Three Way Catalyst and Lean NO_x Trap Modeling for a Lean Burn SIDI Gasoline engine

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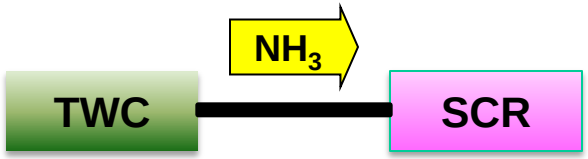
Outline

- Background and objectives
- $DeNO_x$ modeling
  - Three way catalyst (TWC)
  - Lean NO_x trap (LNT)
- Experimental setup
- Simulation results
- Summary

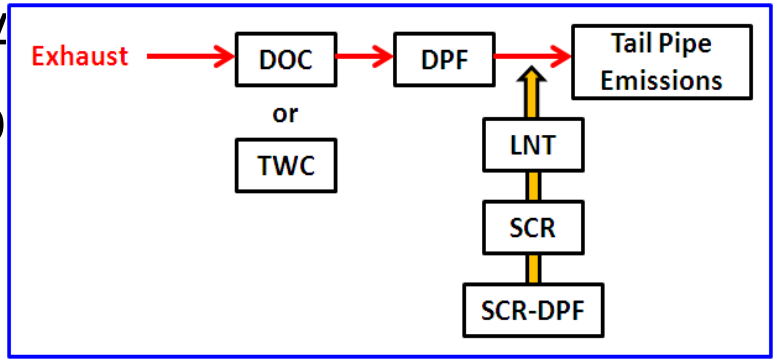
Background

- Lean-burned SIDI engines show great benefit on fuel efficiency and CO_2 reduction
  - Relatively higher nitrogen oxides (NO_x)
- Reduce dependency on conventional fuels
  - Flexible fuel (fuel neutral) engines (e.g. gasoline & ethanol blends)
- Worldwide tightening emission regulations for light duty vehicles
  - NO_x: Tier 2 Bin 5: 70 mg/mile;
  - LEV III: (NO_x+NMOG) 30 mg/mile in 2025;
  - Euro 5+: 96 mg/mile
- Passive ammonia SCR system



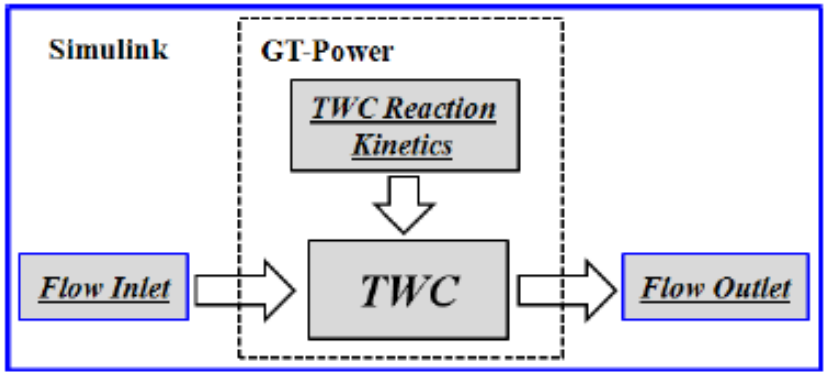
Objectives: Fuel-neutral AT Modeling

- Development of $DeNO_x$ models with global kinetics
  - Reasonable accuracy over a wide range of (fuel neutral) engine exhaust conditions
  - NH_3 kinetics (global)
- Study the overall engine aftertreatment system (e.g. $DeNO_x$ + DeSoot)
  - Interactions among different A
  - Feedback to the engine perfo



TWC Reaction Kinetics

- A single-channel, one-dimensional model
- Using GT-Power to solve conservation equations and chemistry
- 20 surface reactions (Ramanathan et al. 2011) (in Langmuir-Hinshelwood structure)
  - Include kinetics for oxidation of CO, HC, and NO to CO_2, H_2O and NO_2
  - NO_x reduction reactions
  - Water-gas shift and steam
  - Oxygen storage reactions
  - NH_3 kinetics
  - Proposed N_2O kinetics

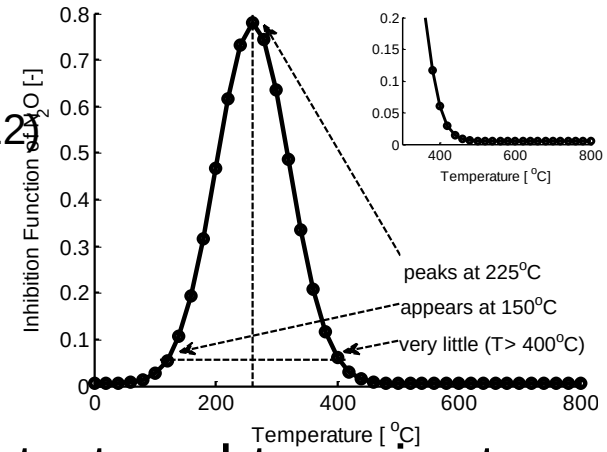


The detail of the TWC kinetics is reported in SAE paper 2013-01-1572

NH_3 and N_2O

NH_3

- Commonly formed during the rich operation of TWC/LNT
- Global mechanism (Ramanathan et al. 2012)
  - $NO+2.5H_2 \rightarrow NH_3+H_2O$
  - $NH_3+1.25O_2 \rightarrow NO+1.5H_2O$
  - $NH_3+1.5NO \rightarrow 1.25N_2+1.5H_2O$

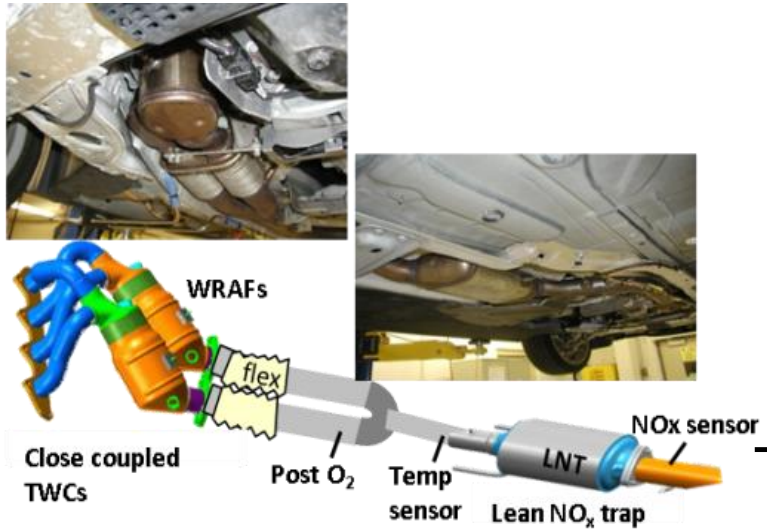


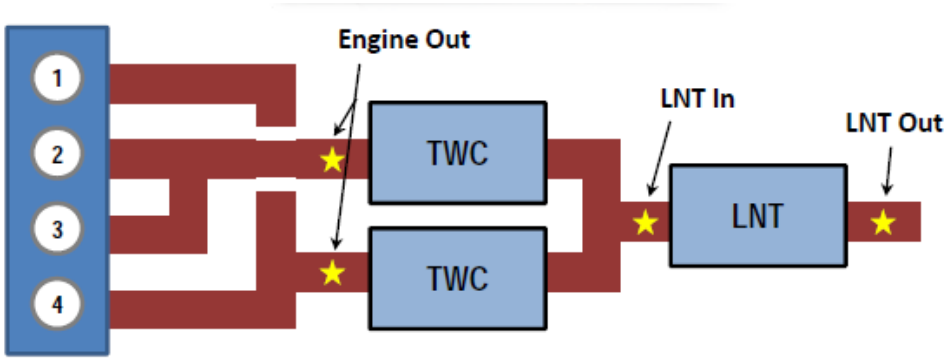
N_2O

- Predominantly formed during <u>cold start</u> and <u>transient</u> operations
  - A byproduct of NO_x reduction by HCs during light-off
- Global mechanism
  - $NO+1/18C_3H_6 \rightarrow 0.5N_2O+1/6CO_2+1/6H_2O$
  - $N_2O+1/9C_3H_6 \rightarrow N_2+1/3CO_2+1/3H_2O$

Experimental Setup

- Lean gasoline vehicle (BMW120i – 2.0L L4) on a chassis dynamometer at ORNL (Parks et al. 2011)

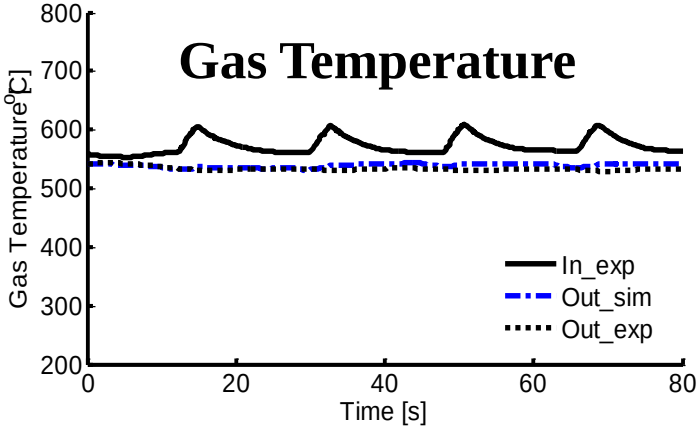


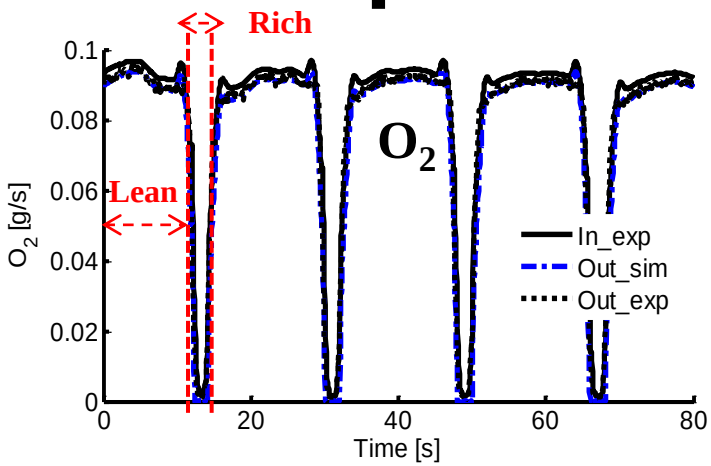


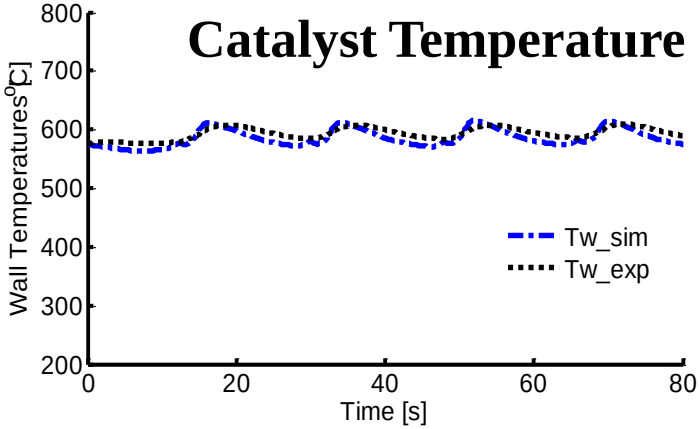
Three different types of data for model validations

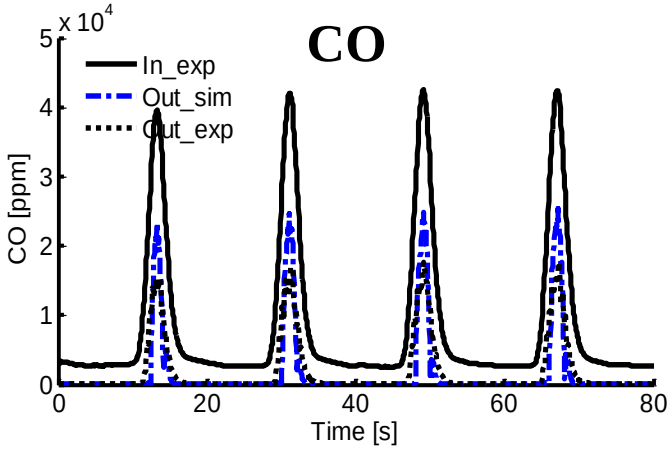
- Time-resolved (transient lean/rich cycle)
- Time-averaged (steady state lean/rich cycle)
- Transient driving cycle

Time-resolved Data: 3500 rpm 30%



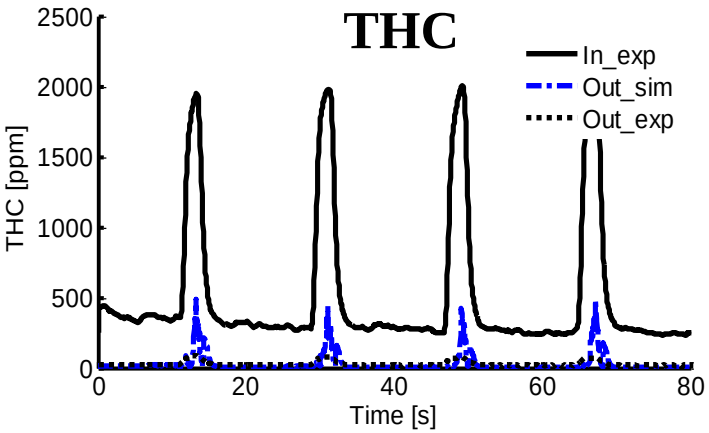


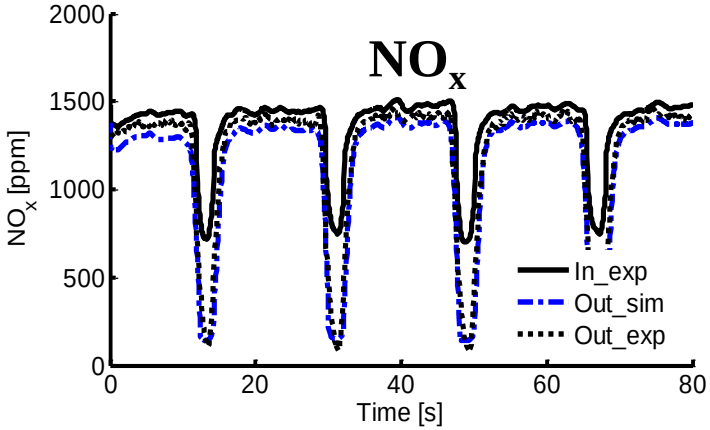


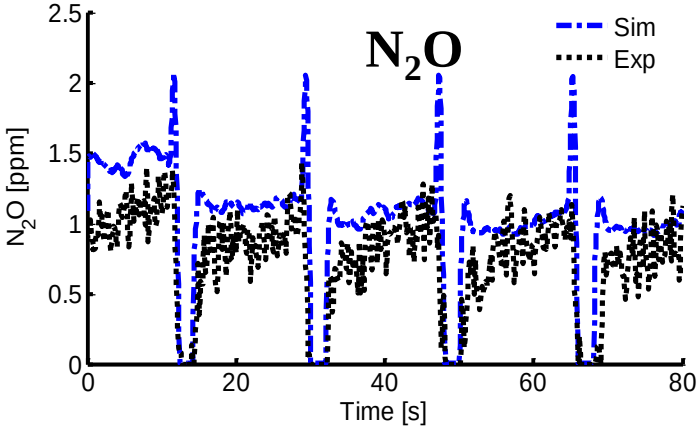


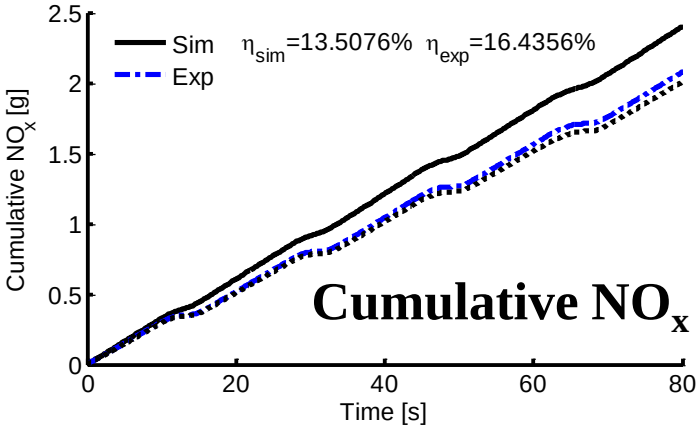
- Gas & Catalyst temperatures match data
- O_2 and CO predictions are good

3500 rpm 30%: THC/NO_x/N_2O



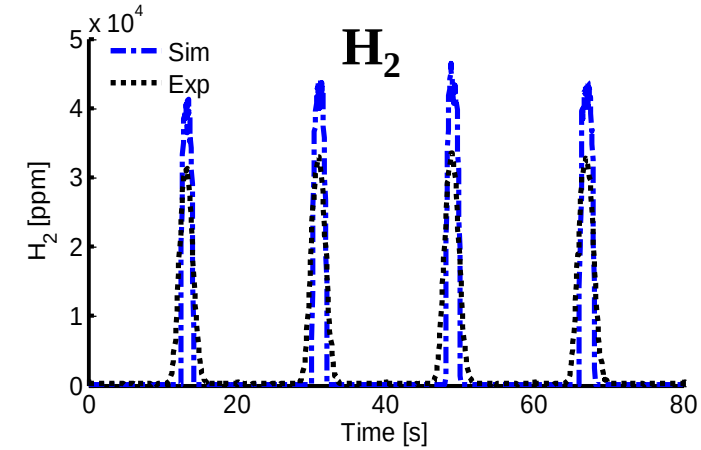


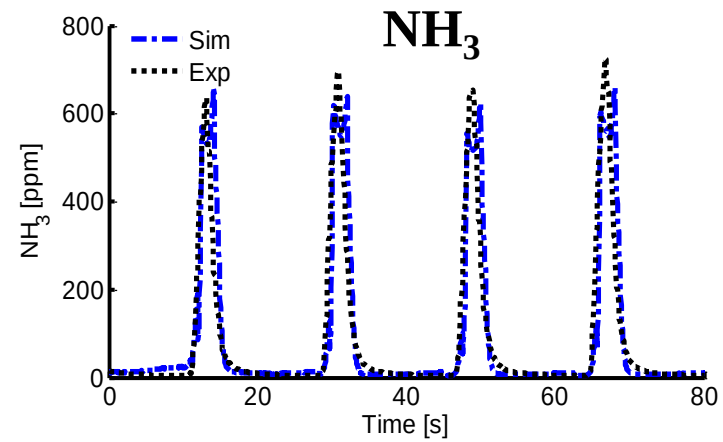


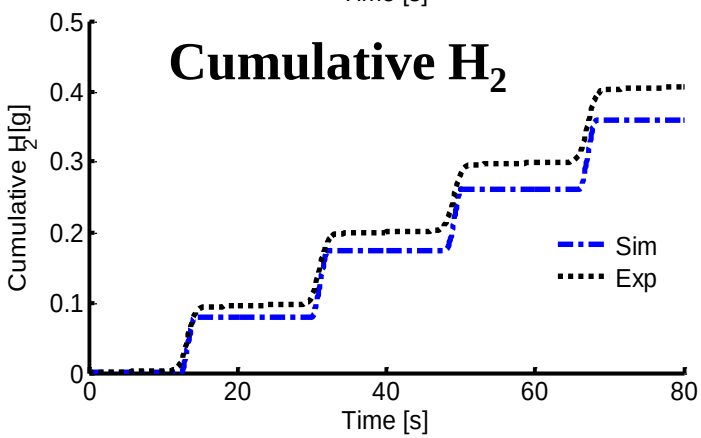


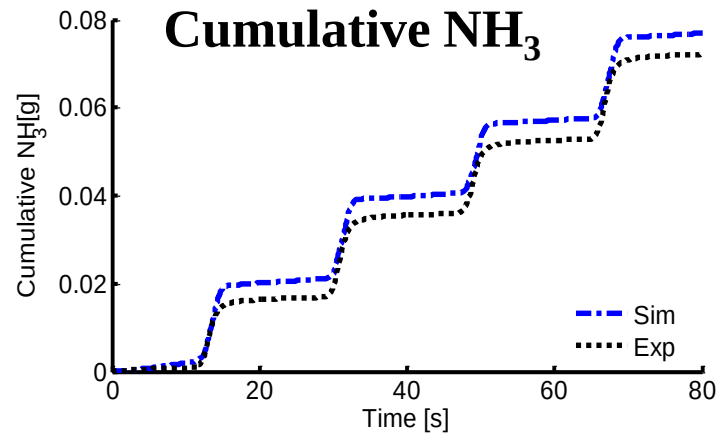
- Good predictions of THC
- Transient N_2O is captured
- Instantaneous NO_x and accumulative NO_x are very comparable

3500 rpm 30%: H_2 & NH_3







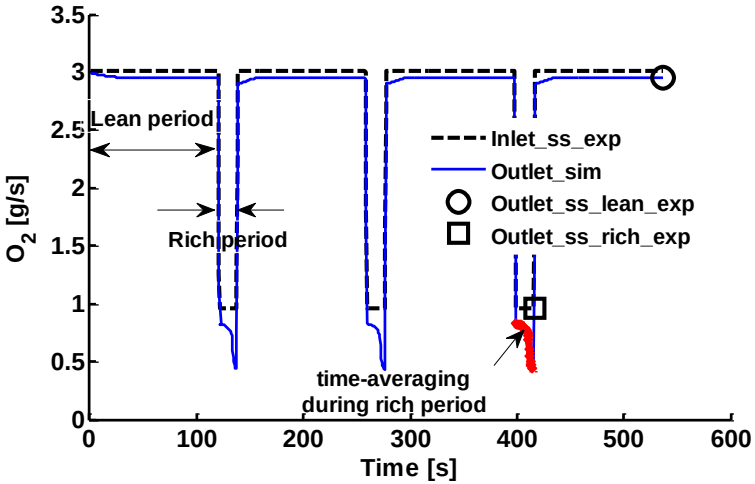


- Slightly high H_2 peak; enough H_2 compared to NO_x
- Instantaneous NH_3 and accumulative NH_3 are very comparable
- NH_3/inlet NO_x = 0.072/2.4 ~ 3%

Time-averaged Data

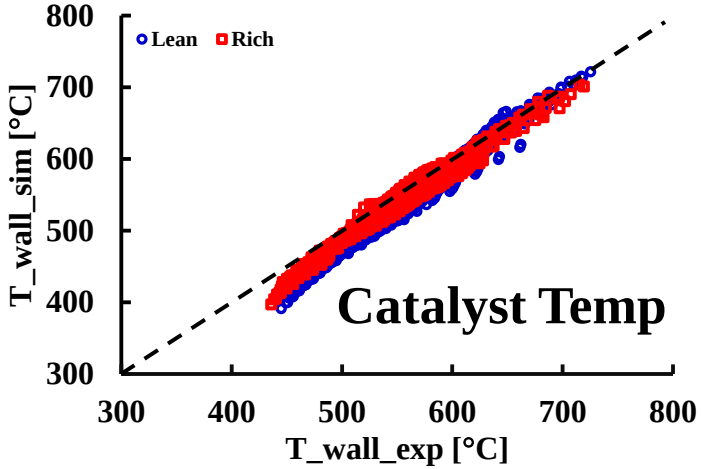
- Speed: 1500 to 4500, Load: 0~120 N·m
  - Total # of steady state operating conditions: **1550** (lean+rich)

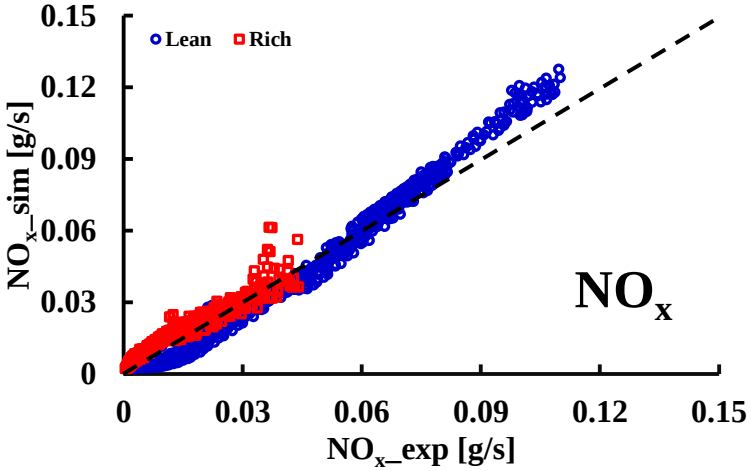
Exhaust	Lean	Rich
Mass flow rate [g/s]	**6.7 ~ 72.1**	**7.0 ~ 46.8**
Space velocity [1/s]	246.5 ~ 3737.4	291.0 ~ 2483.1
Exhaust temp [°C]	**336.6 ~ 716.4**	**412.7 ~ 681.7**
Engine equiratio [-]	**0.46 ~ 0.75**	**1.15 ~ 1.25**
NO_x [ppm]	156 ~ 2527.6	482.6 ~ 1532.7
CO [ppm]	264.6 ~ 4125.7	13937 ~ 34680
HC [ppm]	19.4 ~ 870.5	294.7 ~ 1176.4

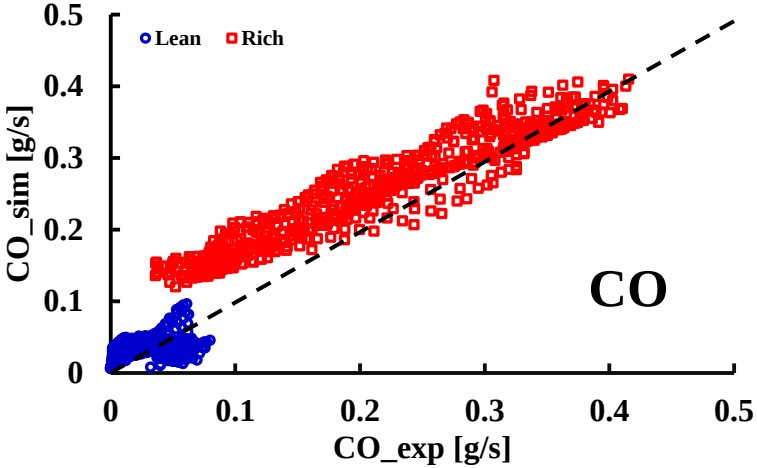


  - <u>No detailed instantaneous species concentrations</u>
  - <u>Examining the kinetics in a wide window of exhaust conditions</u>

Time-averaged Data



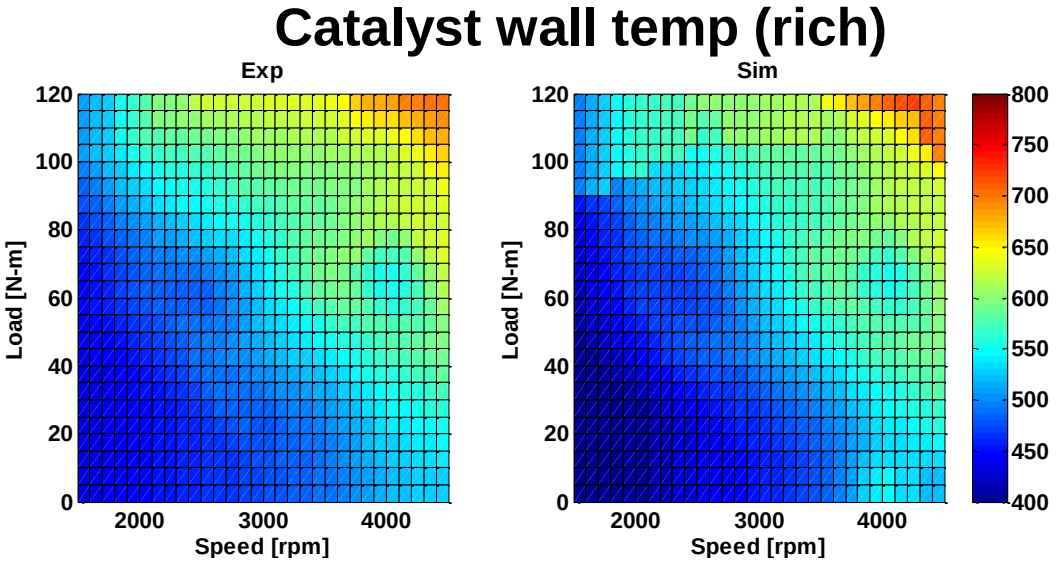


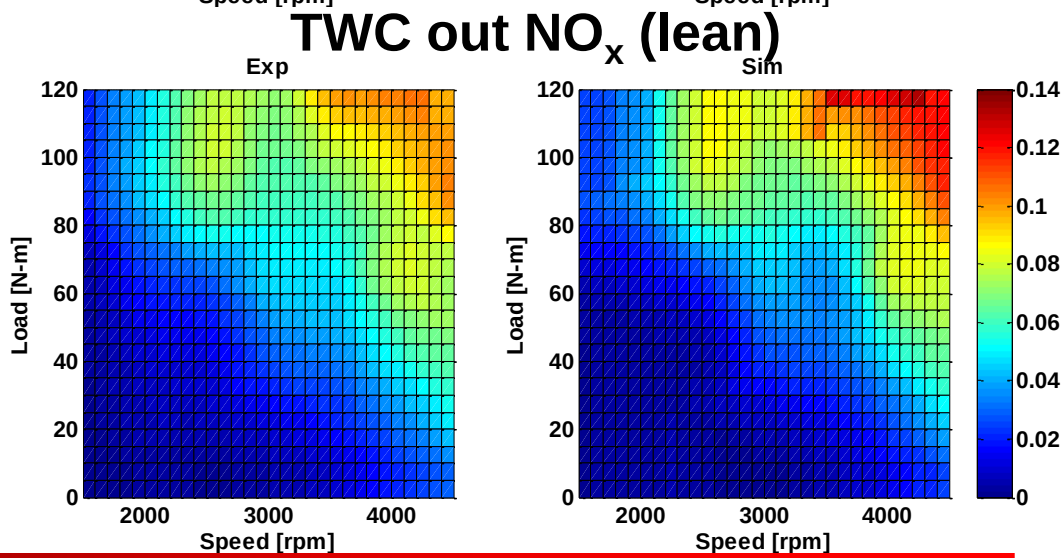


- Good agreement of temperatures and NO_x emissions at lean & rich
- Some discrepancy in CO
  - Consistent with under-predictions of temperatures

Phasing Comparisons

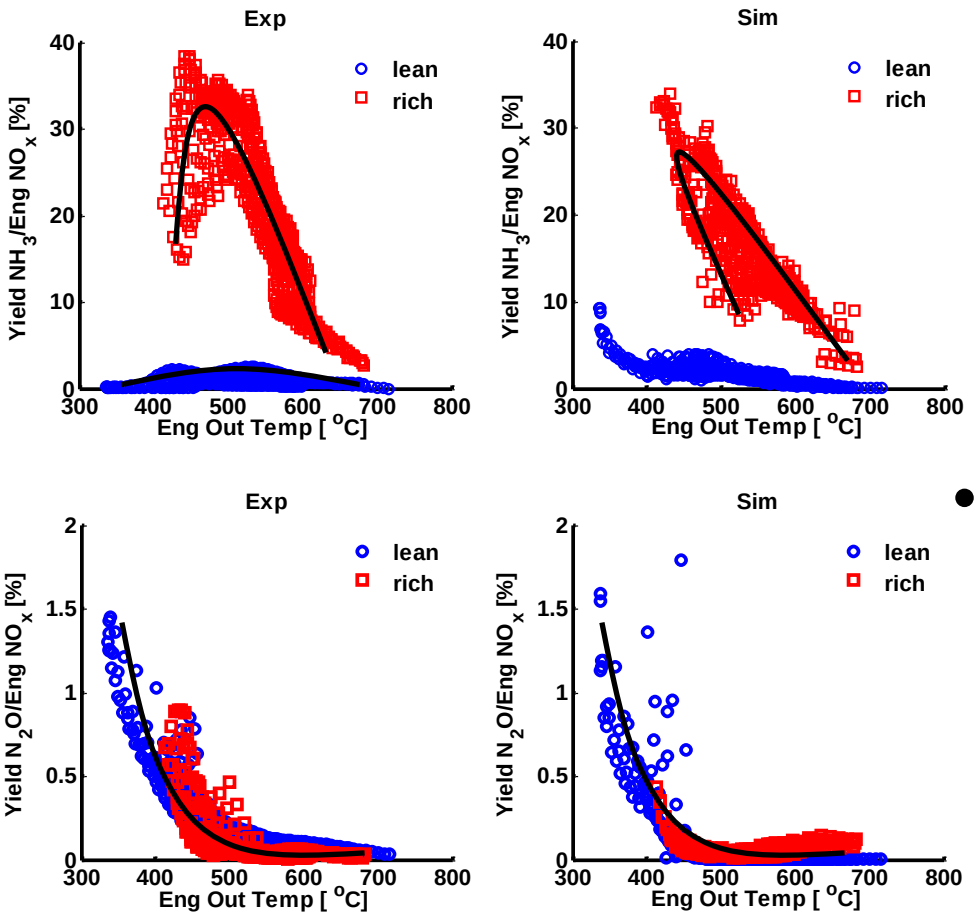
- A good agreement between predicted catalyst temperature, NO_x and experimental data





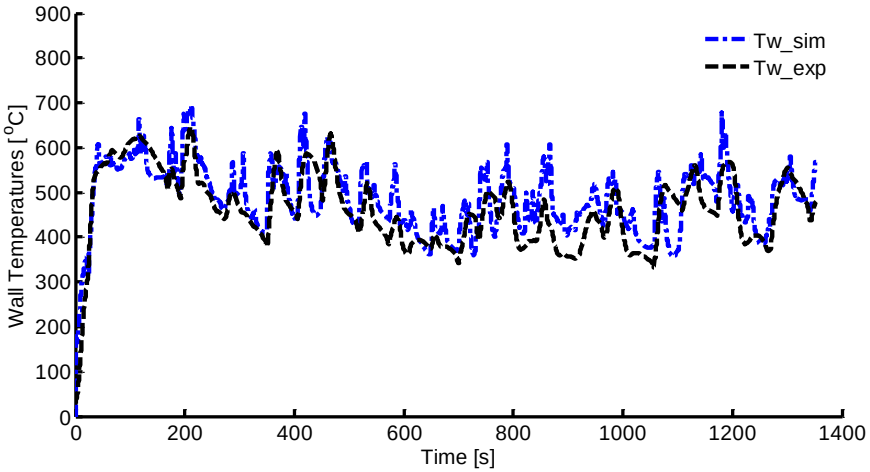
NH_3 & N_2O kinetics

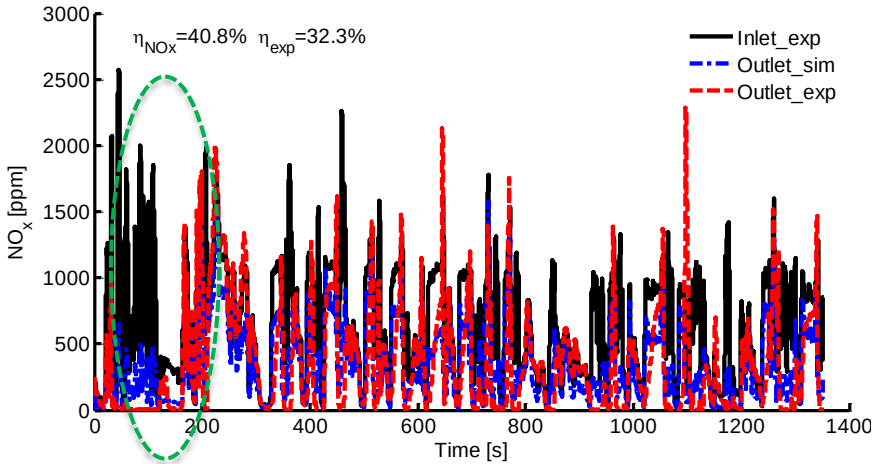
$$\alpha = \frac{\text{yield } NH_3 \text{ or } N_2O}{\text{engine out } NO_x} \times 100\%$$



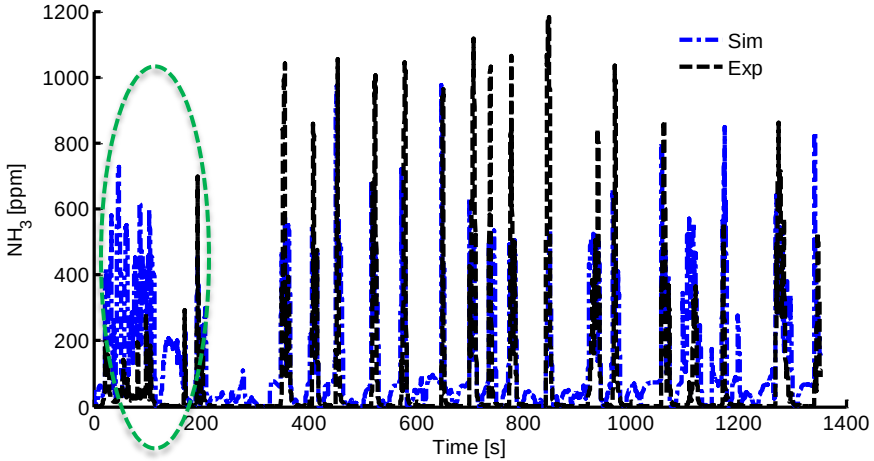
- NH_3
  - mainly formed at rich
  - Some discrepancy at low exhaust temperatures (<400 °C)
  - Over-predicted at lean
- N_2O
  - Independent of AFR
  - Significantly depends on exhaust temperature
    - Favors at low temp

FTP Cycle (cold start)





- Model captures the trends of catalyst temp, NO_x and NH_3
- Higher NO_x and NH_3 in the first 200 seconds
  - Might be some NOx storage functionality in the TWC (not in the model)

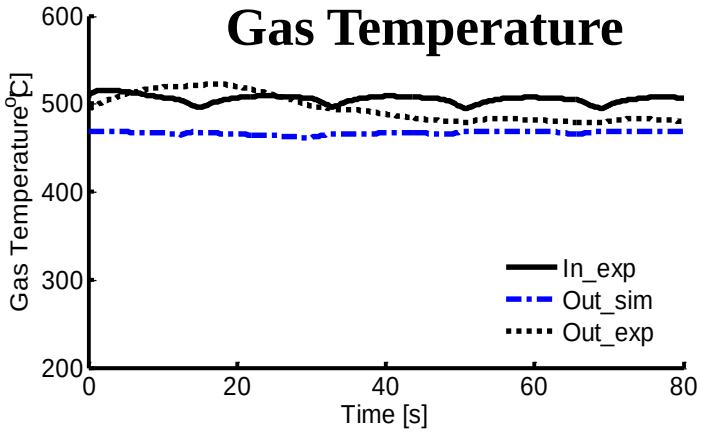


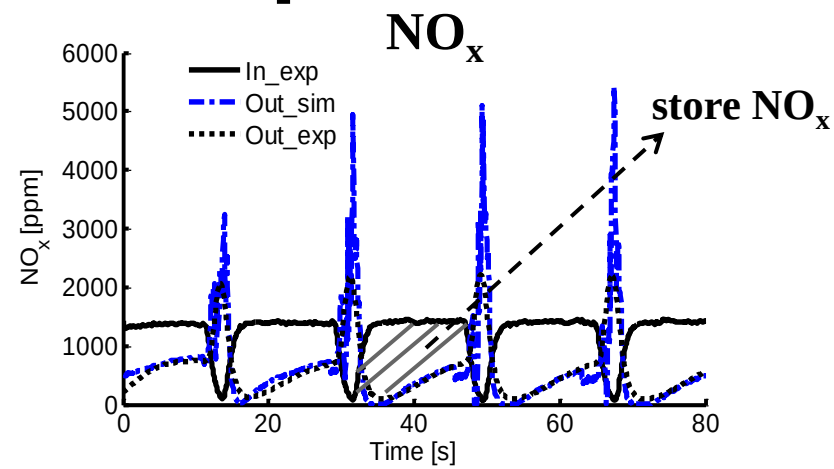
LNT Kinetics

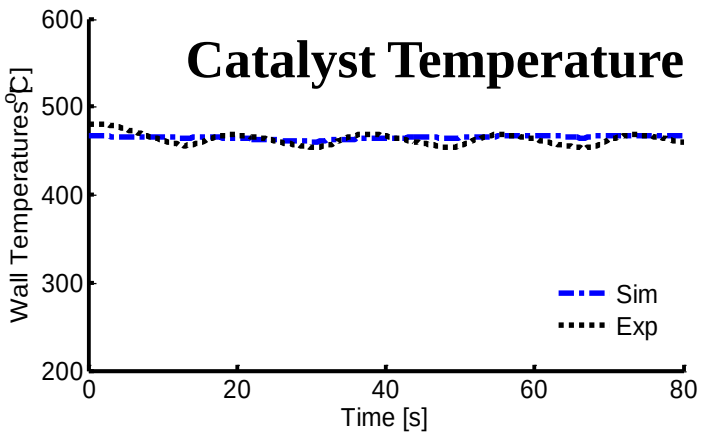
	LNT kinetics	
1	$CO+0.5O_2 \rightarrow CO_2$	Oxidation reactions
2	$C_3H_6+4.5O_2 \rightarrow 3CO_2 + 3H_2O$	
3	$C_3H_8+ 5O_2 \rightarrow 3CO_2 + 4H_2O$	
4	$H_2 + 0.5O_2 \leftrightarrow H_2O$	
5	$NO+0.5\ O_2 \rightarrow NO_2$	NO NO_2 transition
6	$CO + NO \rightarrow CO_2 + 0.5N_2$	NO reduction
7	$1/9C_3H_6+NO \rightarrow 1/3CO_2+1/3H_2O+1/2N_2$	
8	$0.5BaCO_3+NO+0.75O_2 \rightarrow 0.5Ba(NO_3)_2+0.5CO_2$	NO_x adsorption
9	$0.5BaCO_3+NO_2+0.25O_2 \rightarrow 0.5Ba(NO_3)_2+0.5CO_2$	
10	$0.5Ba(NO_3)_2+1.5CO \rightarrow 0.5BaCO_3+NO+CO_2$	NO_x desorption
11	$Ba(NO_3)_2+1/3C_3H_6+CO_2 \rightarrow BaCO_3+2NO+H_2O$	
12	$Ba(NO_3)_2+8H_2+CO_2 \rightarrow 2NH_3+BaCO_3+5H_2O$	NH_3 formation from nitrates
13	$NH_3+0.5Ba(NO_3)_2+0.5CO_2 \rightarrow N_2O+0.5BaCO_3+1.5H_2O$	N_2O formation from nitrates
14	$NH_3+4NO \rightarrow 2.5N_2O+1.5H_2O$	N_2O formation
15	$NO+2.5H_2 \rightarrow NH_3+H_2O$	NH_3 formation
16	$NH_3+1.25O_2 \rightarrow NO+1.5H_2O$	NH_3 oxidation
17	$NH_3+1.5NO \rightarrow 1.25N_2+1.5H_2O$	NH_3 and NO

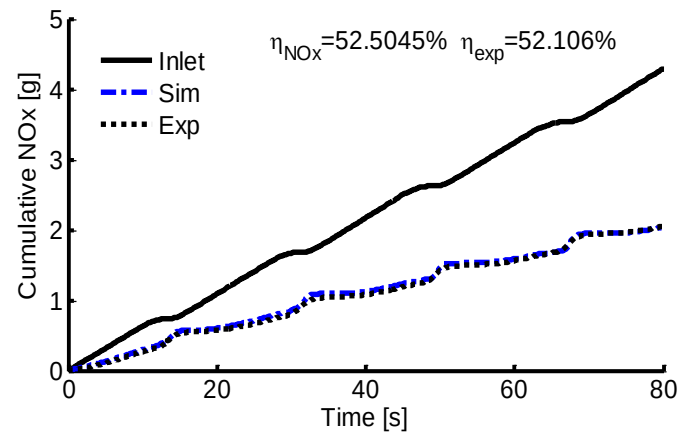
- Total 17 reactions (Olsson et al. 2005)

LNT Validation: 3500 rpm 30%



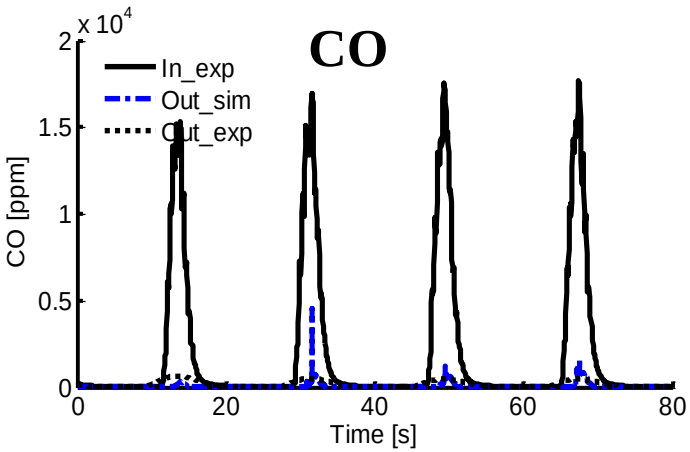


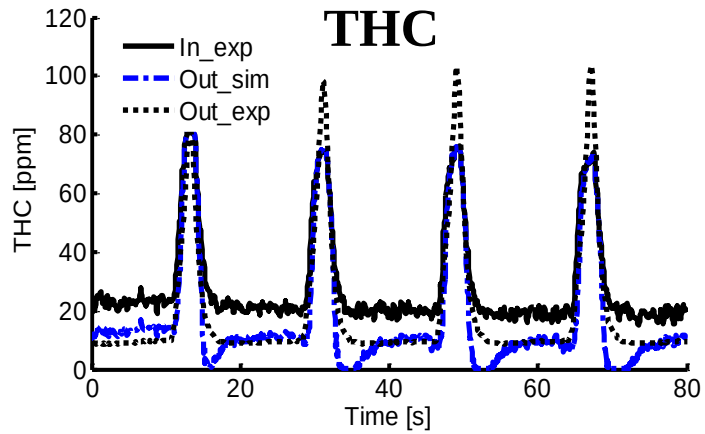


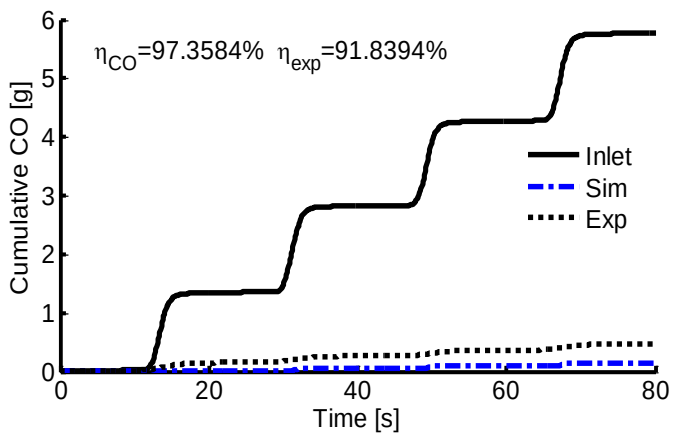


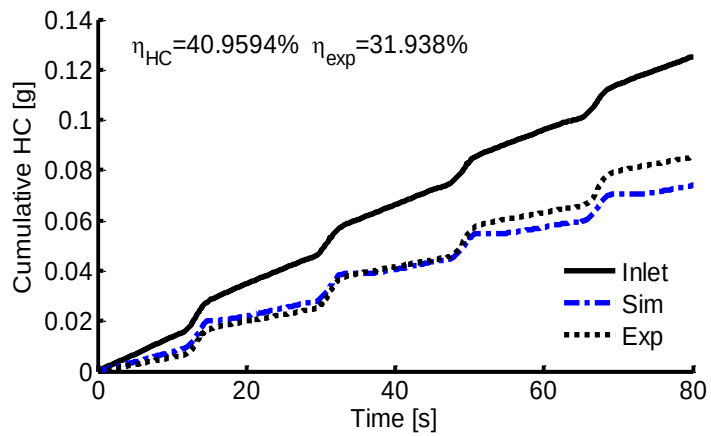
- Temperatures match data
- NO_x adsorption & desorption & reduction are well captured

LNT Validation: CO & THC



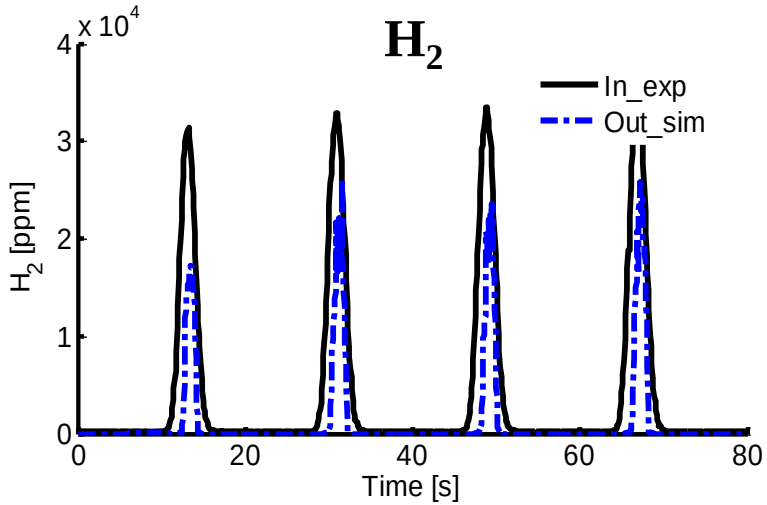


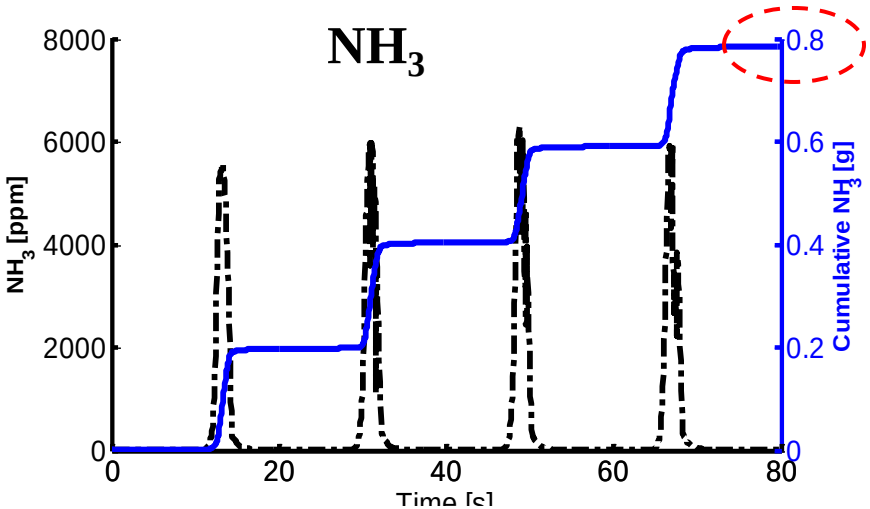




- Slightly lower CO but with reasonable overall conversion rate
- Both instantaneous and accumulative HCs are good

LNT Validation: H_2 & NH_3





- A large amount of H_2 from TWC
- Peak NH_3 is higher than NO_x (6000 vs. 5000)
  - Generated from nitrates (different from TWC)
  - NH_3/inlet NO_x = 0.8/4.2 ~ 20%

Summary

A TWC and a LNT model were developed with global kinetics and validated using experimental data from a lean burn DISI engine

- TWC
  - Validated over a wide range of exhaust conditions
  - Temperature dependences of the conversion rate of NH_3 and N_2O from NO_x were examined
- LNT
  - NO_x adsorption, desorption and reduction were well captured
  - NH_3 formation from LNT could be much more than TWC
  - Need NH_3 kinetics from nitrates

<u>The $DeNO_x$ models are able to predict the temperatures as well as species concentration with a good accuracy.</u>

Acknowledgment

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- ORNL: Emissions & Catalysis Research Group
  - Monthly teleconferences
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Reference

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Thank You !

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