# System Simulations of Hybrid Electric Vehicles with Focus on Emissions


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Sponsor : Lee Slezak
Vehicle Technologies Program
U.S. Department of Energy




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# Background

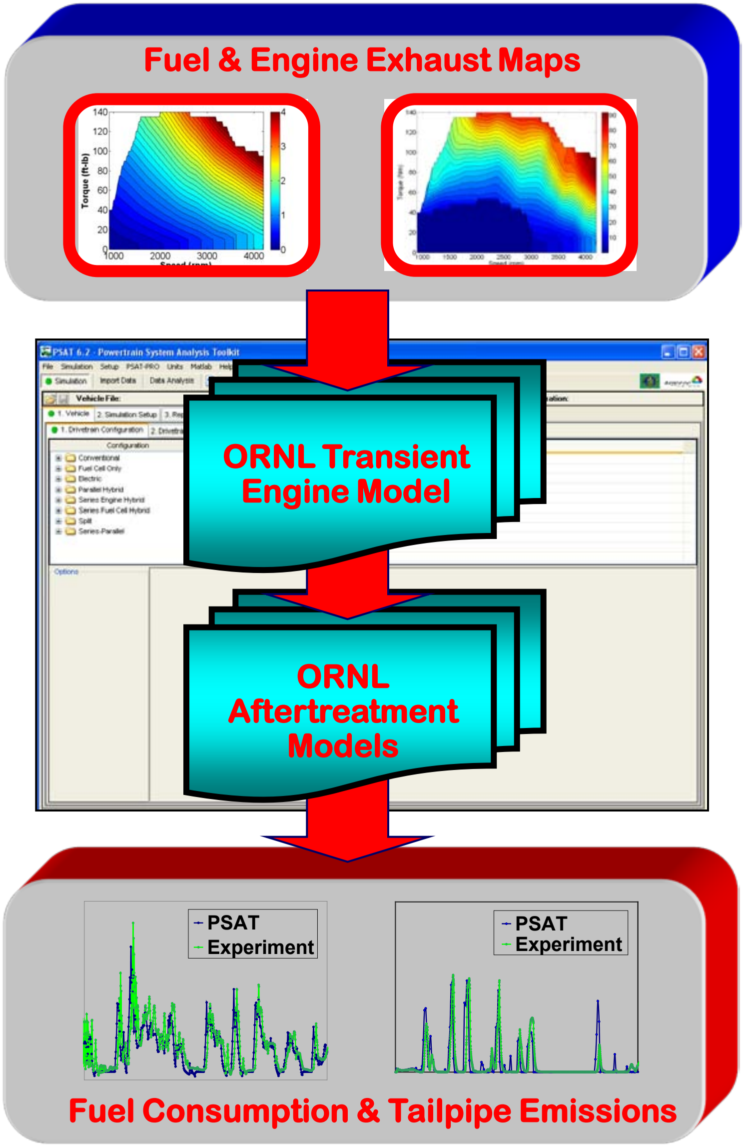
- **US fuel efficiency policy in 2009**
  - Average fuel economy standard of 35.5 mpg in 2016
  - Nearly 10 miles per gallon better than the current average
- **Hybrid electrical vehicles (HEVs) technology**
  - HEV with stoichiometric engines or lean-burn engines
  - Challenges for emissions control in HEVs
    - Intermittent engine operation
    - A longer cold start at the beginning
    - Multiple cold starts during driving cycles
    - For diesel HEV, minimize fuel penalty without hurting emissions
- **DOE Vehicle Systems Analysis Technical Team (VSATT)**
  - Powertrain System Analysis Toolkit (PSAT) developed at ANL
  - ORNL is tasked with studying after-treatment options

# VSATT Modeling Team

- **ORNL team : Stuart Daw, Kalyan Chakravarthy, Zhiming Gao**
- **Testing data support: CLEERS, OEMs, National Labs (ORNL/PNNL)**
- **Our mission is to evaluate the technologies and performance characteristics of advanced automotive powertrain components and subsystems in an integrated vehicle systems context.**
  - **Transient engine model and engine maps**
  - **Diesel Oxidation Catalyst (DOC)**
  - **Diesel Particulate Filter (DPF)**
  - **Lean NOx Traps (LNT)**
  - **Selective Catalytic Reduction (SCR)**
  - **Three-Way Catalyst (TWC)**
  - **HEV & Plug-in HEV**

# HEV simulations are integrated with transient engine and aftertreament models

- **Vehicle simulation framework**
  - PSAT- ANL developed forward-looking simulation package
  - Transitioning to AUTONOMIE, which will replace PSAT
- **ORNL transient engine model**
  - Estimate transient engine exhaust properties and fuel economy based on corrections to steady-state maps
- **Aftertreatment models**
  - Low-order, physically consistent
  - TWCs, DOCs, LNTs, DPFs, SCRs
  - Development ongoing ORNL/PNNL



# ORNL transient engine model demonstrates a good prediction for engine-out emissions, exhaust temperature, and fuel economy associated with cold and warm starting conditions

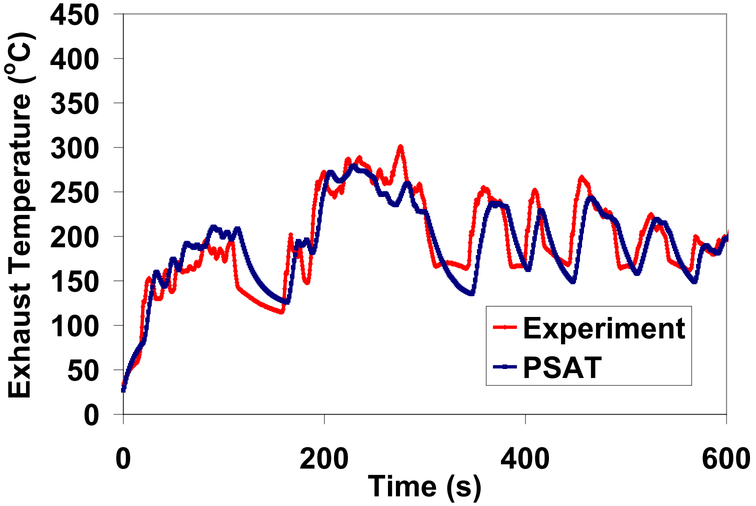
**Example Simulation:**

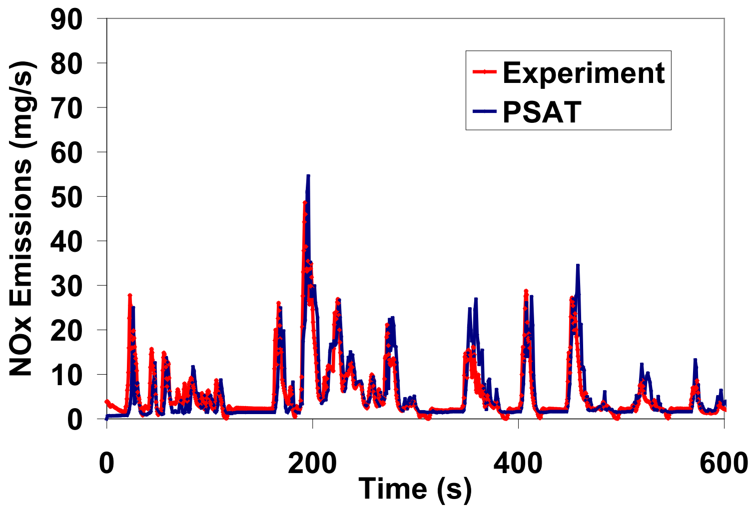
- Mercedes 1.7L diesel engine
- A UDDS cycle with cold start
- Civic vehicle configuration

**Results** :

- Integrated mileage and engine-out emissions*

| | Mileage (mpg) | CO (g/mi) | HC (g/mi) | NOx (g/mi) | PM (g/mi) |
|---|---|---|---|---|---|
| Exp | 40.3 | 2.28 | 0.54 | 0.74 | 0.14 |
| Simu | 40.4 | 2.29 | 0.54 | 0.89 | 0.12 |

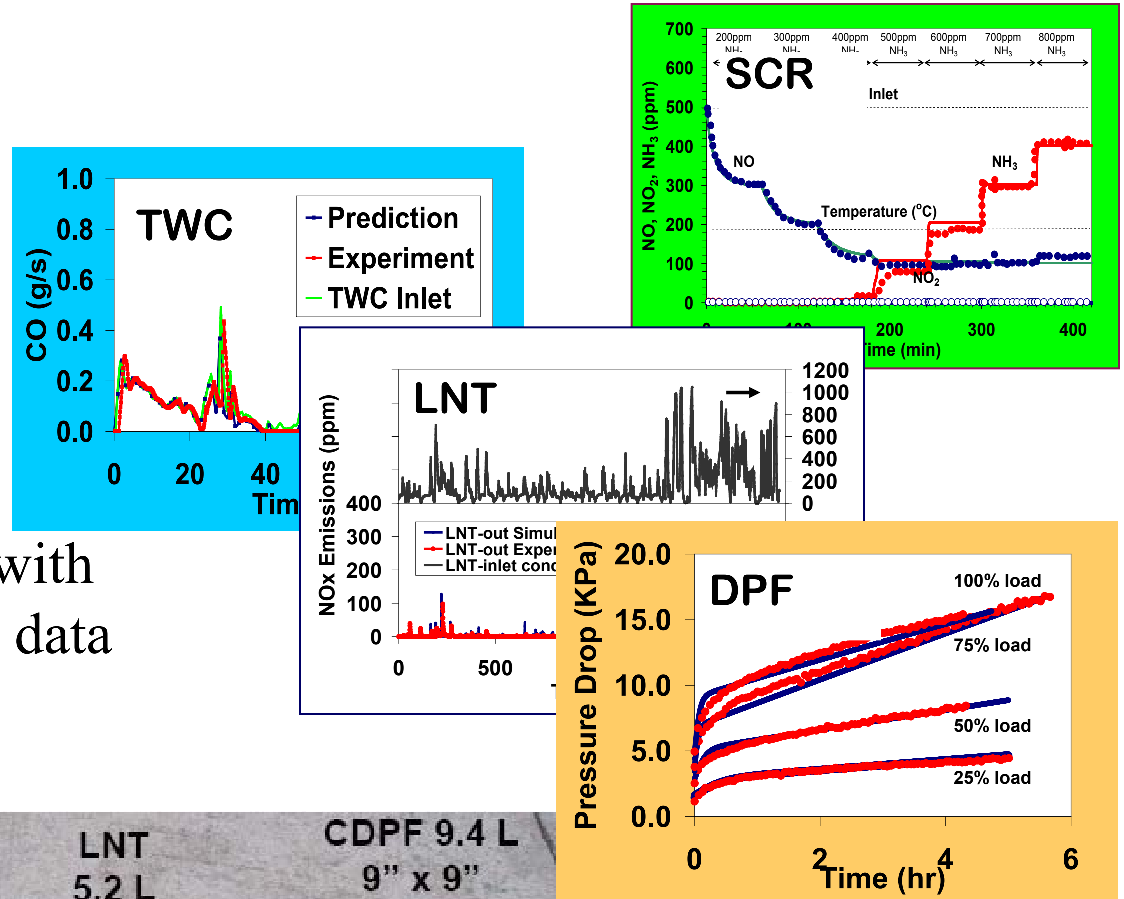



* **Int. J. Engine Res., 11(3), 2010, 137-151**

# Simulated Aftertreatment System

- Stoichiometric engines
  - 1D TWC
- Lean-burn engines
  - 1D LNT (SAE 2010-01-0082)
  - 1D SCR (Cu-ZMS-5)
  - DOC/LNT/CDPF
  - DOC/SCR/CDPF
- The models were validated with public domain experimental data




# Results and Analysis

# Std. gasoline vs. diesel baseline HEV comparison indicates large diesel fuel economy benefit

## Simulation parameters:

- 1450 kg HEV
- One UDDS cycle at hot start
- 1.3 kWhr battery charge (65%)
- 1.5-L gasoline & diesel engines
- No emissions control device

## Diesel vs. Gasoline HEV:

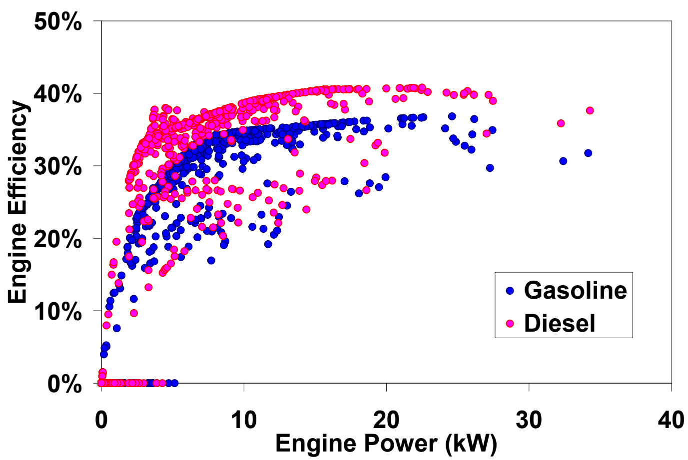
+13% energy density for diesel (+13%)

+6% engine efficiency for diesel (+6%)

= +19% fuel economy for diesel (mpg)

Gasoline HEV without any aftertreatment:
- 70.7 mpg gasoline (71.2mpg @ SAE 2007-01-0281)
- 34% cycle average engine efficiency

Diesel HEV without any aftertreatment:
- 84.2 mpg diesel
- 36% cycle average engine efficiency



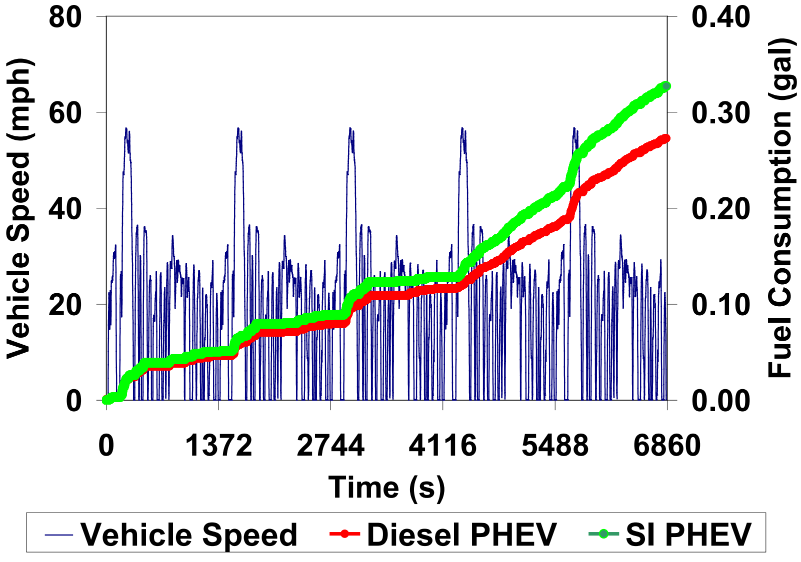

## Engine-out Emissions

| Engine | CO | HC | NOx | PM |
|---|---|---|---|---|
| Gasoline (g/mi) | 3.74 | 0.65 | 1.76 | 0.00 |
| Diesel (g/mi) | 0.44 | 0.11 | 1.14 | 0.62 |

# PHEV baseline comparison also indicates large potential diesel efficiency benefit similar to HEV

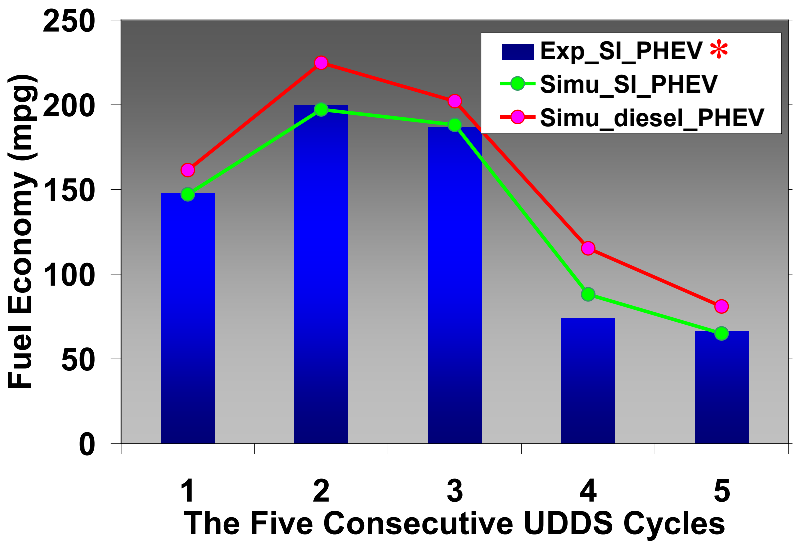
**Simulation condition:**

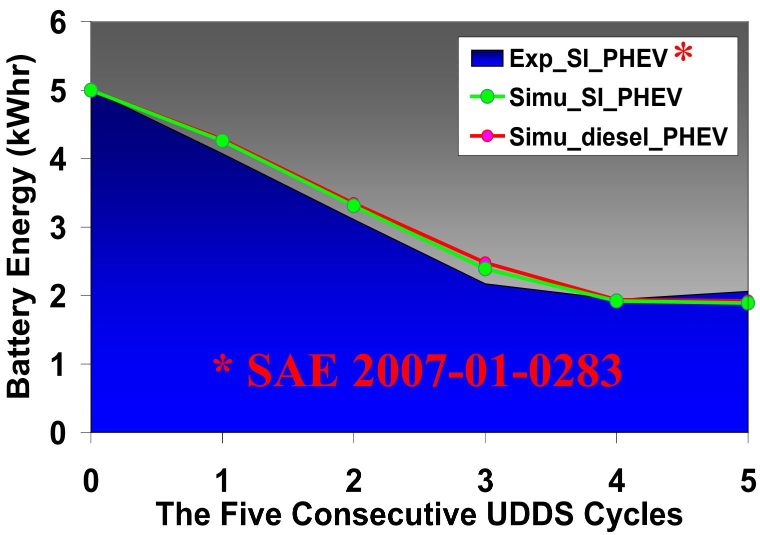
- PHEV (1450kg HEV+120kg battery)
- Cold start, 5 kWh charge (100%)
- 5 consecutive UDDS cycles
- 1.5-L gasoline and diesel engines
- No emissions control device




**Results:**

- Overall 19.9% better mpg for diesel (6% higher energy efficiency)

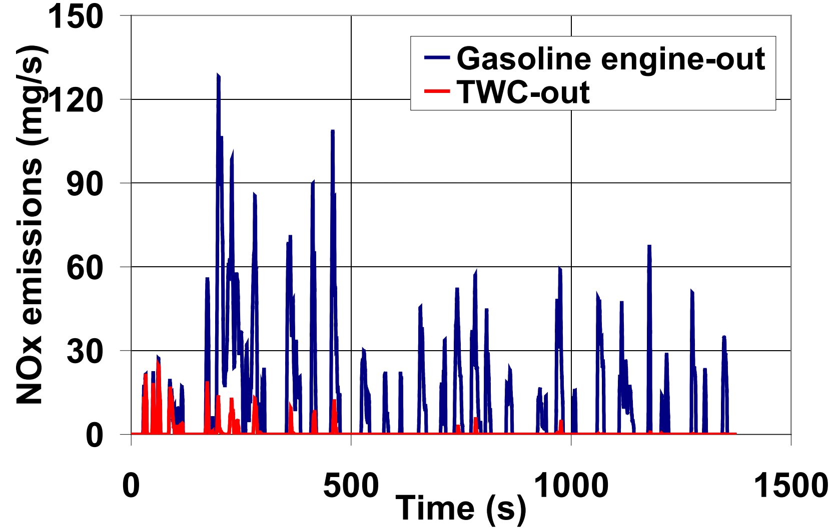


# However, lean NOx control has a big impact on expected diesel HEV efficiency advantage

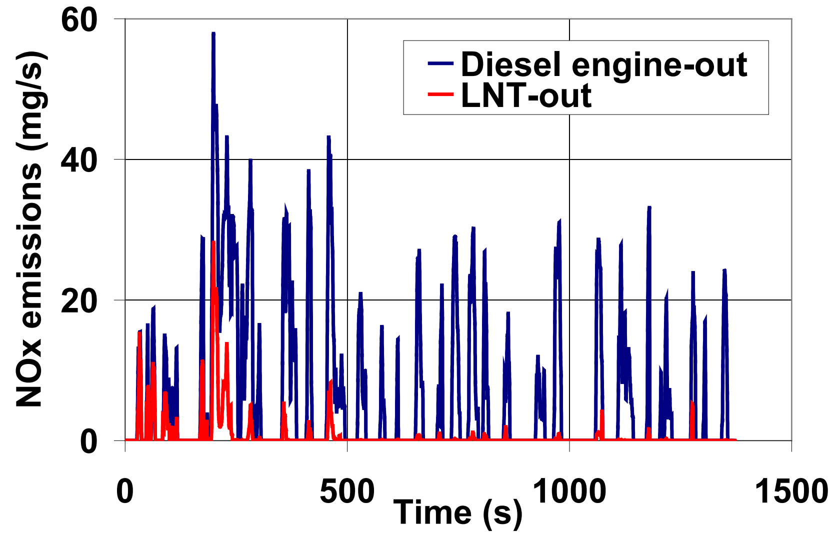
**Simulation parameters:**

- 1450kg HEV 1.3 kWhr battery (65% charge)
- Cold start UDDS drive cycle
- 1.5-L gasoline w/ 2.2-L TWC
- 1.5-L diesel engines w/ 2.4-L LNT
- Engine fueling modulation for LNT regeneration (e.g. 60s lean vs. 3 rich)




**Results:**

- 78.8 mpg diesel vs. 67.3 mpg gasoline
- 0.12 g/mile NOx vs. 0.12g/mile NOx
- LNT fuel penalty for diesel: 2.8%
- With LNT diesel efficiency advantage just over 3%

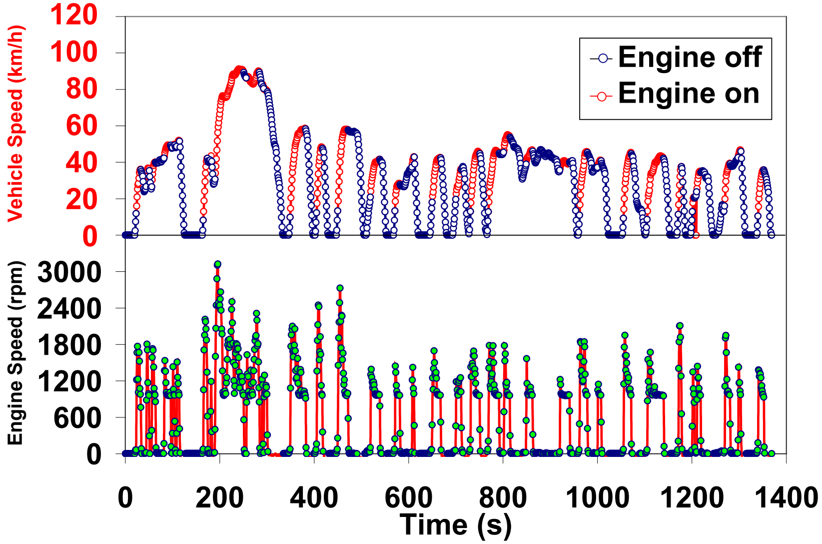



**LNT fuel efficiency penalty has spurred interest in SCR NOx control**

# Urea SCR saves diesel efficiency advantage, but causes extra $NH_3$ slip and a slightly less NOx reduction

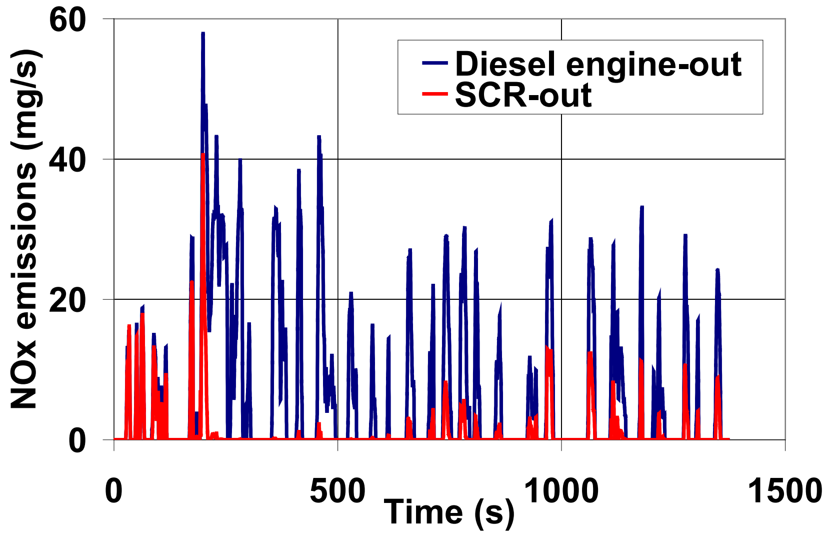
## Simulation parameters:

- 1450kg HEV
- Cold start UDDS drive cycle
- 1.3 kWhr battery (65% charge)
- 1.5-L diesel engines w/ 2.4-L SCR
- Urea inj. for SCR (1:1 $NH_3$ to NO)
- No $NH_3$ slip control for SCR




## Results:

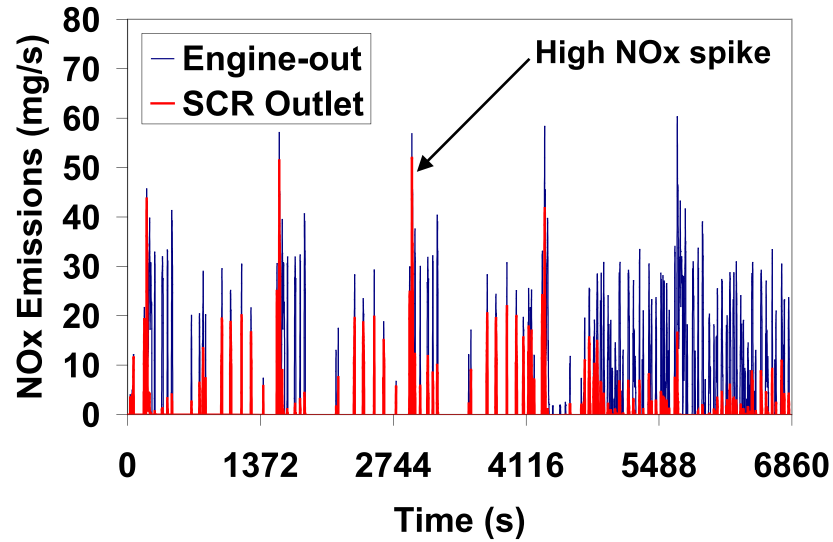
| | TWC | LNT | SCR |
|---|---|---|---|
| Tailpipe NOx (g/mi) | 0.12 | 0.12 | 0.20 |
| Fuel Economy (mpg) | 67.3 | 78.8 | 80.9 |
| Fuel penalty (%) | 0.00 | 2.80 | 0.00 |
| $NH_3$ slip (g/mi) | 0.00 | 0.00 | 0.04 |



# We are using this SCR model to compare PHEVs with different NOx control technologies

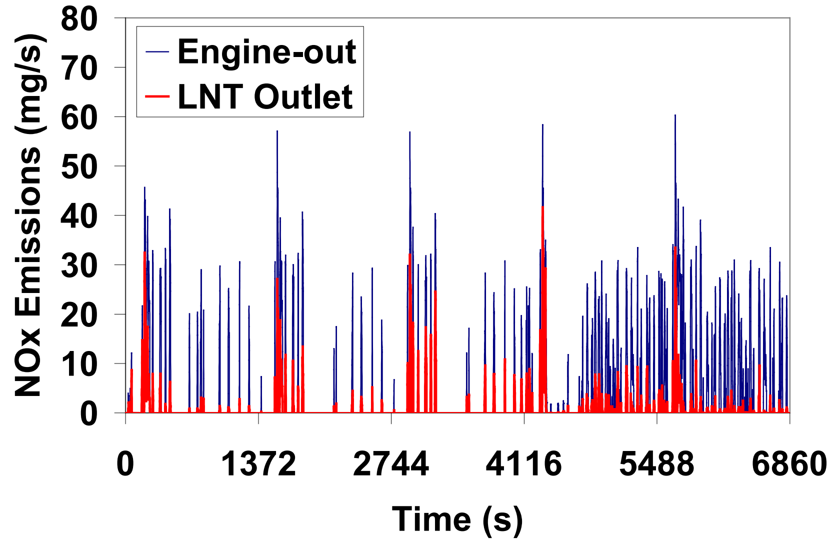
## Simulation parameters:

- PHEV powered by 1.5-L diesel engine
- 5 kWh, 24 Ah battery charge (full charge)
- 5 UDDS cycles beginning with cold start
- 2.4-L LNT, 2.4-LUrea SCR
- LNT regeneration: 60s lean vs. 3 rich
- Urea inj. for SCR (1:1 $NH_3$ to NO)
- No $NH_3$ slip control for SCR




## Results:

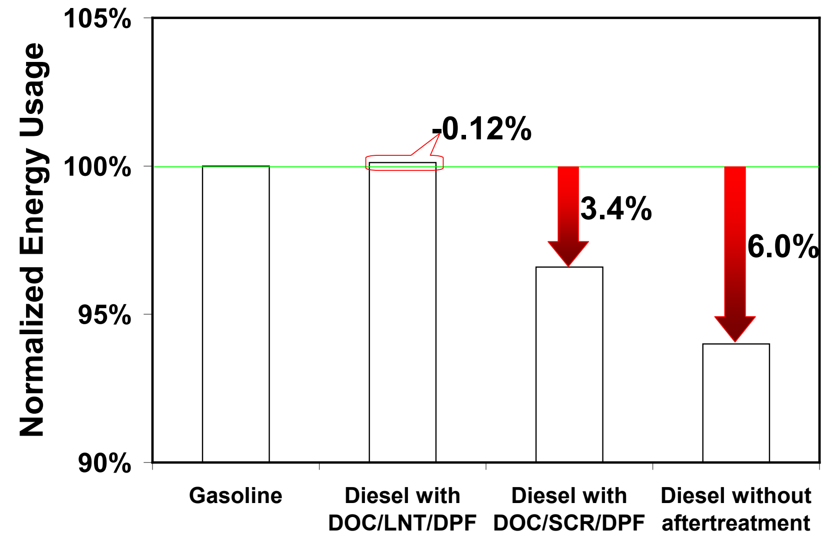
- Tailpipe NOx: SCR=0.16g/mi; LNT=0.15g/mi
- SCR generated 0.068g/mile $NH_3$ emissions
- Fuel econ.: SCR=136.4mpg; LNT=133.8mpg
- 1.9% penalty in fuel efficiency for LNT vs. SCR (less LNT penalty than previous HEV case due to less NOx removal)



# Key issue is the impact of the integration of aftertreatment device models on diesel HEV fuel efficiency and Emissions

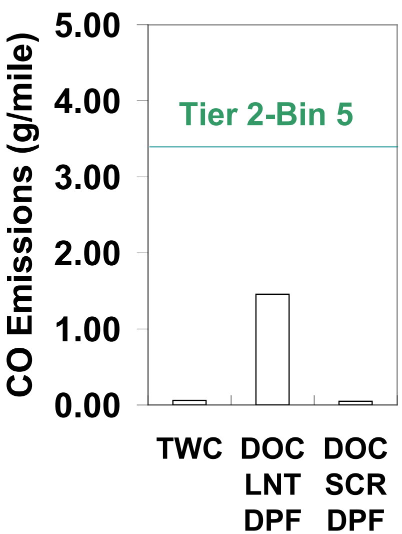
## Simulation parameters:

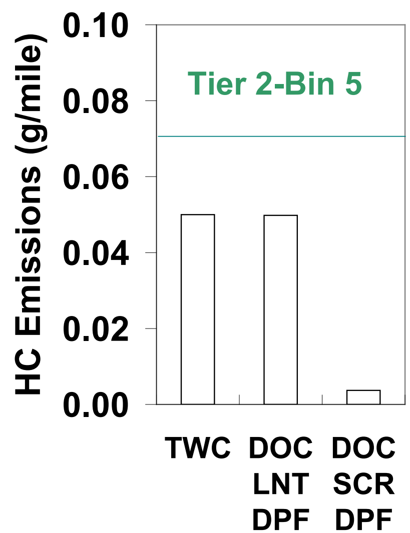
- 1450kg HEV w/ 80 UDDS drive cycles
- 1.5-L gasoline w/ TWC
- 1.5-L diesel engines w/
  1): DOC/LNT/CDPF; 2): DOC/SCR/CDPF
  (DPF regen.: 600s if pressure drop >7.5kPa)

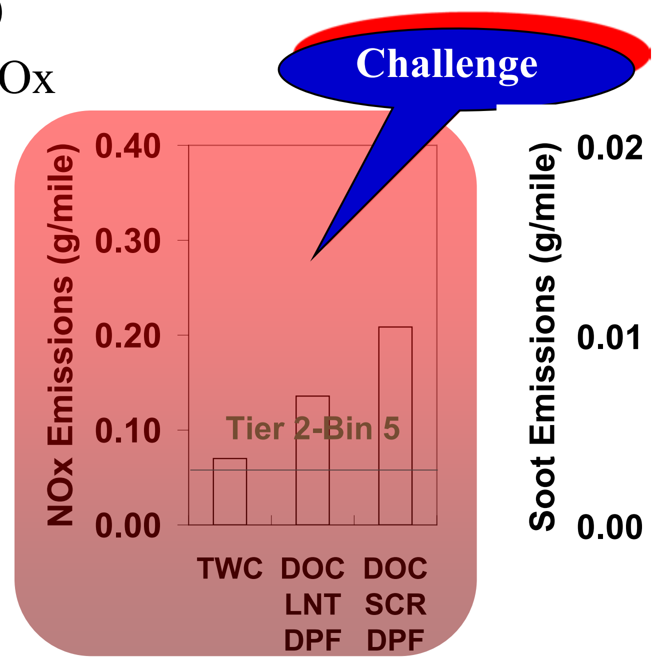


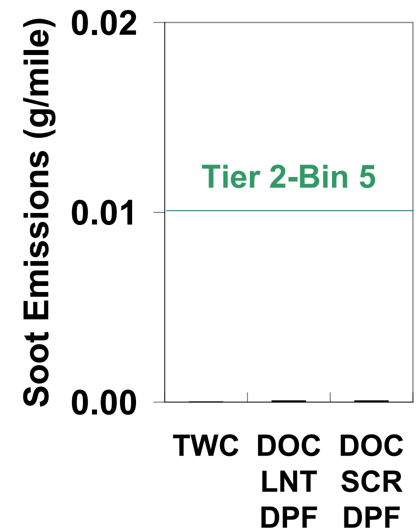

## Results:

- Better fuel economy for DOC/SCR/CDPF
- One DPF regeneration event (for diesel HEV)
- CO, HC, and PM meet Tier 2 Bin 5, except NOx



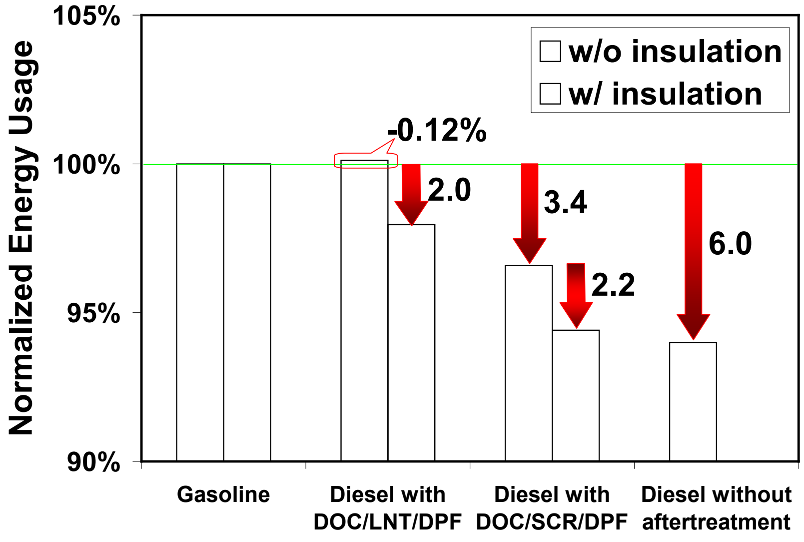
# We recently studied the effect of thermal insulation on HEV fuel efficiency and emissions

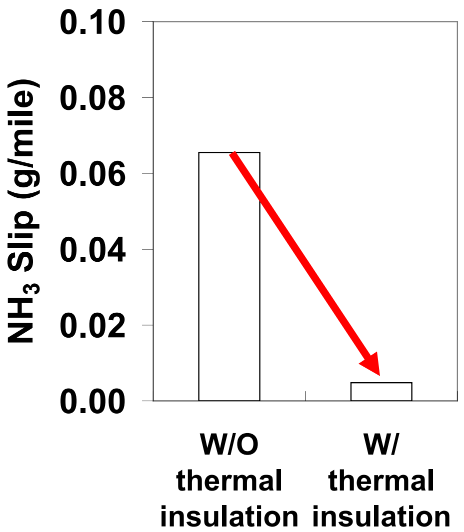
## Simulation parameters:

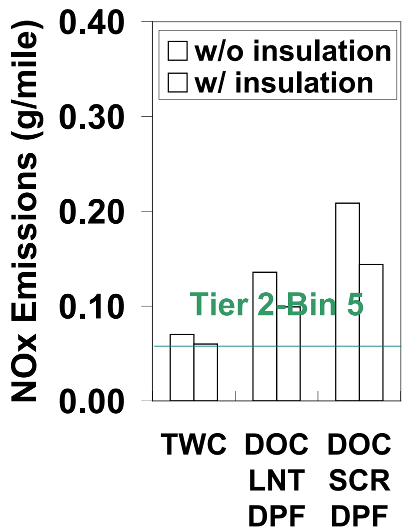
- 1450kg HEV with 80 UDDS drive cycles
- Insulation material: 3.0mm mineral fiber
- Aftertreatment device: Shell, Can, Insulation layer, and Catalyst

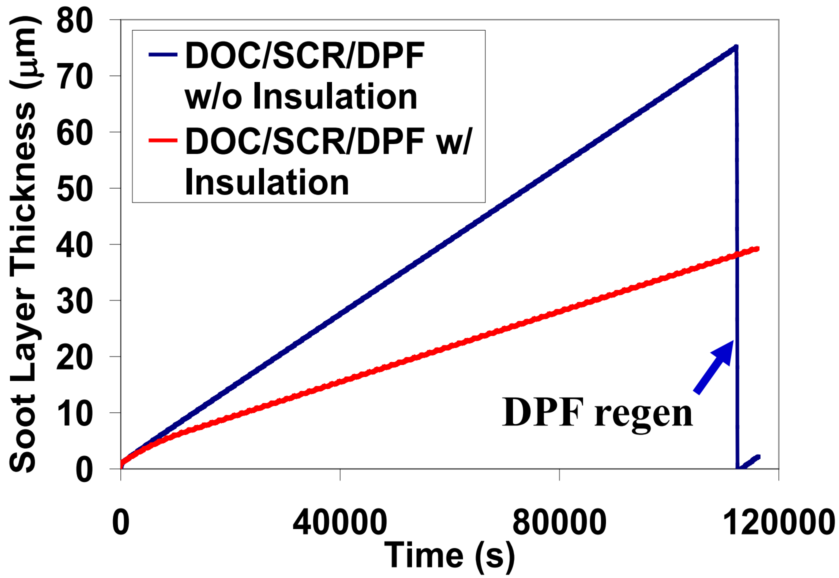
## Results:

- Improve fuel economy
- Enhance CDPF self regeneration
- Reduce NOx and $NH_3$ emissions



# Summary

- **Diesel HEV/PHEV achieve 19% higher fuel economy (mpg) than gasoline HEV/PHEV without emission control device**
  - 13% higher energy density for diesel
  - 6% better engine efficiency for diesel
- **NOx/PM emission control reduce diesel HEV/PHEV fuel efficiency advantages**
  - LNT add about 2%-4% fuel penalty in HEVs
  - SCR saves diesel efficiency advantage, but causes extra $NH_3$ slip
  - DPF add about 2%-3% fuel penalty in HEVs
- **The integrated system of DOC/SCR/CDPF**
  - Save 3.4% diesel efficiency advantage
  - Meet Tier 2 Bin 5 regulation for CO, HC, and PM, except NOx
  - Good insulation boosts diesel efficiency advantage and emission reduction
- **NOx emissions control is still challenging for gasoline and diesel HEV/PHEV**

# Acknowledge

**The authors thank Lee Slezak and U.S. Department of Energy for support to this research**

# Thanks

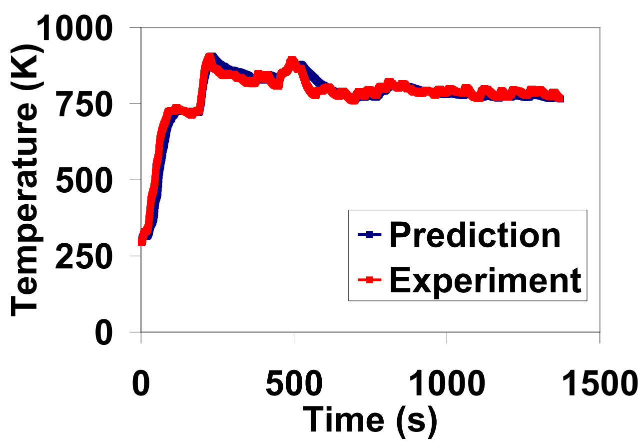
# ORNL 1D TWC model has been validated against independent OEM data

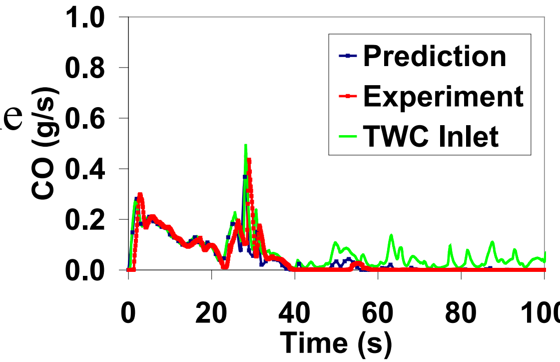
## Model validation conditions:

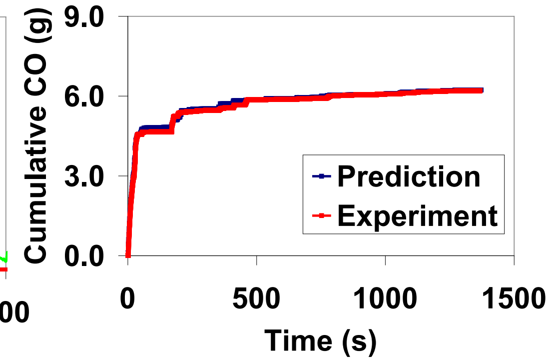
- Vehicle chassis data for gasoline engine
- Supplied by OEM collaborator
- UDDS cycle, cold start

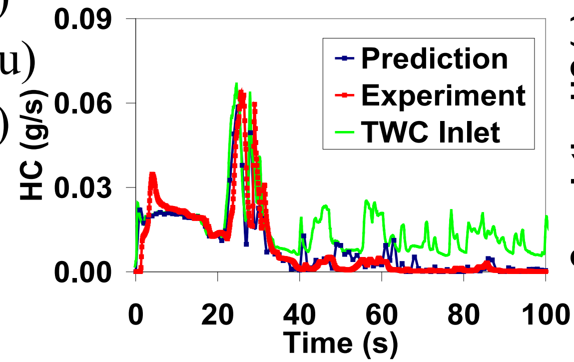
## Integrated emissions:

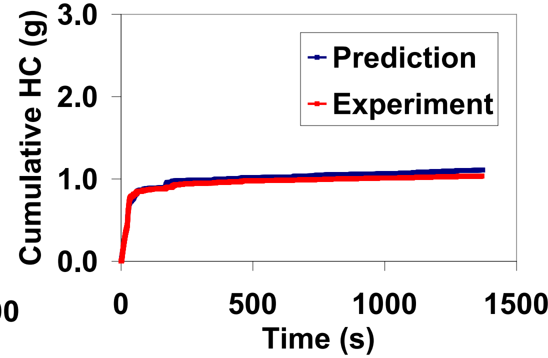
- CO (g/mi): 0.833(exp) vs. 0.836(simu)
- NOx (g/mi): 0.156(exp) vs. 0.157(simu)
- HC (g/mi): 0.139(exp) vs. 0.148(simu)

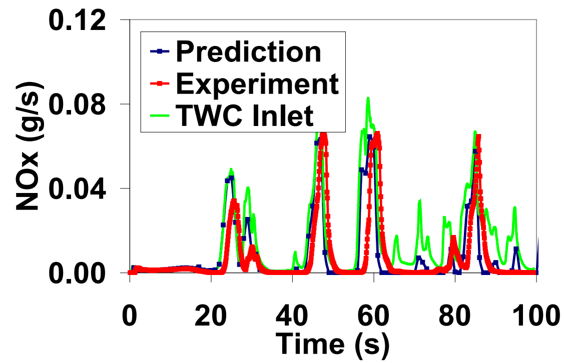


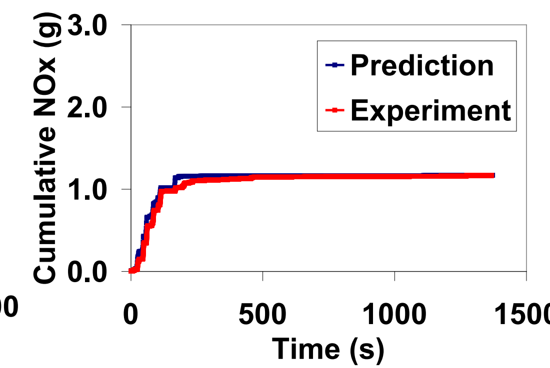



# ORNL basic 1D DOC model has been validated against open literature experimental data

## ORNL DOC model

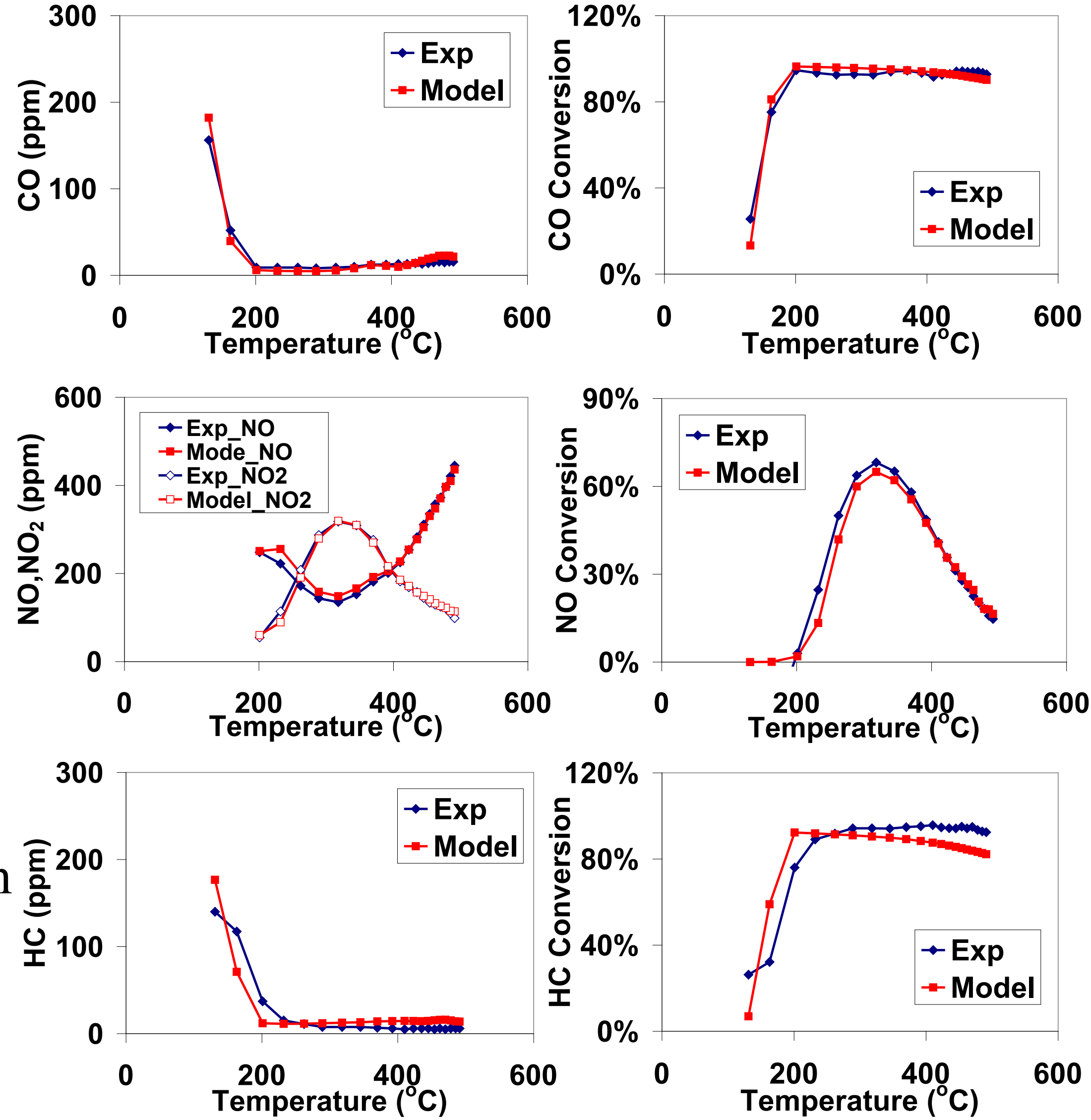
- Three global reactions: (1) CO oxidation, (2) NO oxidation, (3) HC oxidation

## Model validation conditions:

- Experimental data from the open literature (**P. Triana, Dissertation, MTU, 2005)**

## Example results

- 5%-100% engine load at the engine speed of 1400rpm-2200rpm



# We have utilized literature data to construct an initial 1-D transient Simulink module for SCR-NOx control

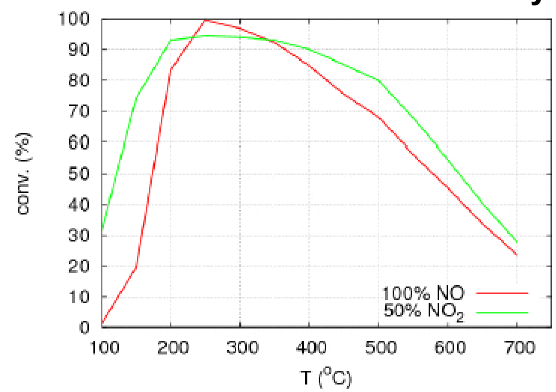
## SCR model assumptions:

- Currently CuZSM5 catalyst
- $NH_3$ adsorption/desorption
- NO SCR reaction
- $NO_2$ SCR reaction
- Fast SCR reaction ($NO + NO_2$)
- NO and $NH_3$ oxidation

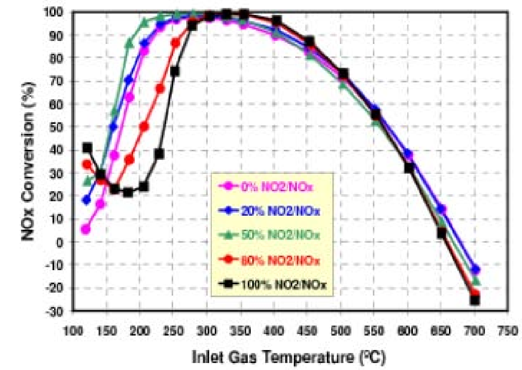
## SCR vs. LNT:

- SCR uses urea for NOx reduction
- SCR does not require PGM catalyst
- No modulation of engine is required
- LNT causes fuel penalty for NOx reduction
- LNT requires PGM catalyst

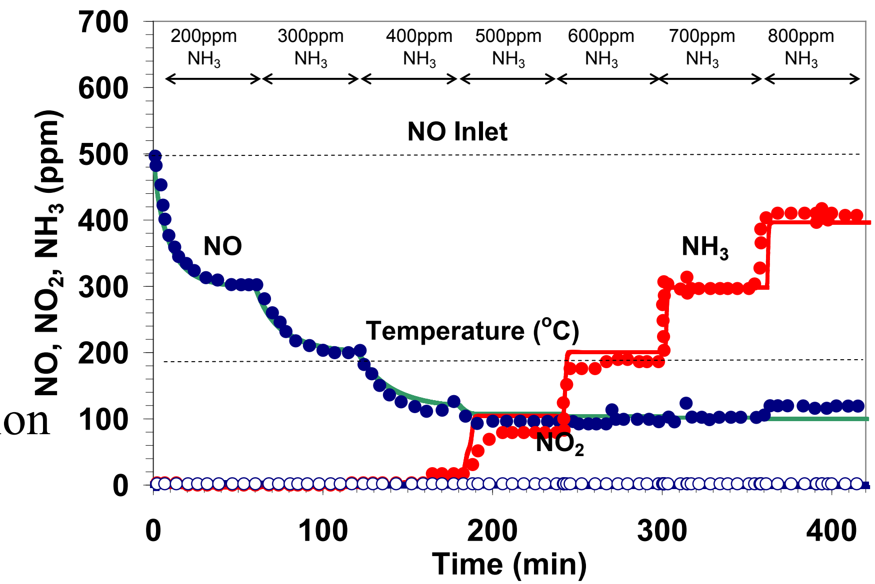
**Steady State Response**




**ORNL Model**




**SAE 2009-01-0897**

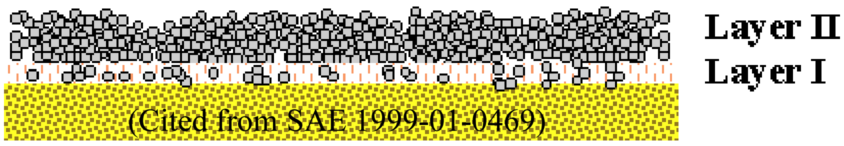


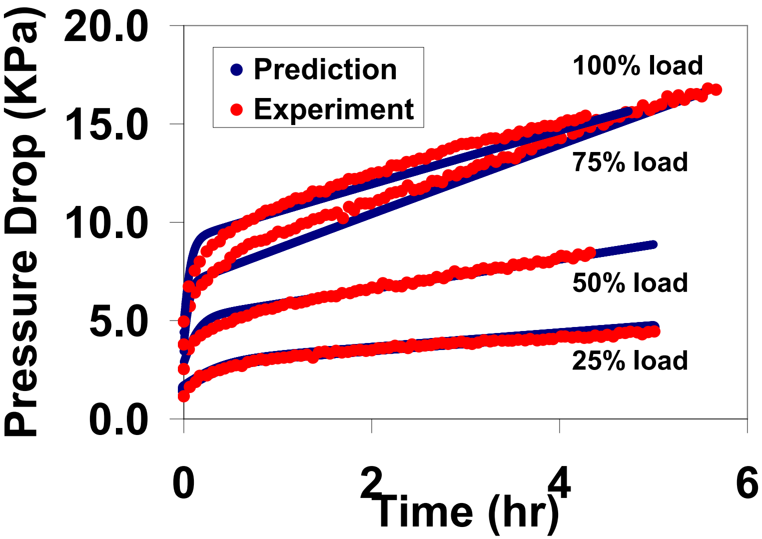

**Points from experiments by Olsson et.al, Applied Catalysis B: Environmental, 81(2008), 203-217. Lines from ORNL simulation.**

# ORNL DPF model for simulating soot emissions filtration compares well with open literature

**CDPF model assumptions:**

- Two-layer model
- Thermal and catalytic oxidation reactions




**Model validation conditions:**

- Experimental data from the open literature (SAE 2003-01-0841)

**Validation Results:**

- 25%-100% engine load at the engine speed of 1800rpm

**Cumulative soot**

| Engine load | 25% | 50% | 75% | 100% |
|---|---|---|---|---|
| Exp (g) | 18 | 35 | 103 | 55 |
| Model (g) | 18 | 34 | 108 | 53 |

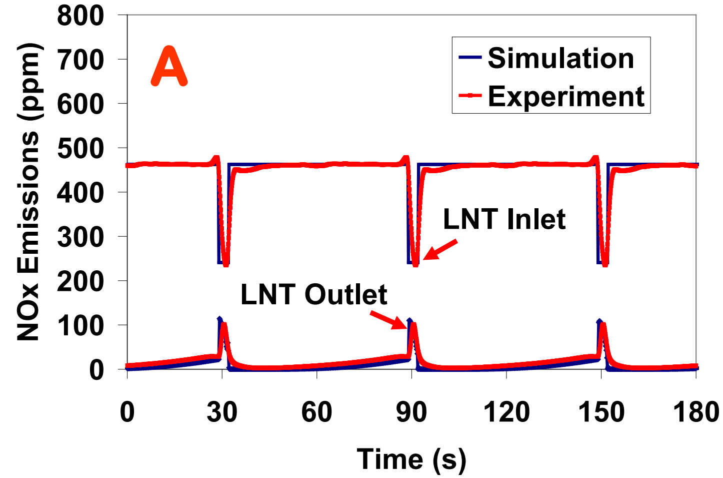
# ORNL LNT model for simulating lean NOx emissions compares well with observations

<u>**Simualtion Parameters**</u>

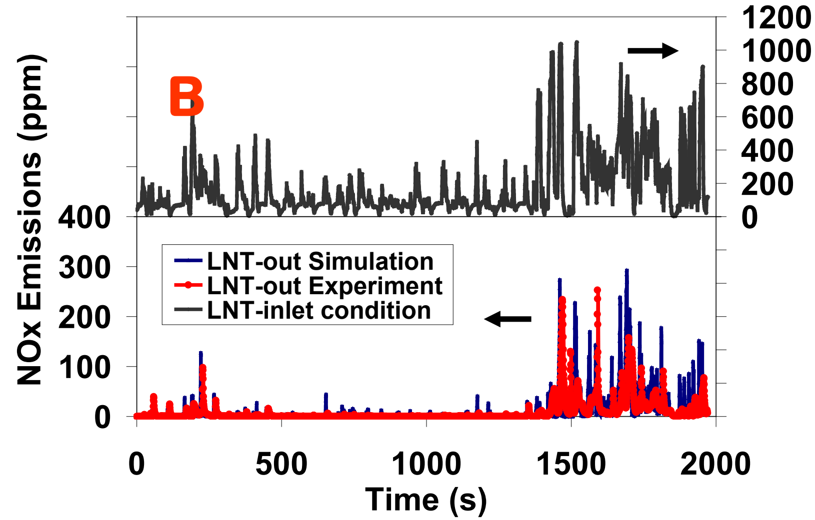
- Engine: 1.7-L Mercedes diesel engine
- Steady-state engine operation (A): 57s Lean burn and 3s rich combustion
- FTP driving engine operation (B): a combined driving cycle of UDDS and US06

| | LNT-out NOx (g/mi) | NOx Reduction (%) |
|---|---|---|
| Simu | 0.05 | 94.1 |
| Exp | 0.04 | 95.5 |

**Successfully demonstrates reasonably agreement with observations for both steady-state and FTP driving engine operation (SAE 2010-0882).**




**Steady-state operation**

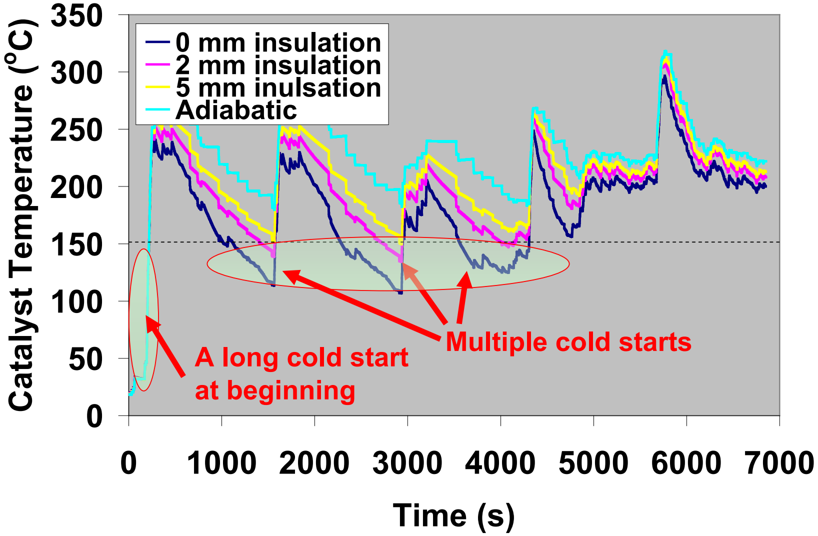


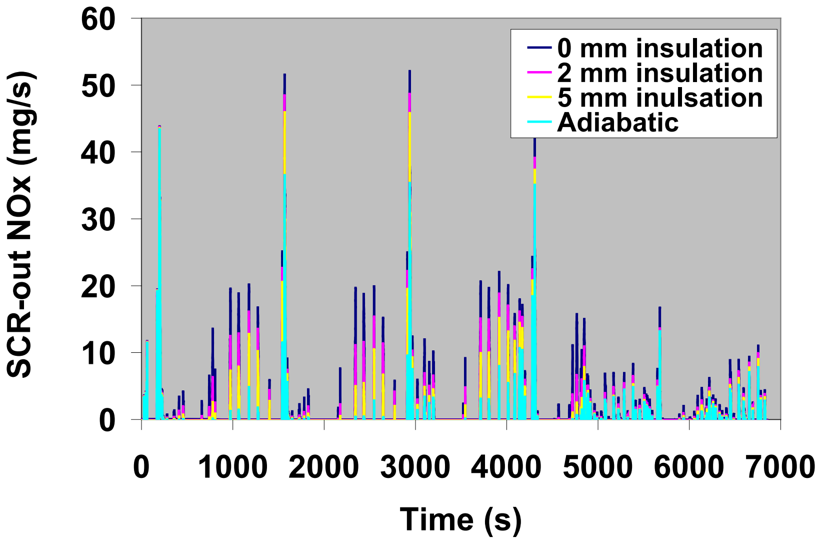

**FTP driving operation**

# Thermal insulation improve on aftertreatment device thermal operation conditions

## Simulation parameters:

- PHEV powered by 1.5-L diesel engine
- 5 kWh, 24 Ah battery charge (full charge)
- 5 UDDS cycles beginning with cold start
- 2.4-LUrea SCR (Cu-ZSM-5 catalyst)
- Insulation material: 3.0mm mineral fiber
- Aftertreatment device: Sheel, Can, Insulation layer, and Catalyst




## Results:

- Avoid multiple cold start in PHEV
- Reduce NOx and $NH_3$ emissions

# Objectives

- Develop engine maps and aftertreatment models for simulating the performance of conventional, advanced hybrid and plug-in hybrid vehicles operating with gasoline, diesel and alternative fuels as well as advanced engine combustion modes

**In the presentation**

**We focus on reporting simulated comparison of gasoline and diesel HEVs with explicit consideration of the impacts of emissions control**

# Future work

- **Smart control strategies for utilization of ammonia in SCRs and reductant in LNTs**
- **Potential impact of cold start or low temperature emissions traps technology**
- **Optimization of integrated DOC/LNT/SCR/CDPF systems**
- **Effects of advantage engine combustion (e.g. GDI, HCCI, PCCI) on improving fuel economy and emission reduction**
- **Effects of waste energy recovery on improving fuel economy and emission reduction**
- **Coordination**
  - Close to coordination with OEM, national laboratories, and universities to maintain relevance to the latest engine/emissions technologies for HEV/PHEV and industry needs