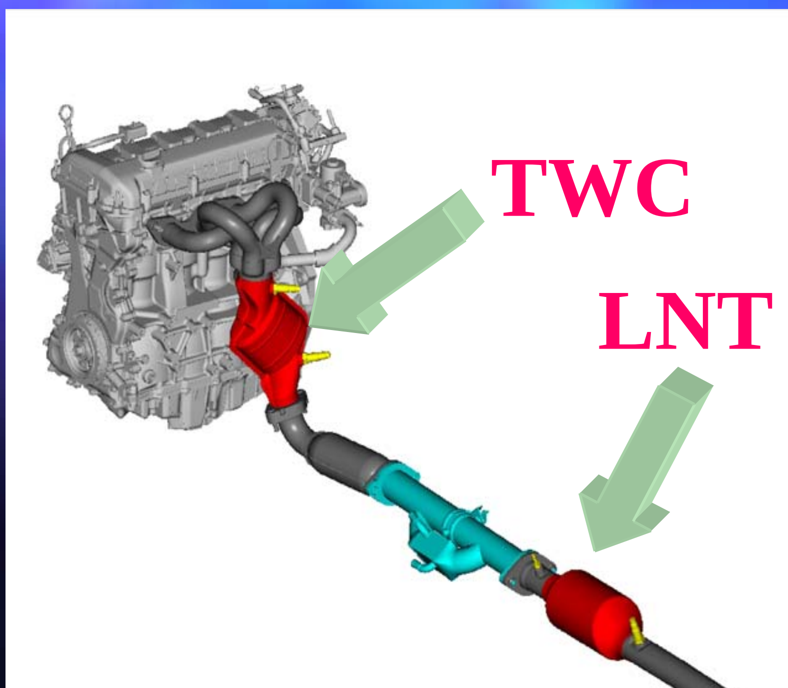
Lean NOx Trap: Adsorptive Catalytic Reactor



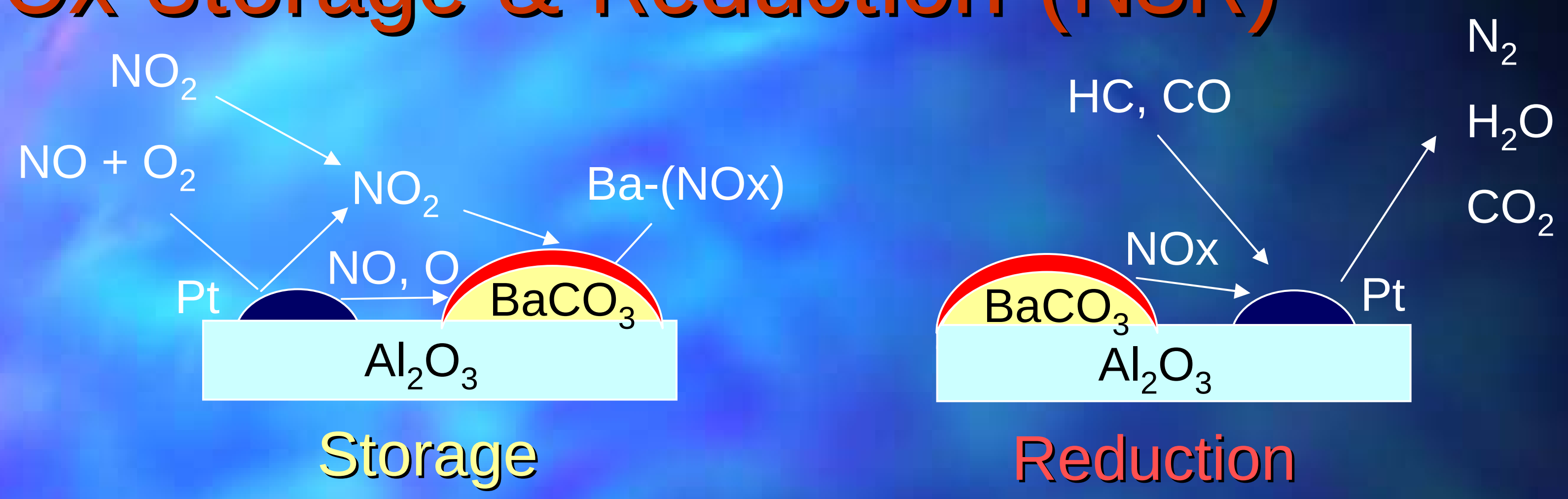


Engine Exhaust → LEAN NOx TRAP → Clean Exhaust



- Challenges
  - Maximize NOx conversion
  - Maximize reductant conversion
  - Minimize fuel penalty
  - Achieve robust control

NOx Storage & Reduction (NSR)



- NOx Storage
  - Trap NO/NO_2 as surface species, nitrite, nitrate
  - Need high trapping efficiency (> 95%)
  - Catalytic adsorbent: Pt/Rh/Alkali Earth Oxide/Support
- NOx Reduction
  - Reduce NOx on Pt/Rh during rich purge
  - Need high conversion of NOx to N_2 (> 90%)
  - Ensure high conversion of reductant via oxidation

LNT Research Methodology

Experiments ⟷ *Modeling*

Steady-state lean NOx reduction

Lean NOx storage

NOx storage & reduction

Transient kinetics studies (TAP)

Bench-scale reactor studies

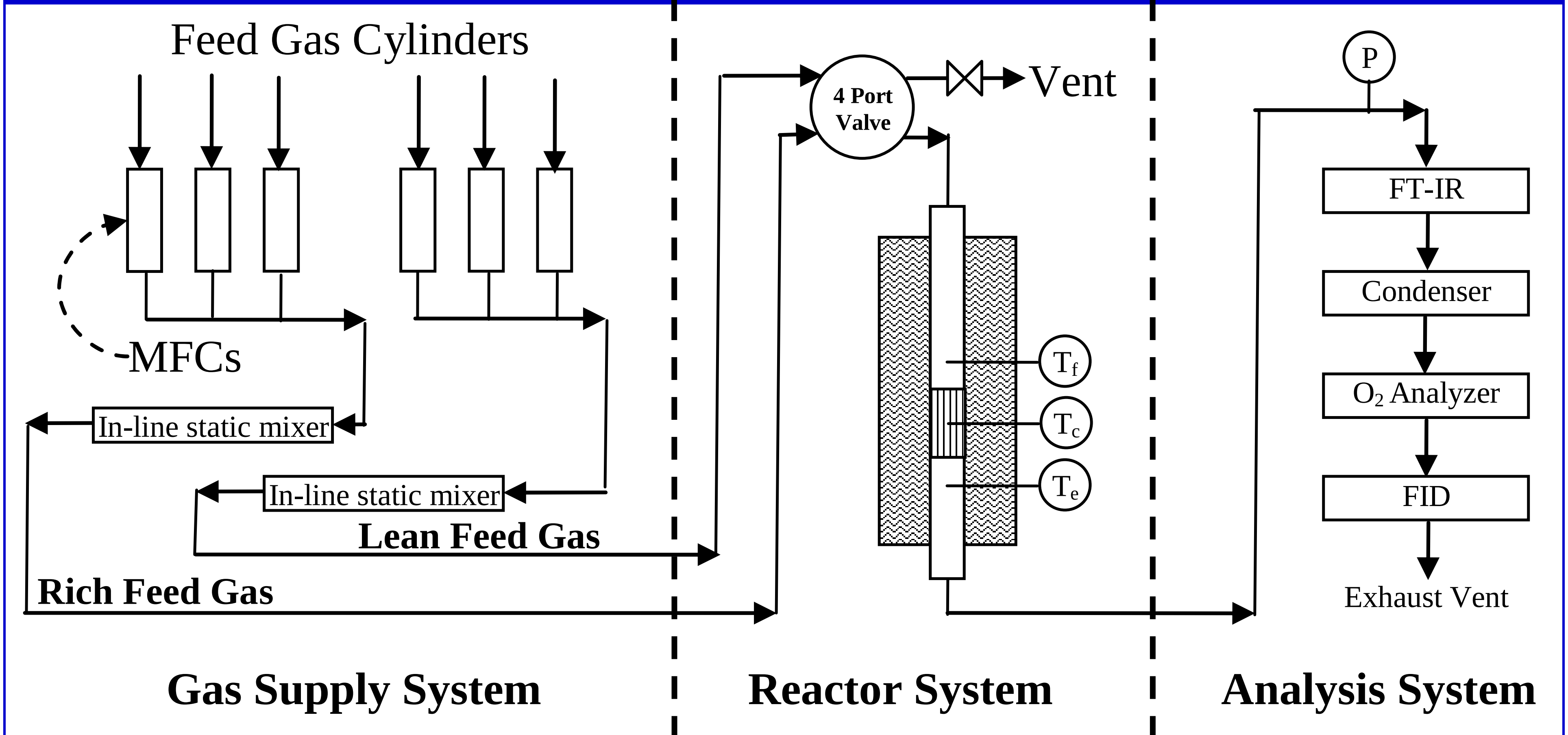
Kinetic Modeling

- *Microkinetic*

Reactor Modeling

- *Isothermal, pseudohomogeneous*
- *Nonisothermal, interphase*

Bench-Scale Monolith Reactor System



Typical Transient Profiles

2.2% Pt
16% BaO

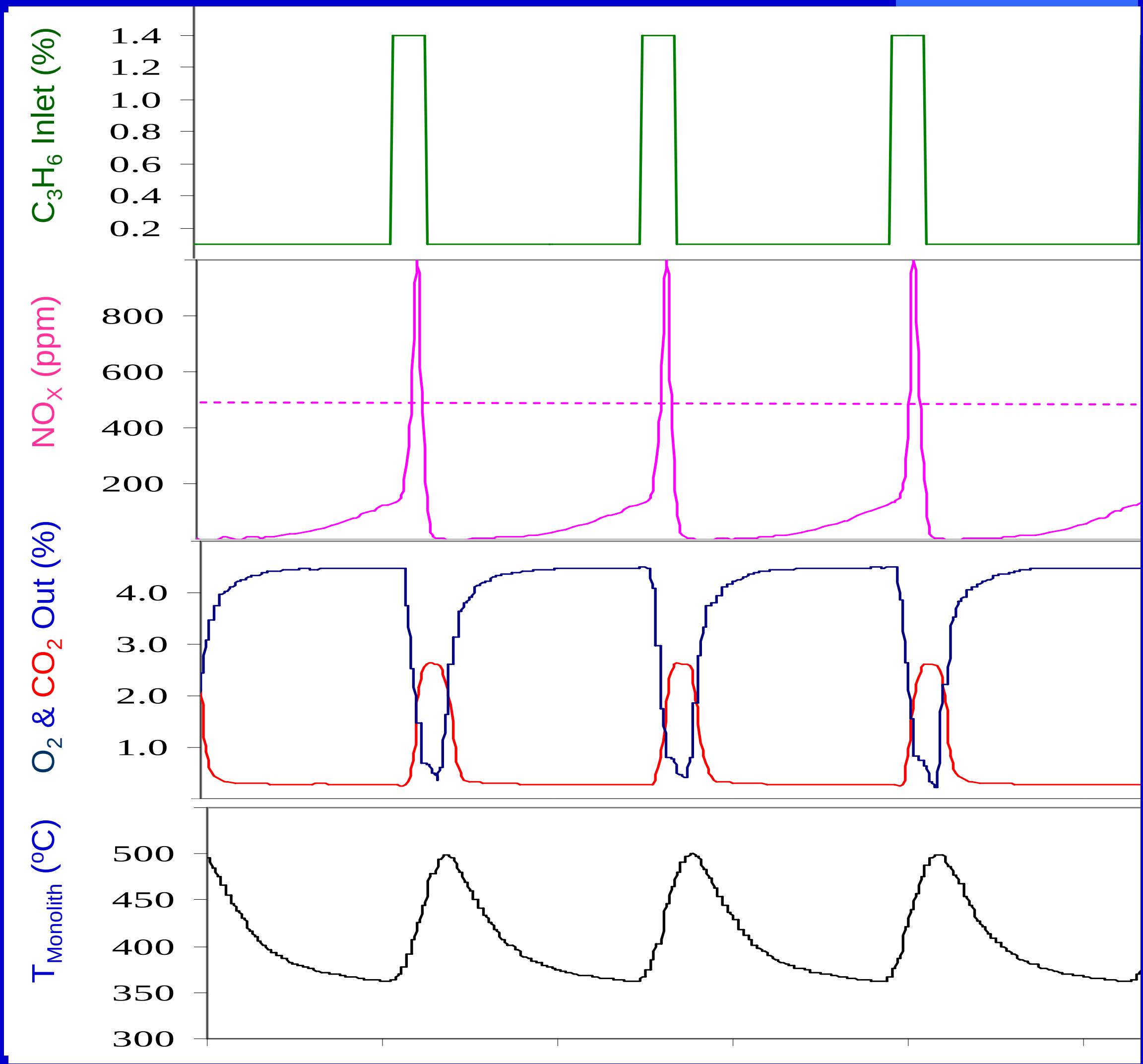
Inlet Concentrations:
500 ppm NO
5% O_2
1000 ppm C_3H_6

$S_{N,Pulse} = 0.8$
(1.4% C_3H_6 during pulse)

$$S_N = \frac{2[O_2] + [NO]}{9[C_3H_6]}$$

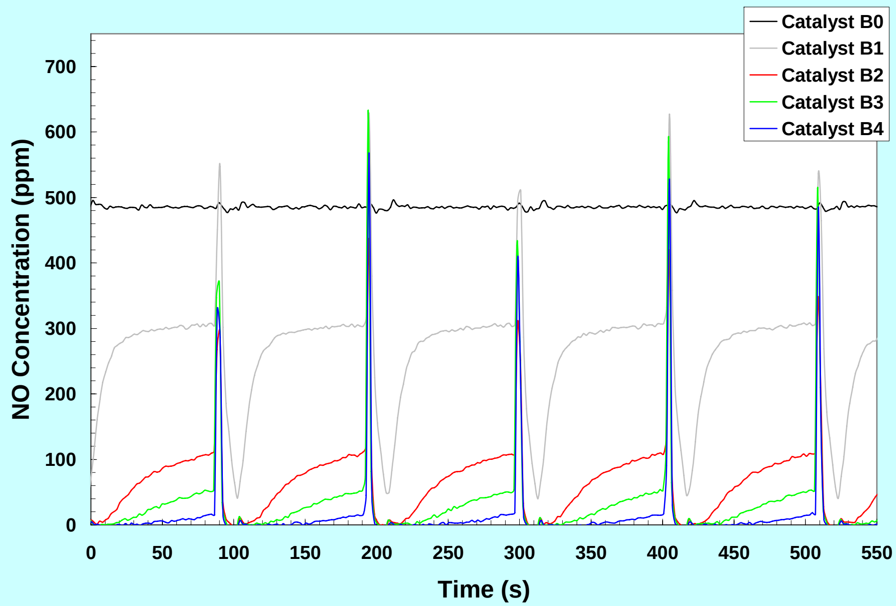
t_{Pulse} = 10 seconds
t_{Cycle} = 70 seconds

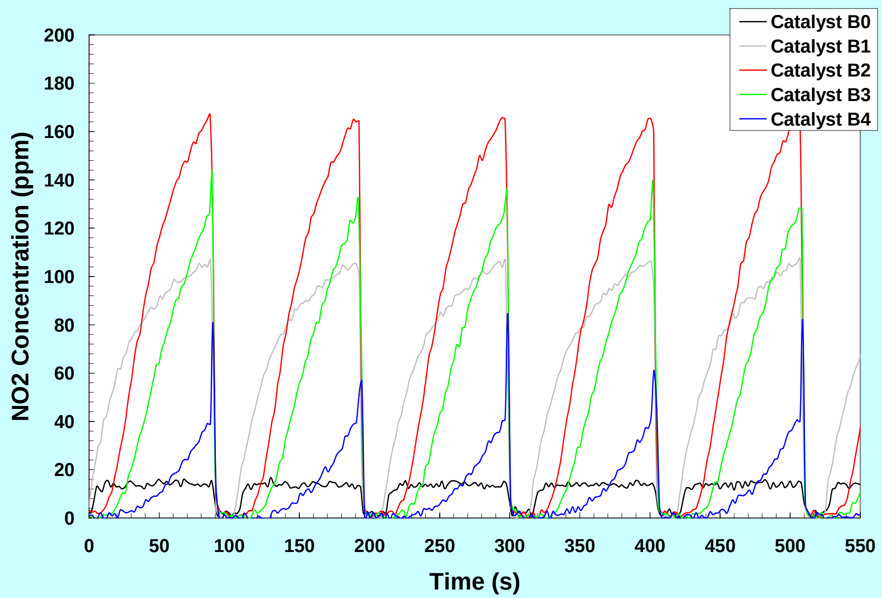
$T_F = 300^oC$



NSR: Effect of Pt Loading

LEAN: 500 ppm NO; 5% O_2 90 s; RICH: 0.7% C_3H_6; 500 ppm NO; 5% O_2 14 s

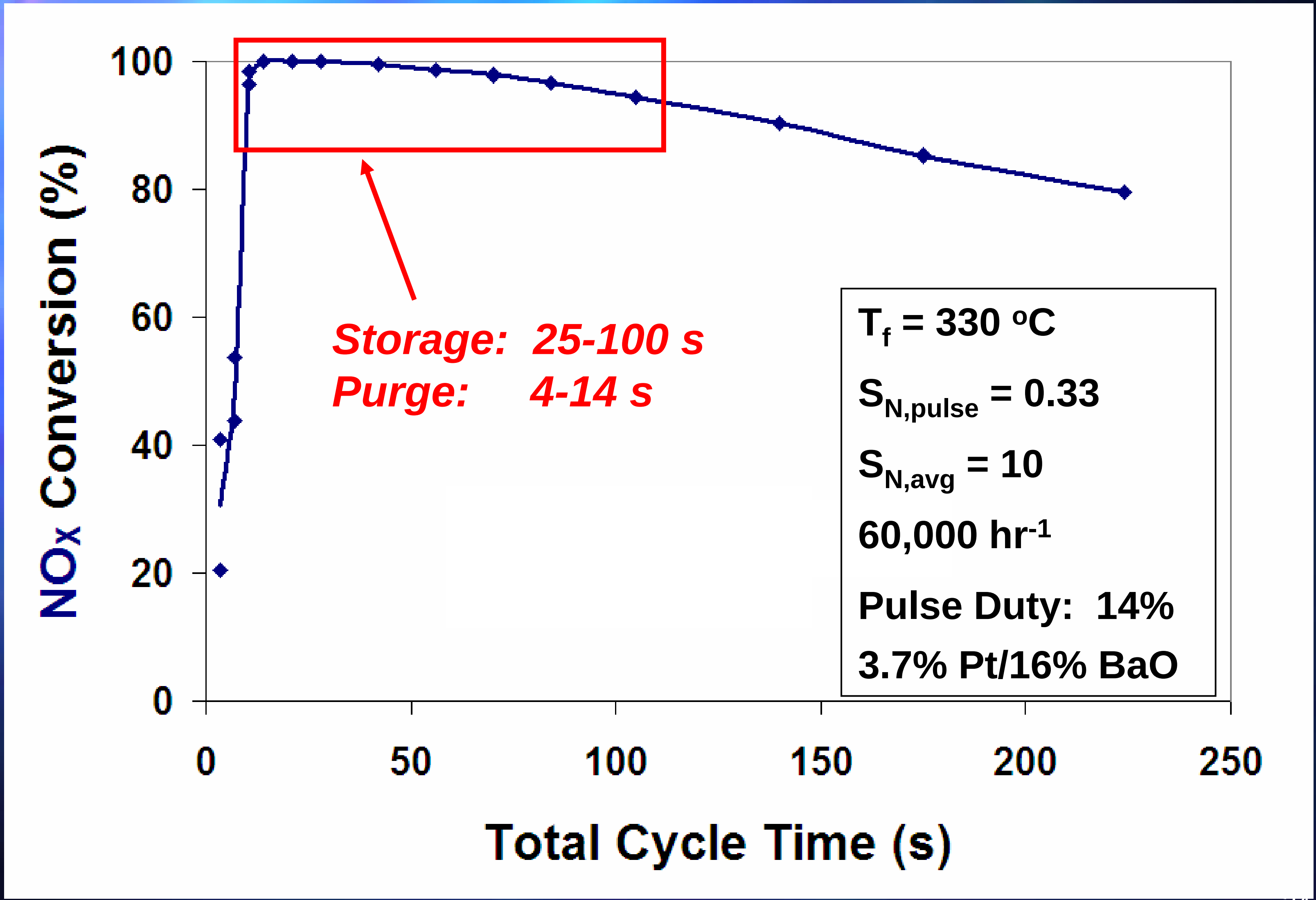




NO_2 + $BaCO_3$ ←→ $BaONO_2$ + CO_2 (Storage & Reduction)

NO_2 + BaO ←→ $BaONO_2$ (Storage)

Effect of Total Cycle Time



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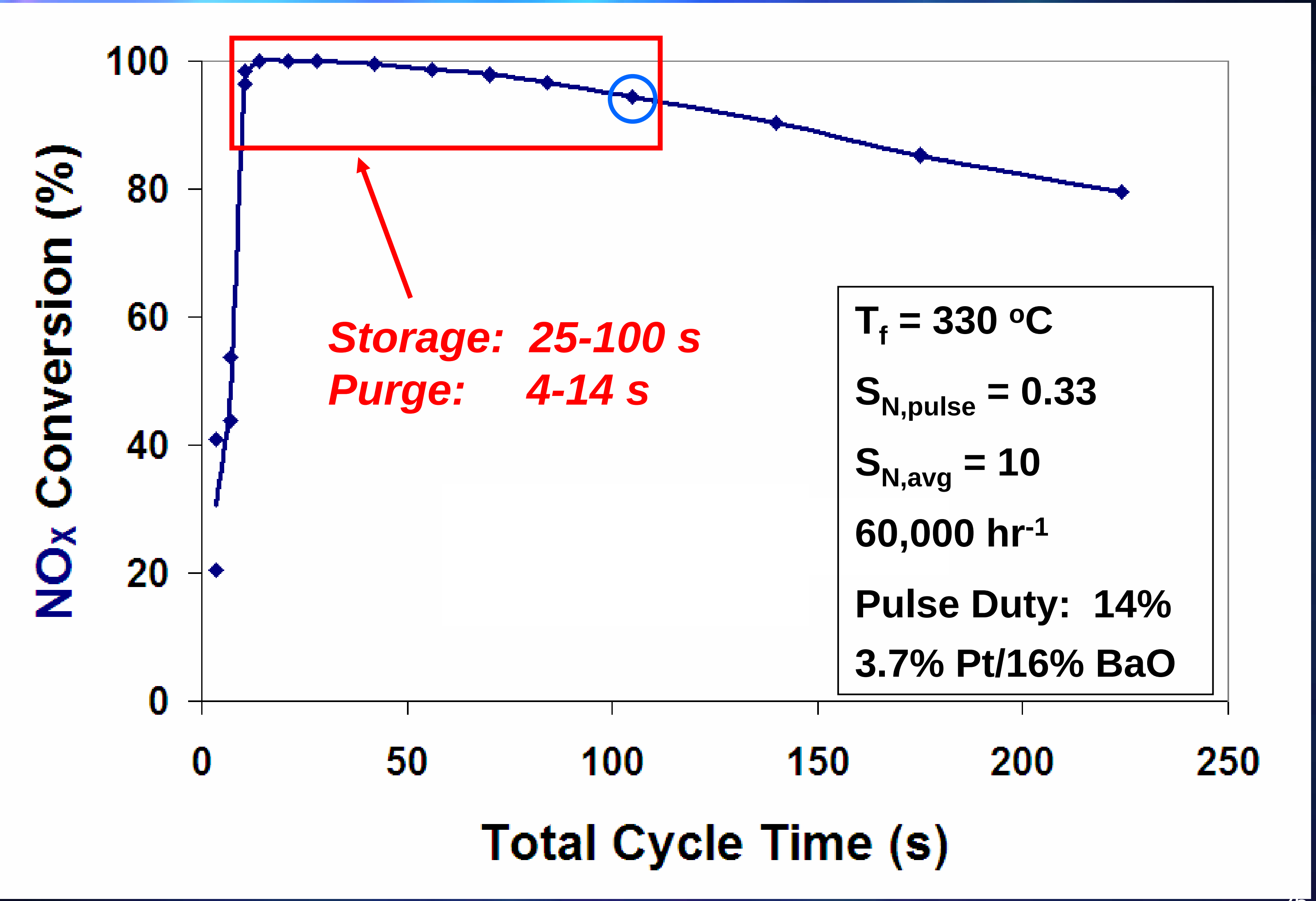
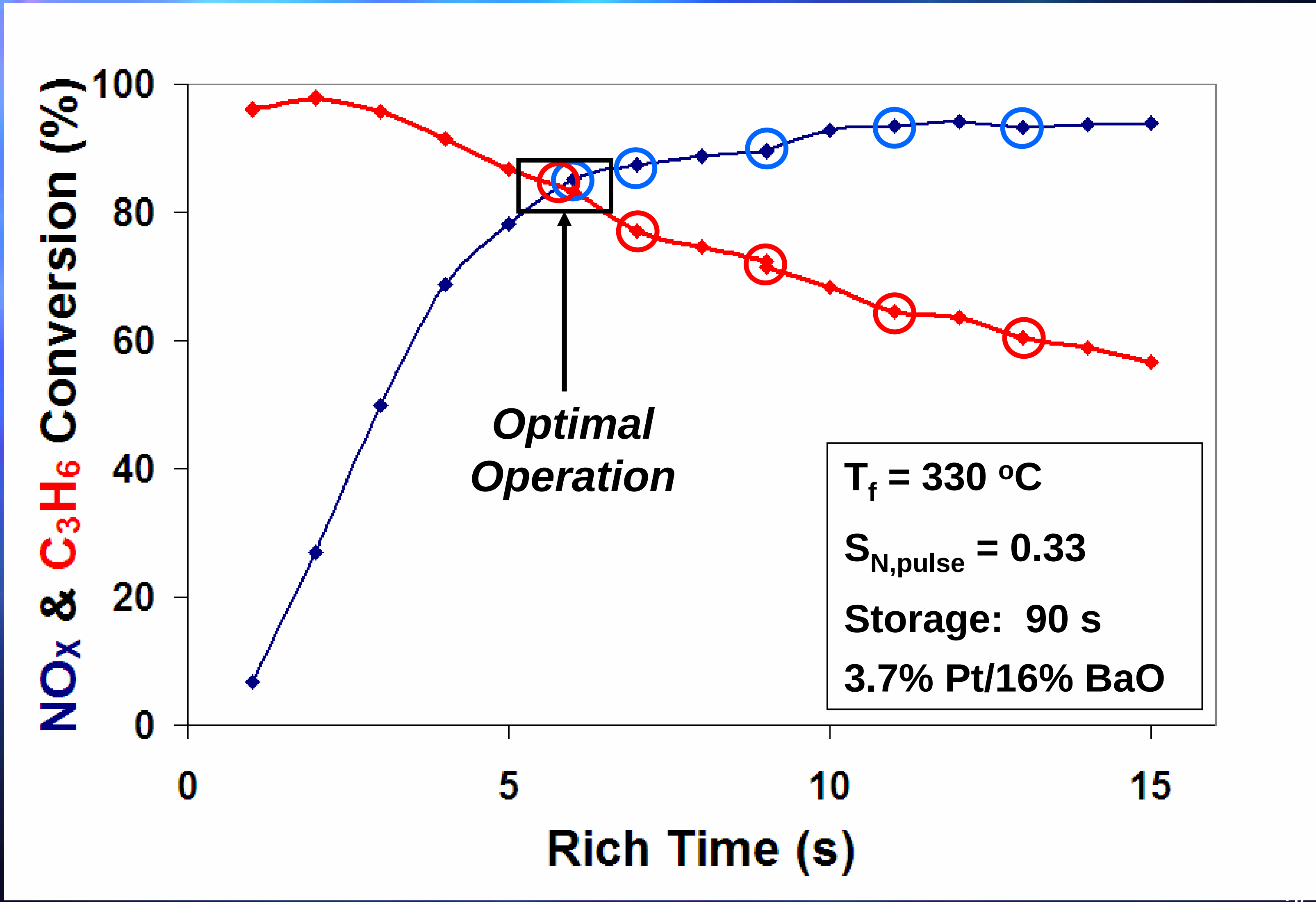
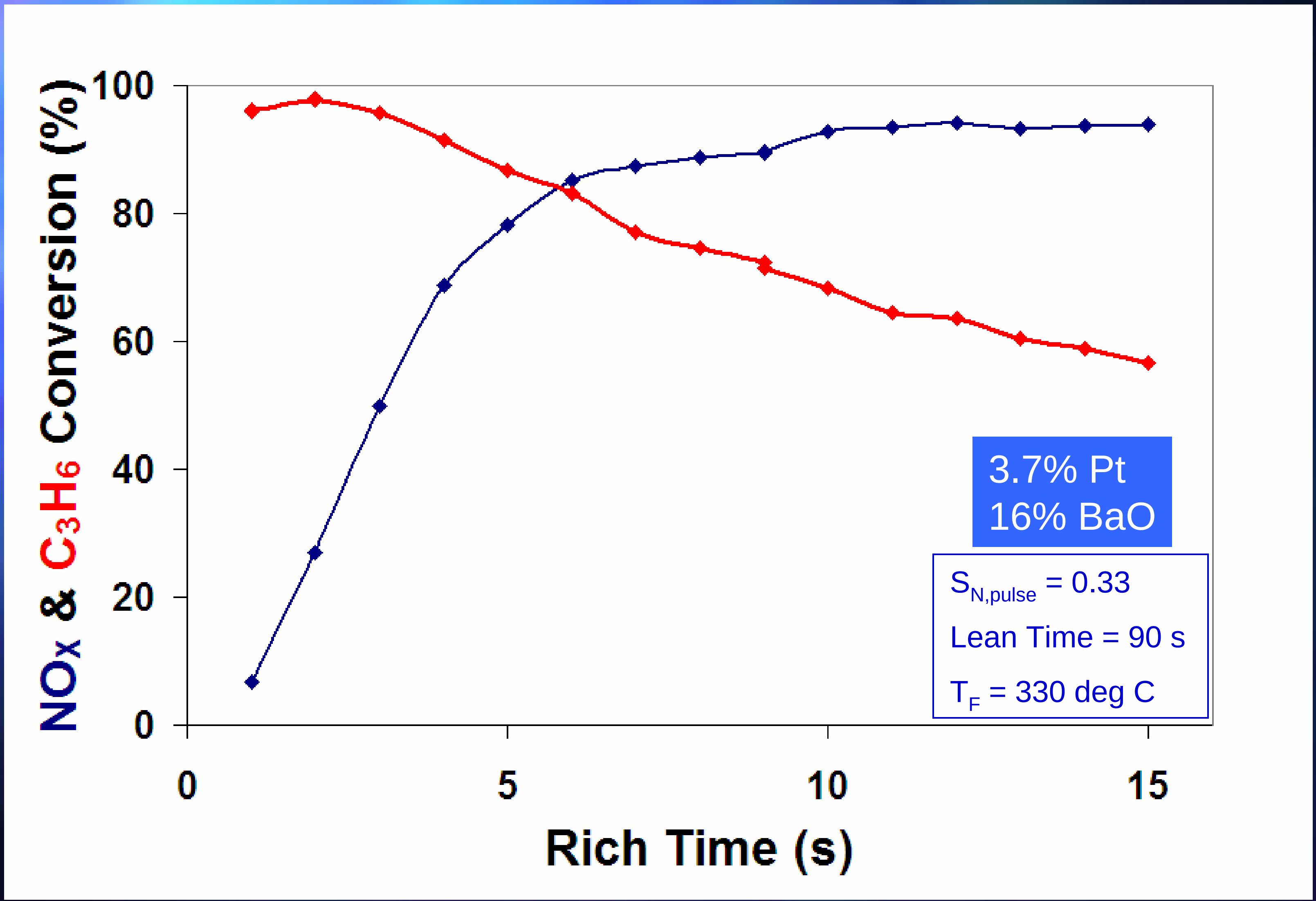


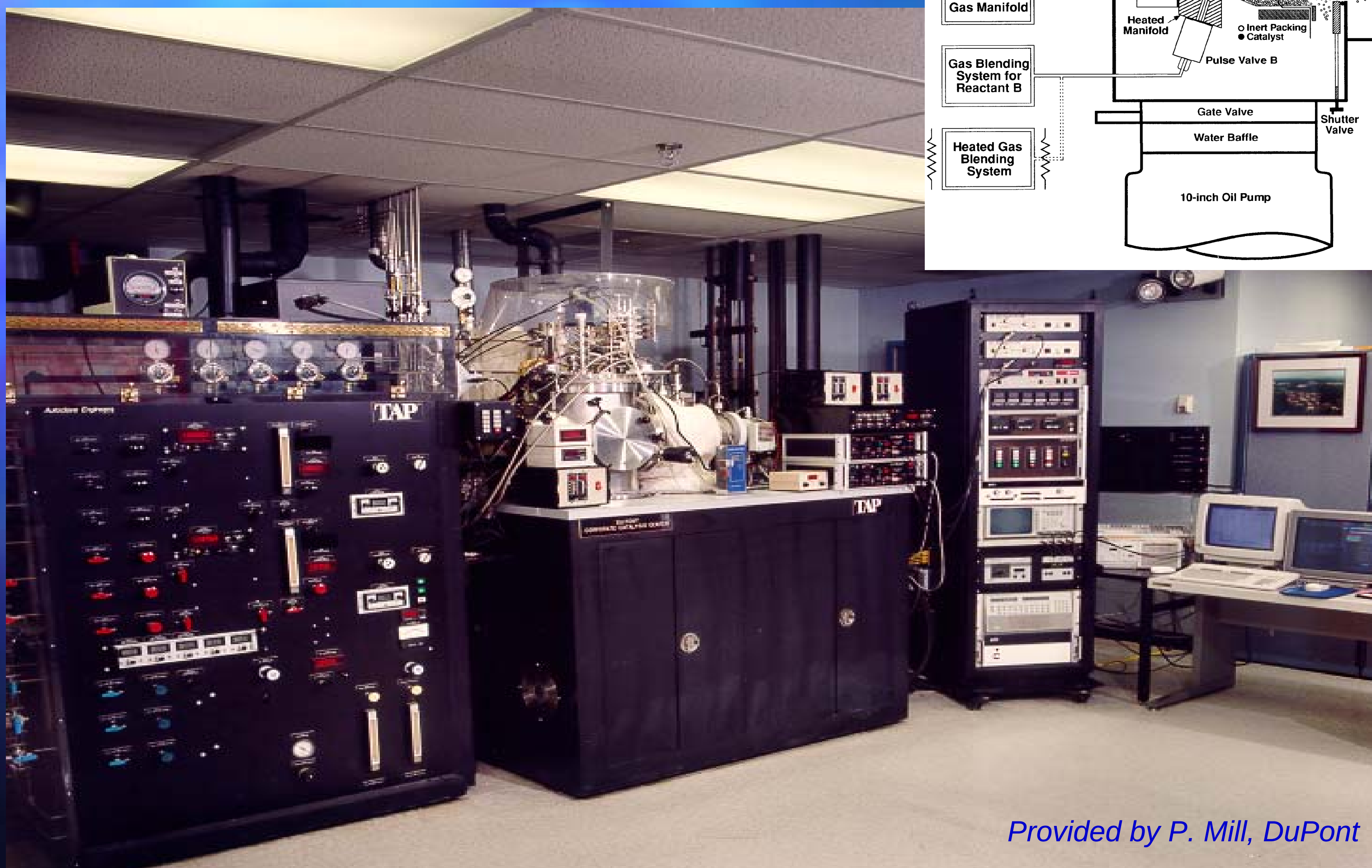
Effect of Purge Time (Pulse Duration)

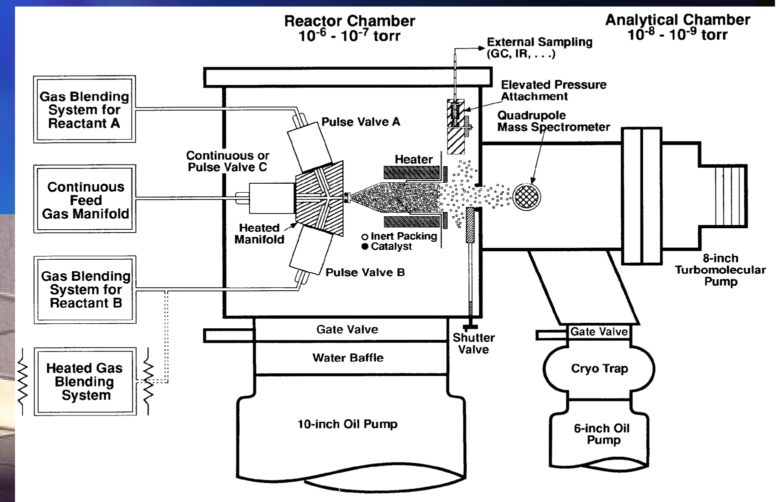


Effects of Rich Time (Pulse Duration)



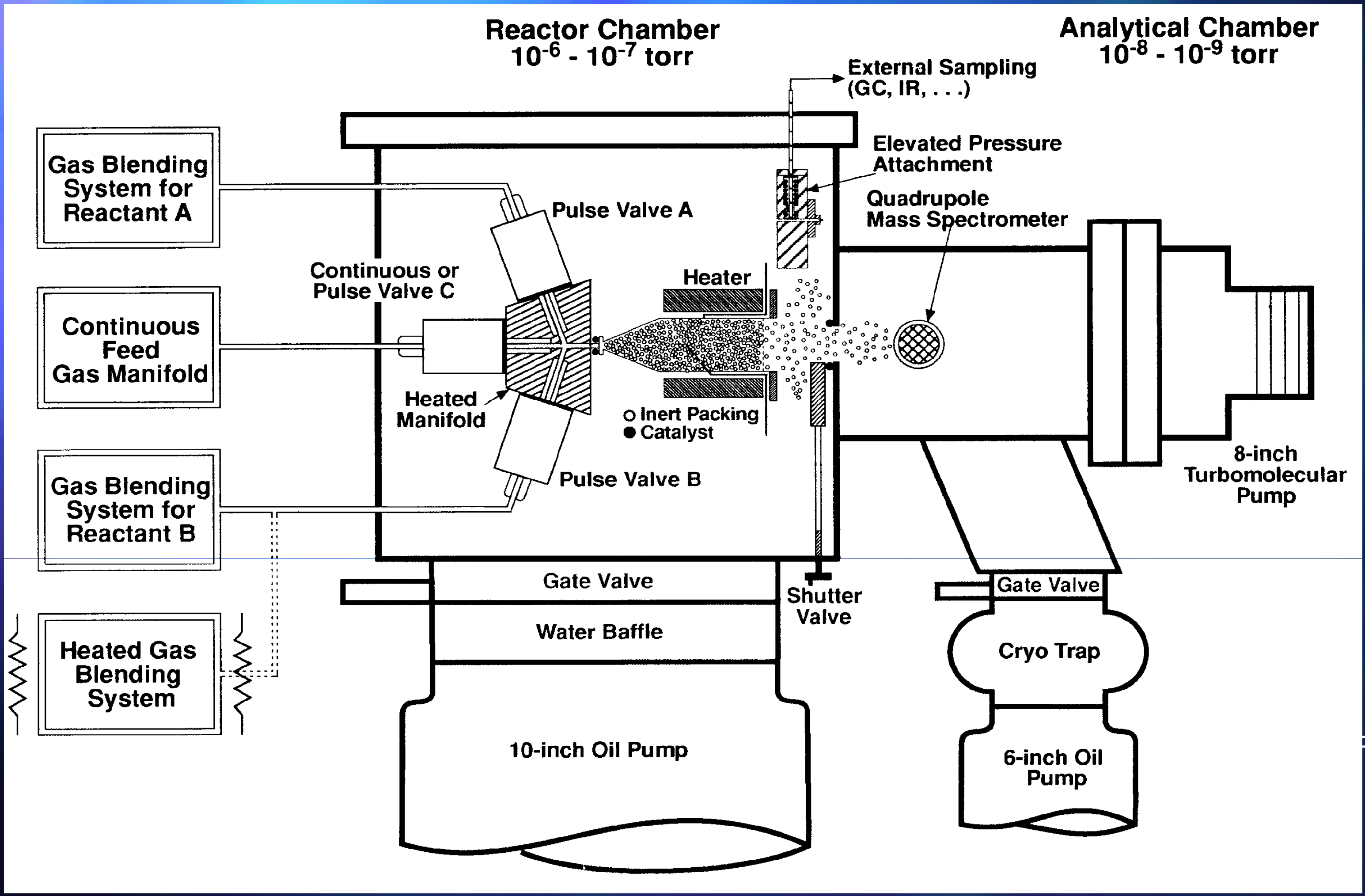
Temporal Analysis of Products (TAP) Reactor System





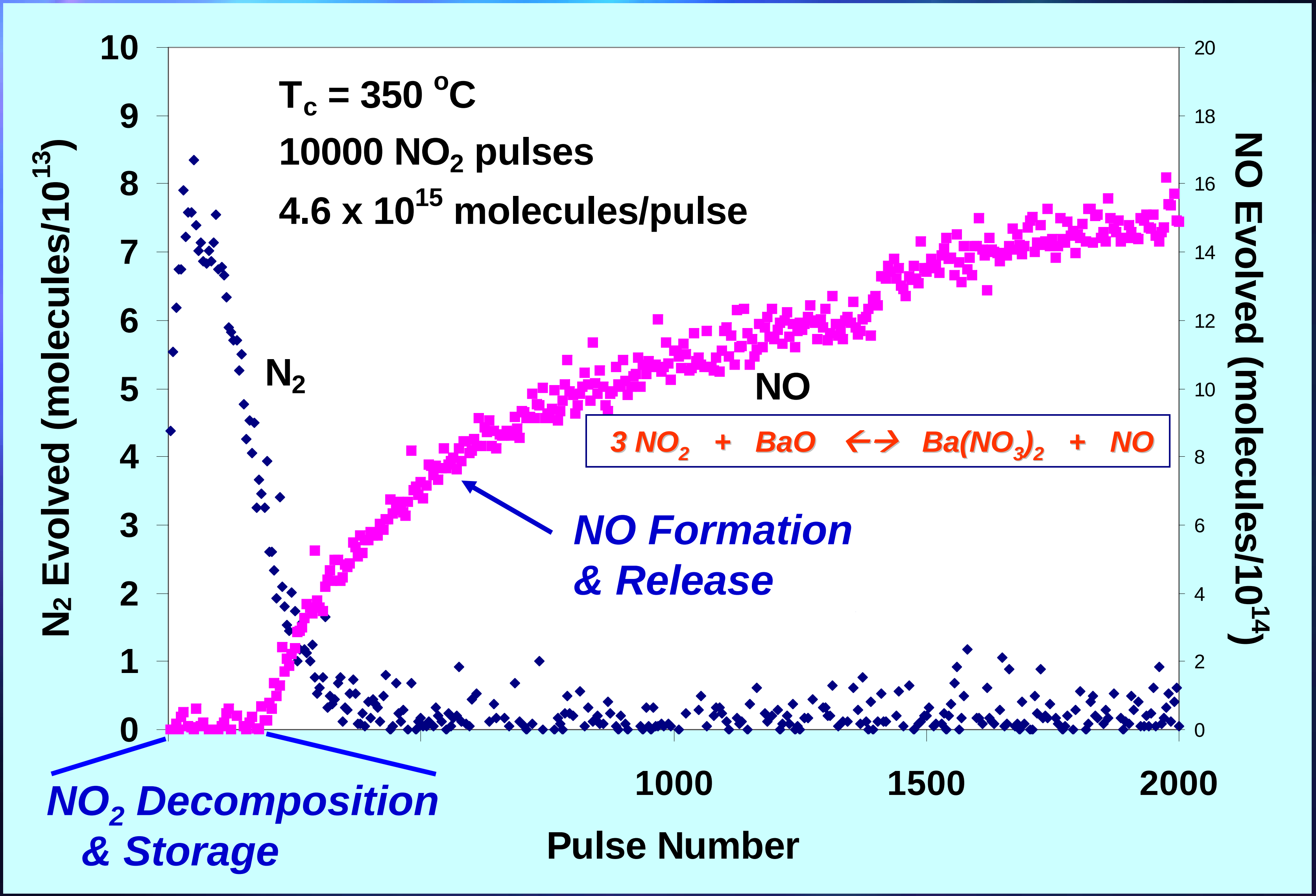
Provided by P. Mill, DuPont

TAP Reactor Schematic



P. Mill, DuPont

N_2 & NO Evolution During NO_2 Pulsing



NO_x Storage Pathways

SHORT TERM STORAGE

$NO + 0.5\,O_2 \overset{Pt}{\leftrightarrow} NO_2$

Pt, BaO

Pt, BaO

BaO

NITRITE PATHWAY

$BaO + 0.5\,O_2 \overset{Pt}{\leftrightarrow} BaO_2$

$BaO_2 + NO \overset{Pt}{\leftrightarrow} BaONO_2$

$BaONO_2 + NO \overset{Pt}{\leftrightarrow} Ba(NO_2)_2$

$Ba(NO_2)_2 + O_2 \overset{Pt}{\leftrightarrow} Ba(NO_3)_2$

$BaO + 2\,NO + 1.5\,O_2 \leftrightarrow Ba(NO_3)_2$

$BaO + 2\,NO_2 + 0.5\,O_2 \leftrightarrow Ba(NO_3)_2$

NITRATE PATHWAY

$NO_2 + BaO \leftrightarrow BaONO_2$

$BaO_2 + NO_2 \leftrightarrow BaO\text{-}NO_3$

$BaO\text{-}NO_3 + NO_2 \leftrightarrow Ba(NO_3)_2$

$BaO + 3\,NO_2 \leftrightarrow Ba(NO_3)_2 + NO$

Principal Collaborators

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