Lean NOx Trap Regeneration Studies on a Light-Duty Diesel Engine with In-Cylinder Air-to-Fuel Control

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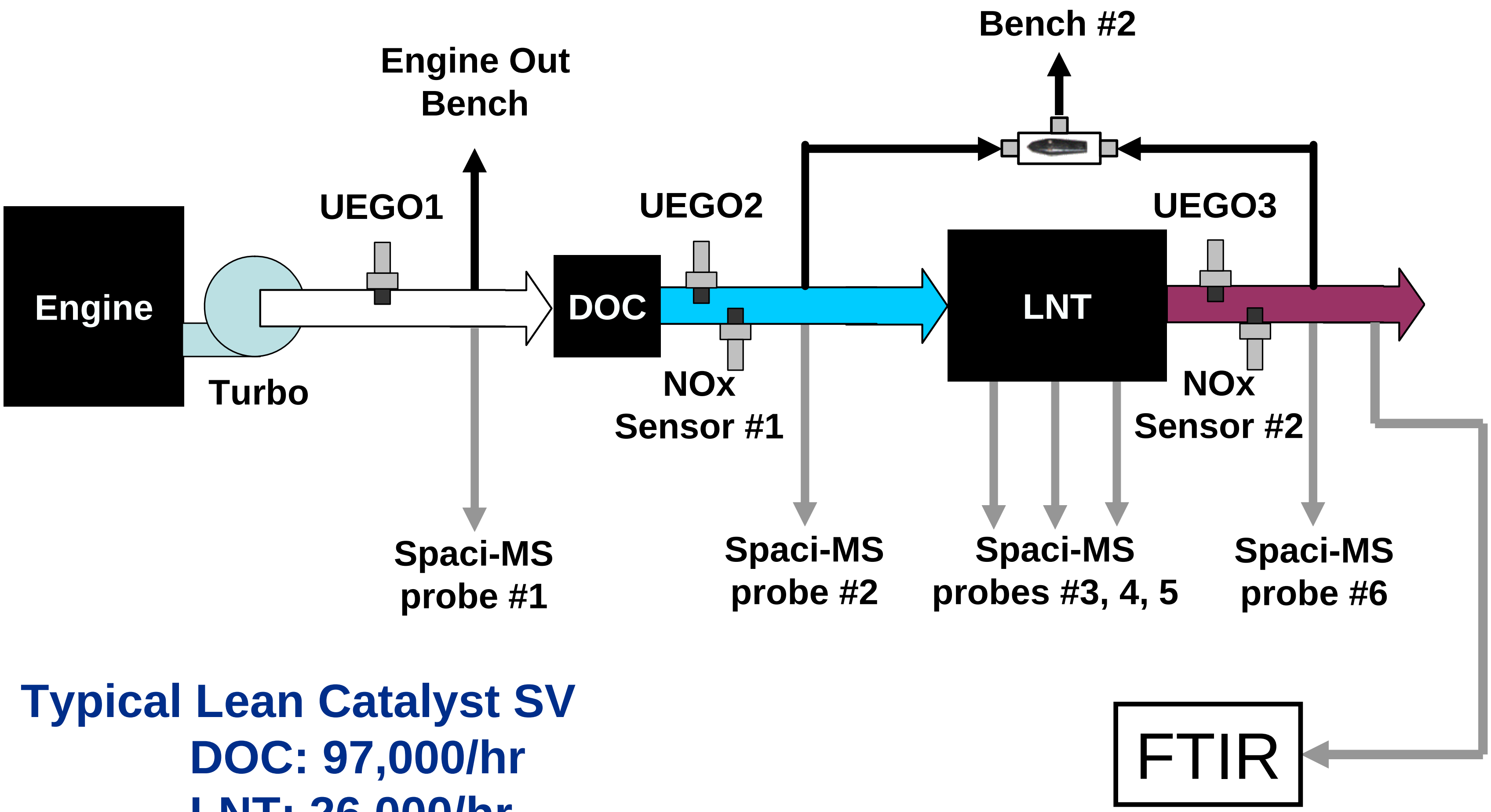
Outline

- Reductant Production from In-Cylinder Regeneration Strategies
- N_2 Selectivity of Lean NOx Trap Regeneration Processes
  - Bench Flow Reactor Studies
  - Engine Studies

Acknowledgements

- U.S. DOE Office of FreedomCAR and Vehicle Technology
- Program Managers: Gurpreet Singh, Ken Howden, and Kevin Stork

Schematic of Experimental Setup [MECA Supplied DOC and LNT]



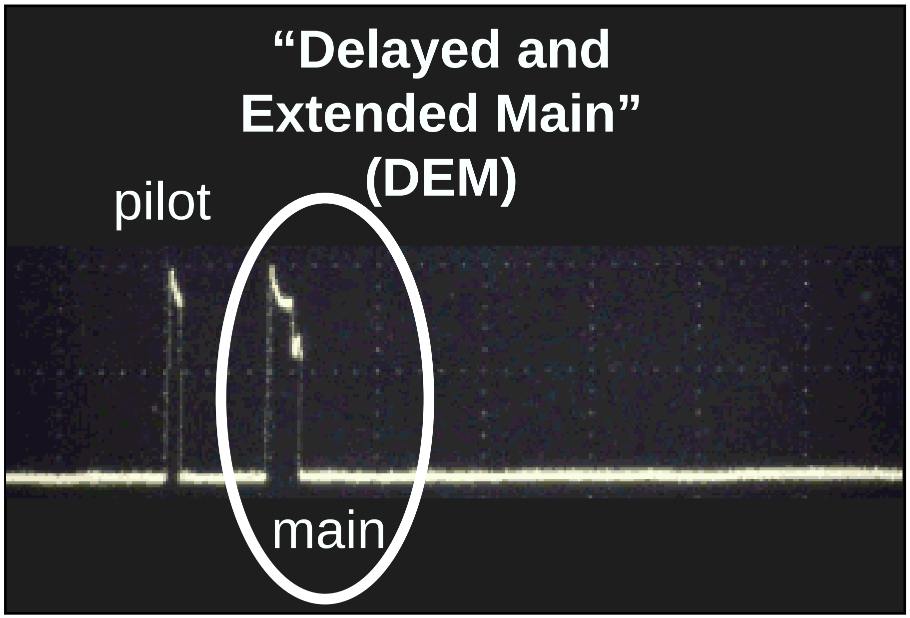
Typical Lean Catalyst SV

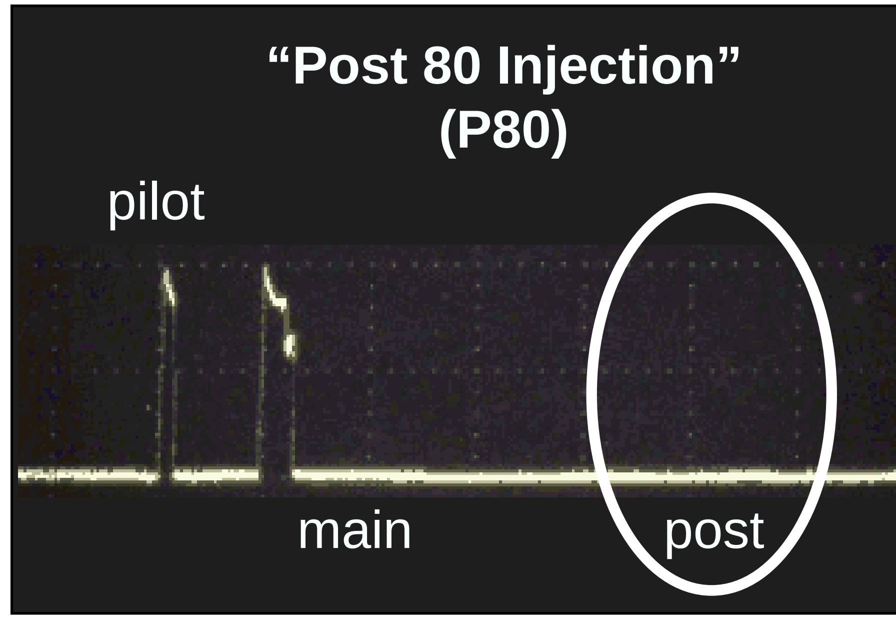
DOC: 97,000/hr

LNT: 26,000/hr

Comparison of three strategies for achieving intermittent rich combustion

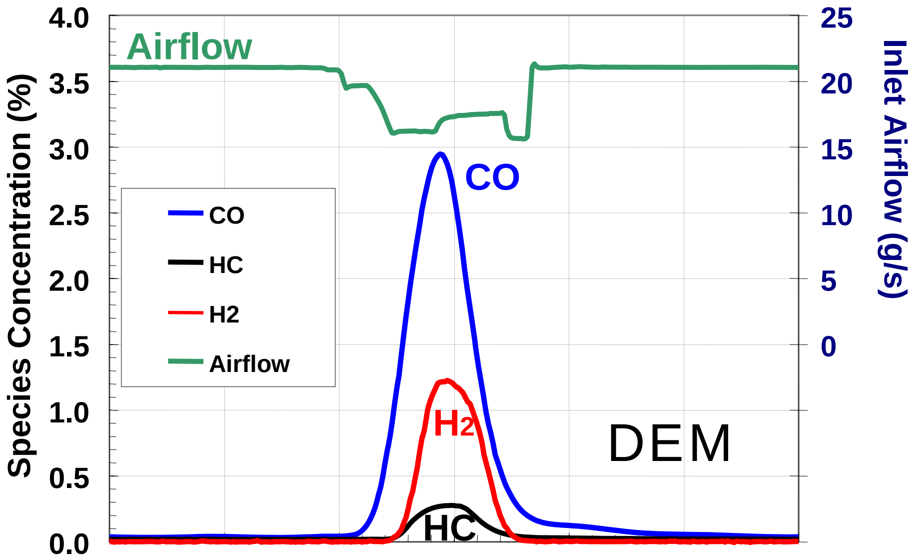
- **Two strategies employ no EGR for highest engine-out NOx (fastest adsorber loading)**
- **Rich excursion is achieved by a combination of intake throttling and the following injection strategies:**

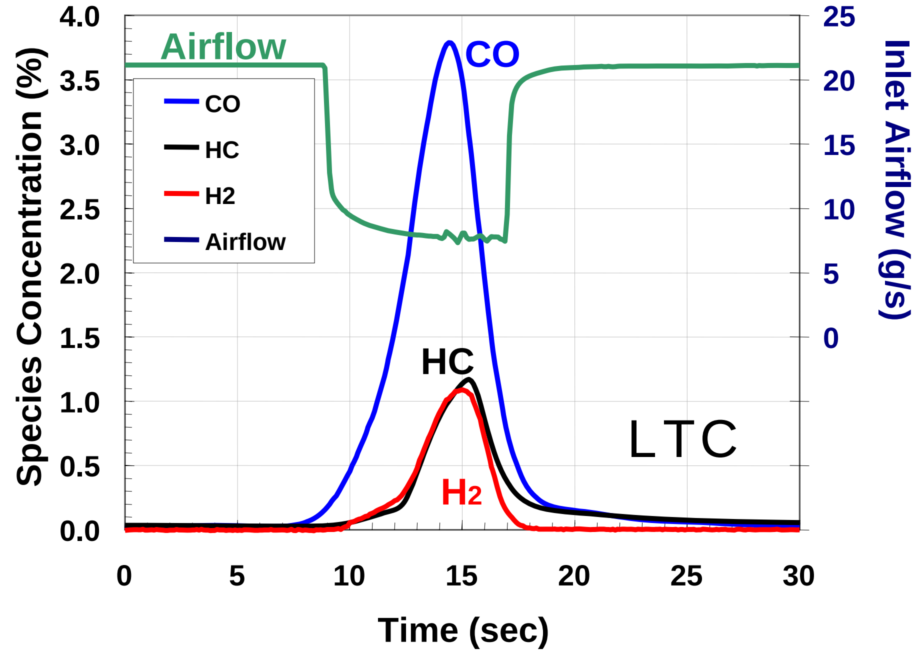


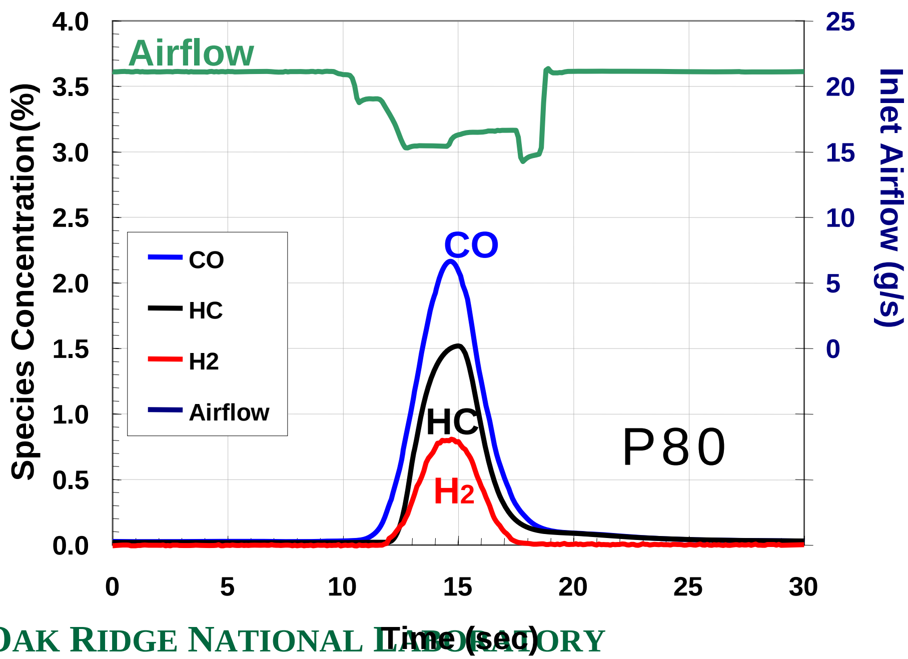


3rd strategy investigated uses high EGR to enter LTC during rich excursion

Real-time data highlights approach of strategies



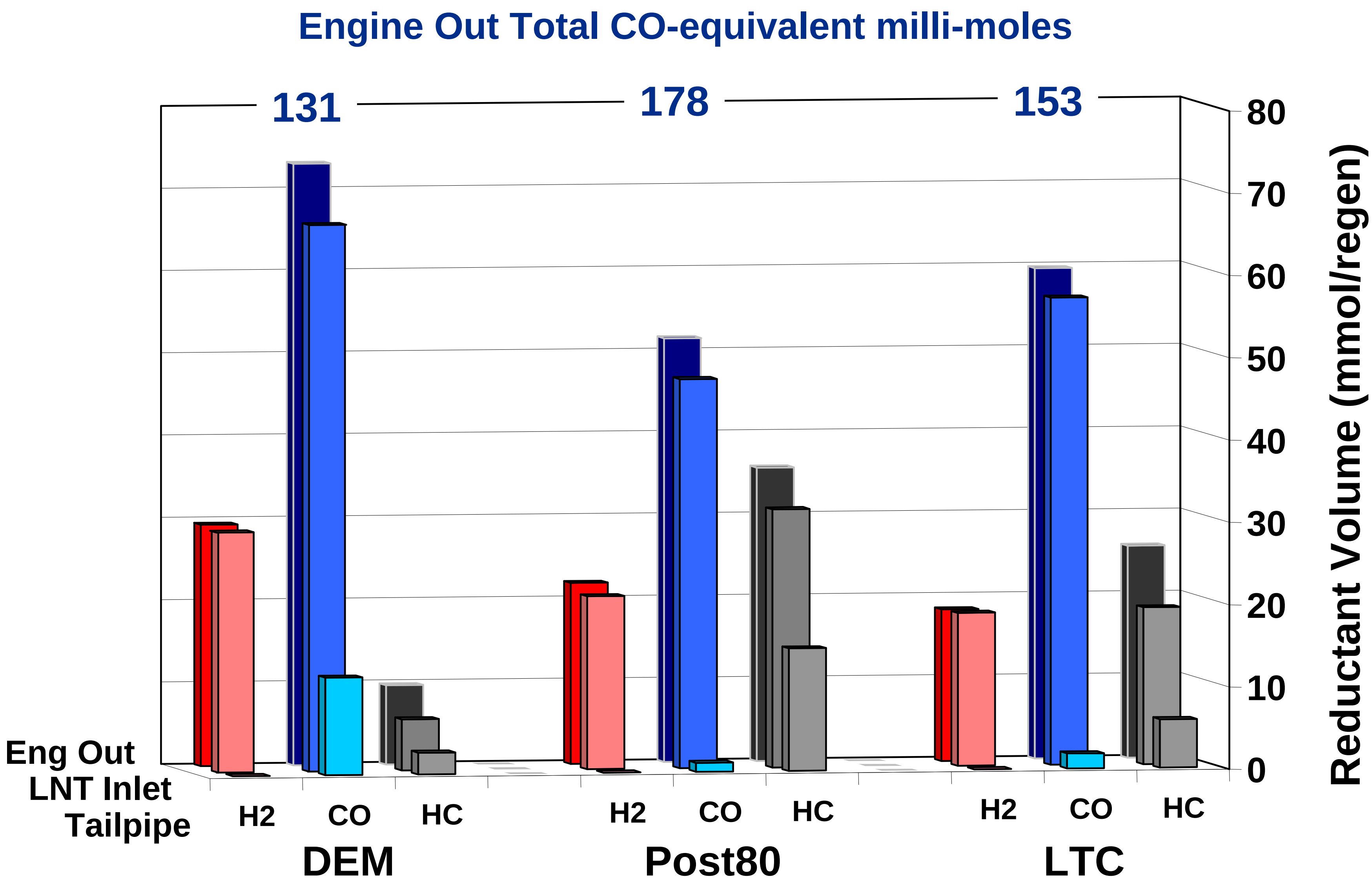




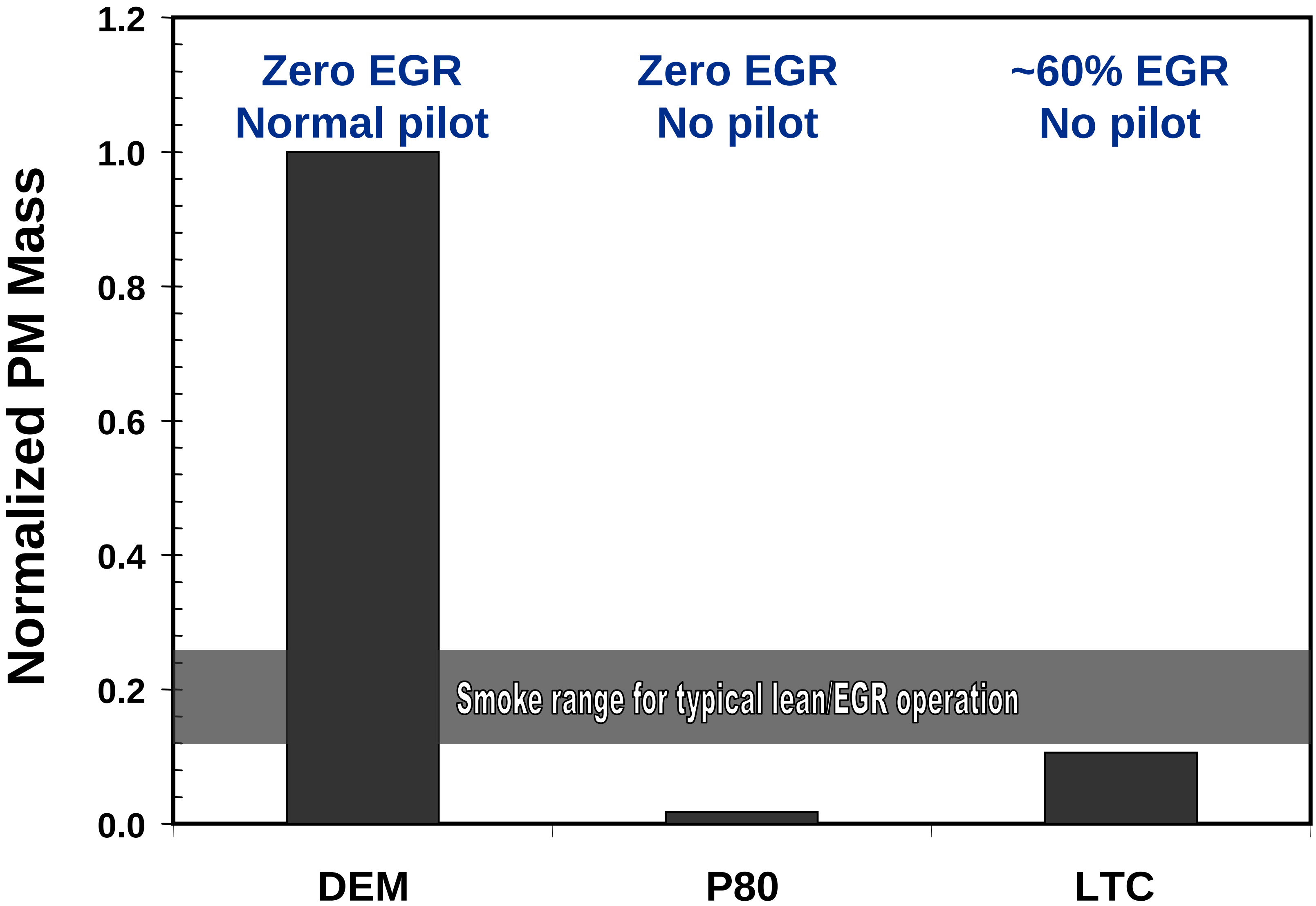
- **DEM and P80 strategies employ identical throttling schedule, similar reduction in intake air mass (reduction of AFR)**
  - **Approach to excess fuel addition affects reductant species formed, concentrations**

- **"LTC" strategy uses EGR and nominal injection control for rich transition**

Total Reductant Moles for Strategies: Reductant Split Differs for Strategies

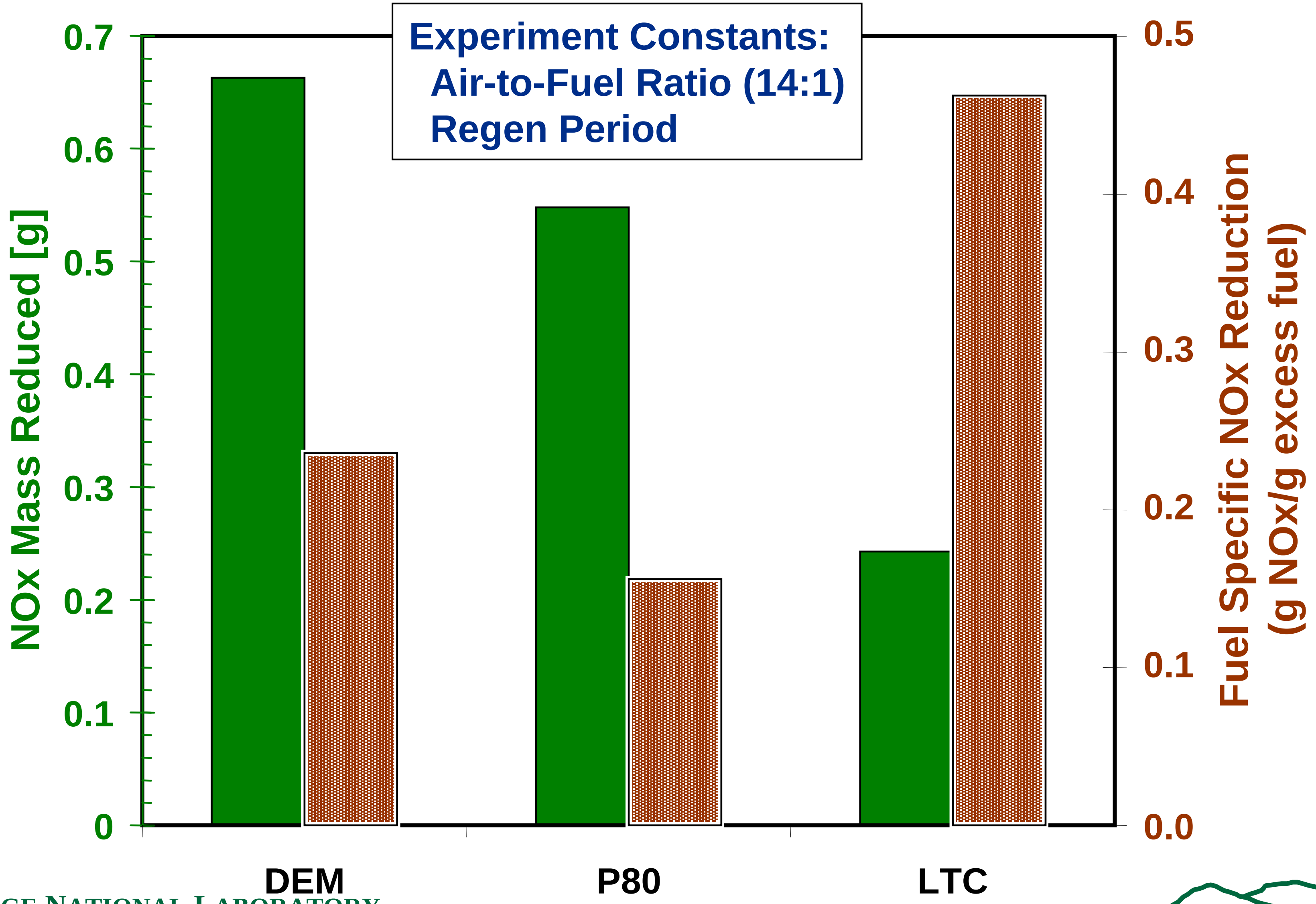


DEM Generates High Level of PM; P80 and LTC Strategies Produces Very Low PM



Comparison of Mass of NOx Reduced and Fuel Efficiency of NOx Reduction

Strategies not optimized for FEP, NOx, torque, etc.



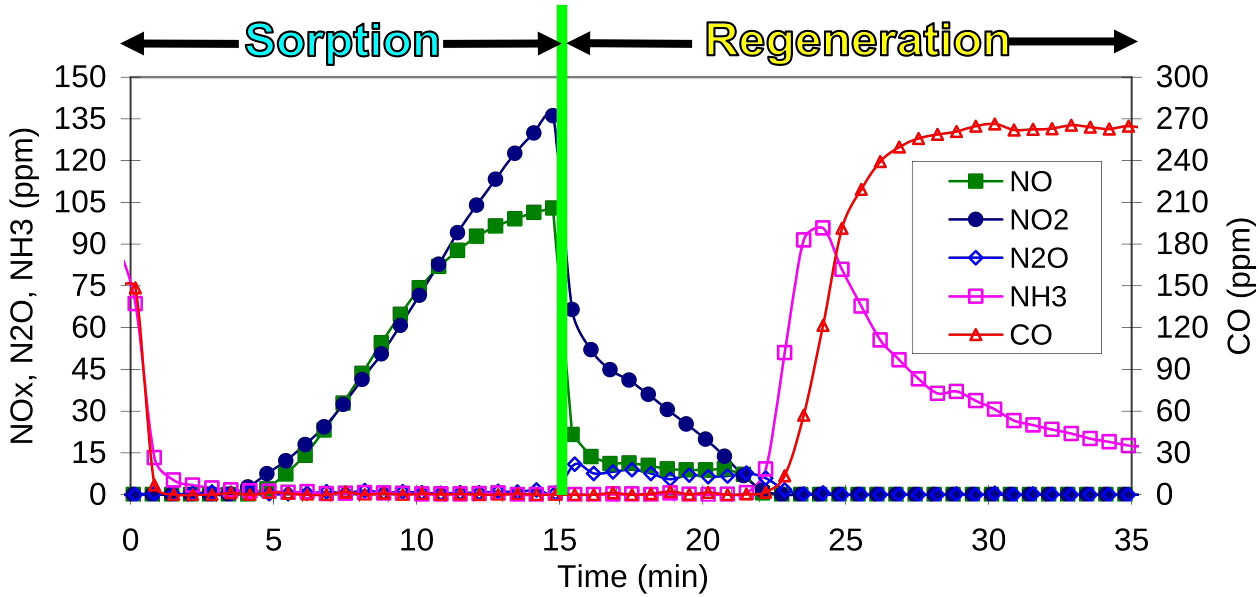
Summary 1: Regeneration Exhaust Species Highly Dependent on Strategy

- **DEM (Delayed Extended Main) Strategy**
  - **High H_2 and CO Levels**
  - **Best Overall NOx Reduction**
  - **High PM Levels**
- **P80 (80º After Top Dead Center) Strategy**
  - **High HC Levels, Lower H_2 and CO**
  - **NOx Reduction Performance Less than DEM**
  - **Lowest PM Levels**
- **LTC (Low Temperature Combustion) Strategy**
  - **Low PM Levels (less than typical lean/EGR operation)**
  - **Best Fuel-Efficiency for Regen (g NOx/g excess fuel)**

Engineered Systems May Use Portfolio of Regeneration Strategies

General Observations Regarding N_2 Selectivity

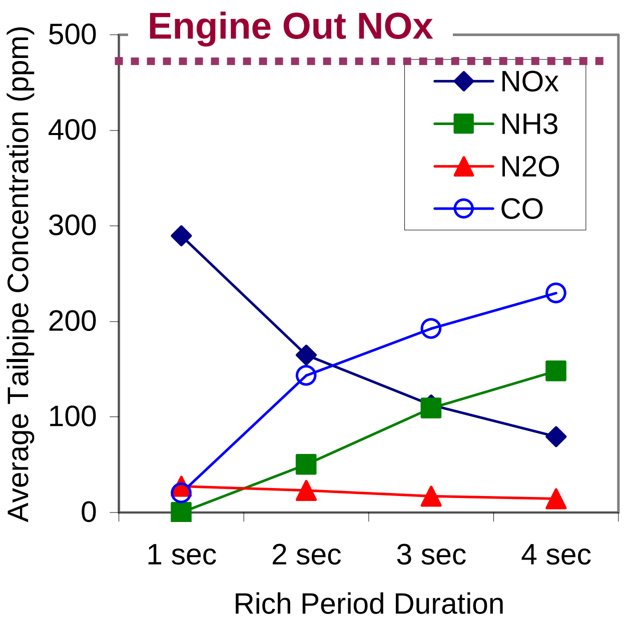
- **ORNL bench reactor results for engine-aged core sample shown**
- **N_2O and NH_3 are both formed during regeneration, but …**
  - ***only*** **when NOx has been stored on the catalyst**
    - **N_2 + reductant = NH_3 is not likely**
- **NH_3 appears after initial main NOx release/reduction spike**

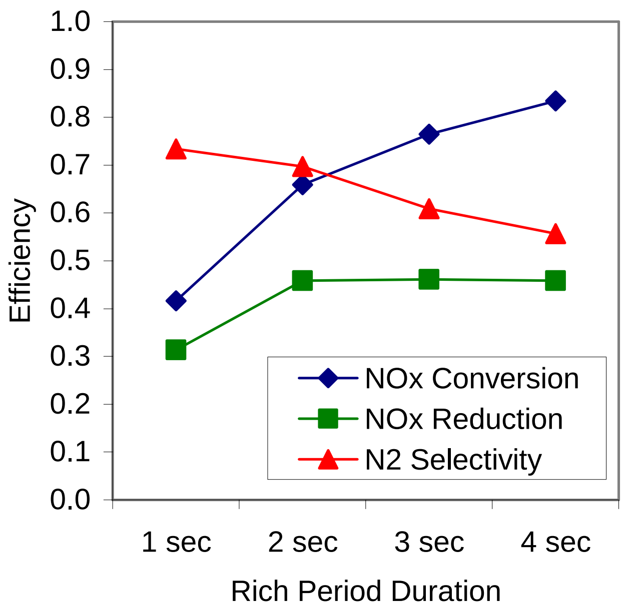


See Castoldi et. al, *Cat. Today* **96** (2004) 43-52 for NH_3 vs. sorbate loading

NH_3 Production During Extended Regeneration Observed in Engine Studies

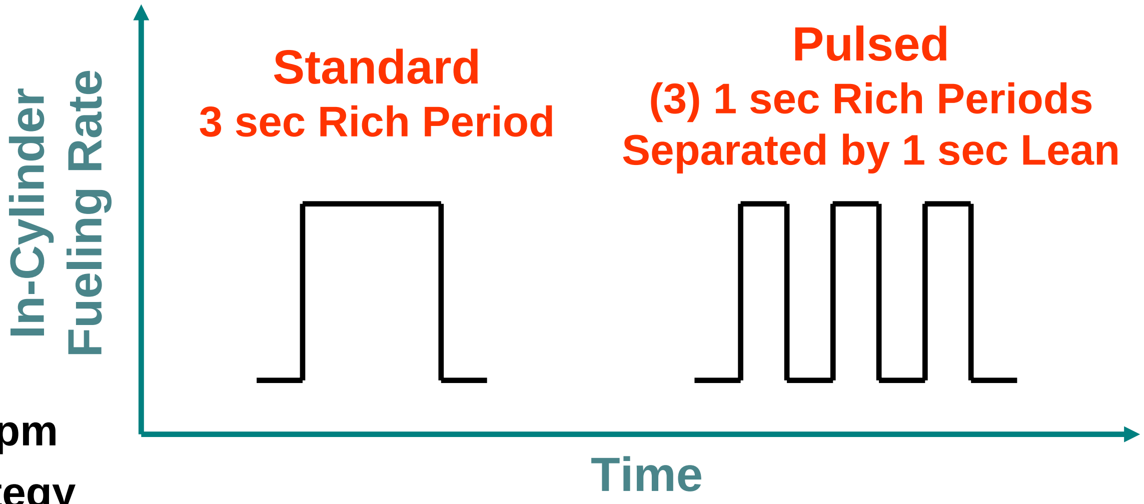
- **NH_3 and N_2O measured at tailpipe via FTIR (cycle averaged analysis)**
- **Experimental parameters chosen to enhance NH_3 formation**
  - DEM, 13:1, 300ºC, 60s Cycle
  - "Over-regeneration" with high NOx saturation of LNT
- **Excess reductant leads to high NH_3 emissions and reduced NOx to N_2 reduction efficiency**





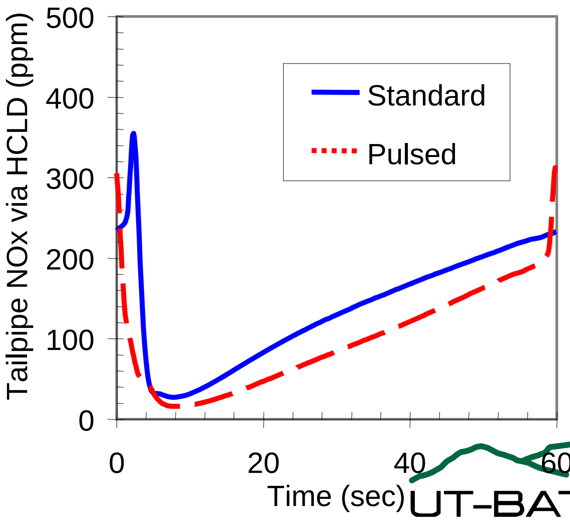
Engine Regeneration Strategies Can Be Developed to Optimize N_2 Selectivity

- **Comparison for (2) regeneration strategies**
  - **Same fuel penalty**
  - **Same base parameters**
    - **Temperature=300ºC**
    - **Cycle period=60 sec**
    - **Engine Out NOx~500 ppm**
    - **DEM regeneration strategy**
    - **13:1 A/F target**



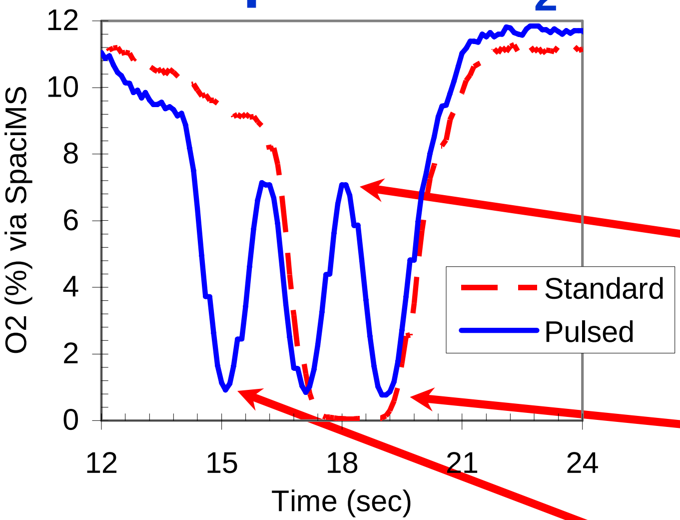
Pulsed Strategy Gives Lower NH_3 *AND* Equivalent NOx Reduction

	Standard	Pulsed	Difference
Engine Out NOx (ppm)	472.1	457.3	-3.1%
Avg. Tailpipe NOx (ppm)	138.7	98.6	-29.0%
Avg. Tailpipe NH3 (ppm)	217	73	-66.4%
NOx Capacity (g/l)	0.311	0.317	2.2%
BSFC (lb/bhp-hr)	0.381	0.390	2.3%
Catalyst Temperature (C)	331.5	342.6	3.4%



Tailpipe O_2 Analysis Shows O_2 Purge for Pulsed Case

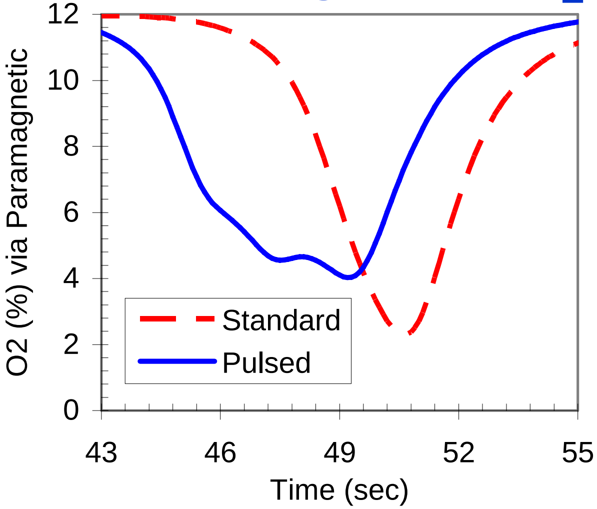
SpaciMS O_2



Standard

Pulsed

Paramagnetic O_2

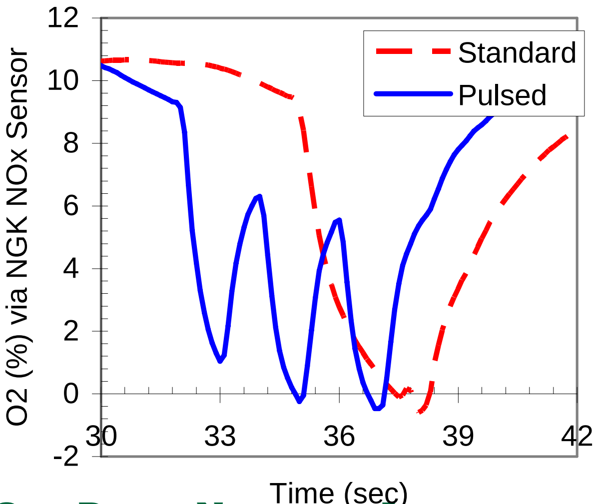


O_2 purge during Pulsed strategy

Zero O_2 during Standard strategy

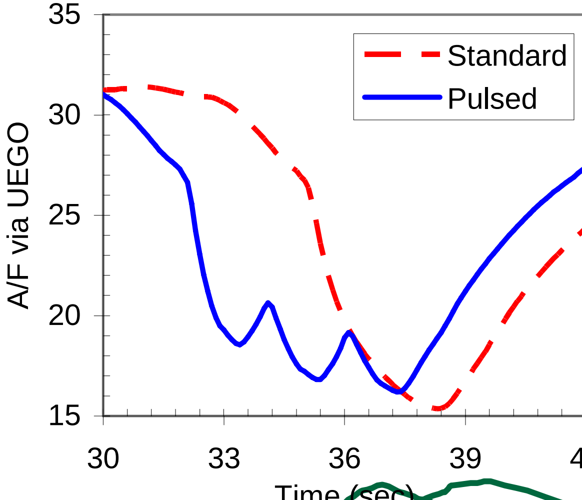
Non-Zero O_2 minimum during Pulsed strategy ???

NGK Sensor O_2



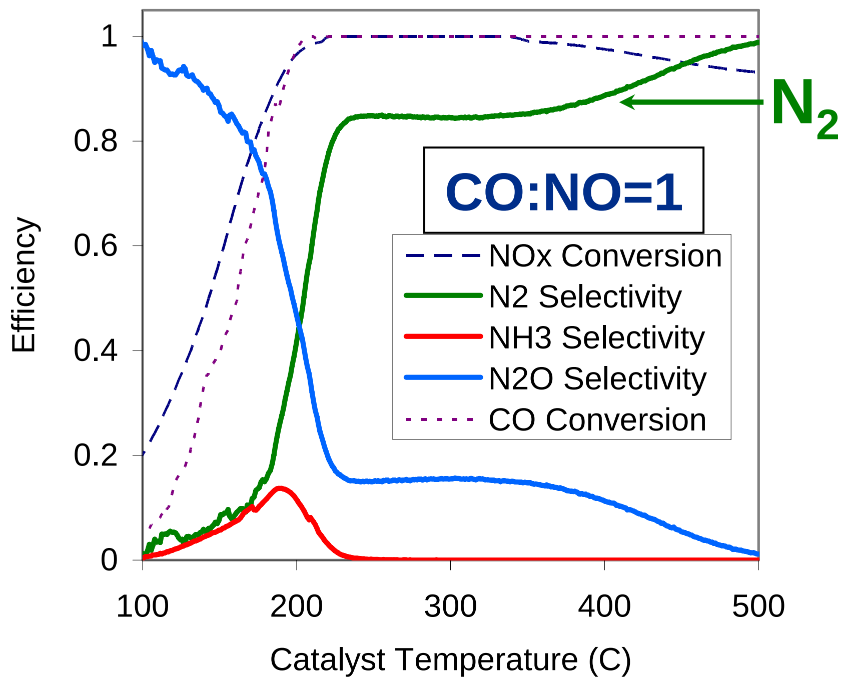
Note:
Assuming no mixing, catalyst residence time is ~0.1s

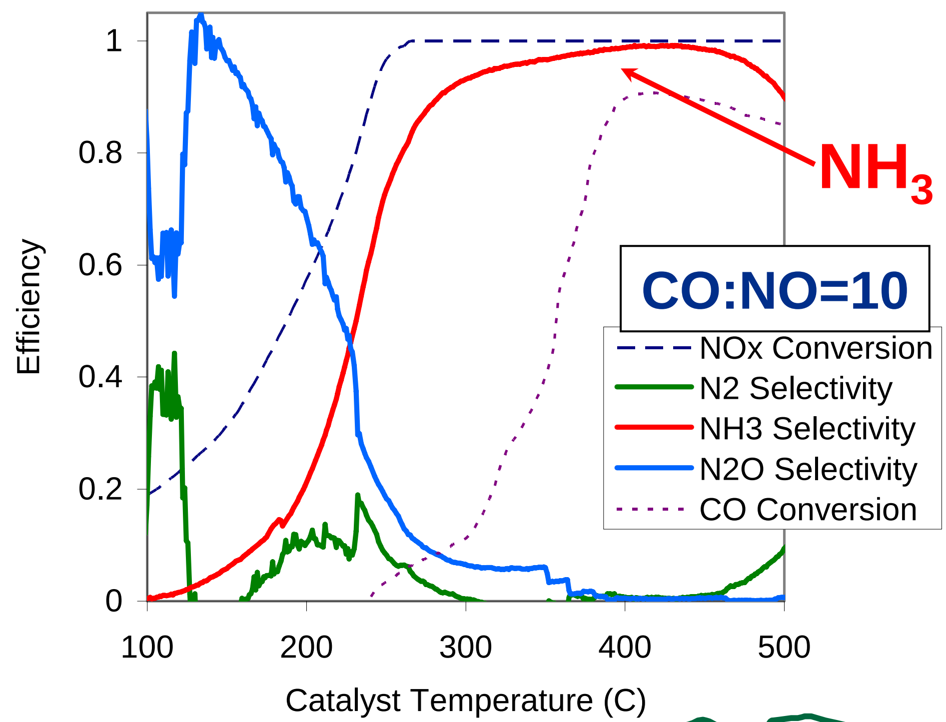
UEGO A/F



N_2 Selectivity Highly Dependent on Reductant:NOx Ratio

- **Bench Flow Reactor Temperature Programmed Reduction (TPR) Experiments at 100,000/hr SV**
- **Reducing Conditions: CO and NO Into Catalyst**
  - At CO:NO=1, N_2 Selectivity High – N_2 Preferred
  - At CO:NO=10, N_2 Selectivity Low – NH_3 Preferred
- **Same Trend Holds for H_2 Reductant and NOx as NO_2**
- **See Josh Pihl (U. of Wis.) Poster for More Details**





Theories for NH_3 Formation

- **N_2 and reductant (H_2, etc.) react to form NH_3 on precious metal site during regeneration**
  - No supporting data found to date
- **Isocyanate surface species formed on Pt plays role in NH_3 formation [Lesage et.al., *Phys. Chem, Chem. Phys*., 5 (2003)]**
  - 2 NCO + 3 H_2O ➔ 2 NH_3 + 2 CO_2 + 0.5 O_2 **[Rich: NCO ➔ NH_3]**
  - 2 NCO + O_2 ➔ N_2 + 2 CO_2 **[Lean: NCO ➔ N_2]**
  - Engine studies show reduced NH_3 formation via O_2 purge during regeneration
- **NH_3 formed from gaseous NOx released from catalyst in reactions with surrounding reductants (H_2, CO, etc)**
  - High dependence on reductant to NOx ratio observed
  - Bench reactor experiments show decay of NH_3 formation with time suggesting slow NOx release from catalyst is source of NH_3

No Supporting Data (first bullet)

Supporting Data Observed (second and third bullets)

Summary 2: Strategy Dictates N_2 Selectivity

- **NH_3 and N_2O can be formed during LNT regeneration**
  - **Produced from NOx stored on catalyst**

- **Selectivity toward N_2 vs. NH_3 is highly dependent on ratio of reductant to NOx during regeneration**
  - **It is critical to match reductant to NOx ratio in dynamic process**

- **Strategy details critical for minimal fuel penalty and optimal NOx reduction to N_2**

- **Lean-rich pulsing during regeneration gives lower NH_3 formation *AND* Equivalent NOx reduction**
  - **Transient analysis of tailpipe O_2 with SpaciMS shows:**
    - **O_2 purge during regeneration (supports isocyanate and other theories)**