PHEV Engine and Aftertreatment Model Development

Project ID: vss008

<u>Stuart Daw (PI)</u>, Zhiming Gao, Kalyan Chakravarthy,

Oak Ridge National Laboratory

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

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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Overview

- **Timeline**
  - Start
    - 2005
  - Finish
    - Ongoing
- **Budget**
  - FY08 Funding
    - $725K
  - FY09 Funding
    - $700K
  - FY10 Funding
    - $350K
    - Reorganized modeling team and reduced work scope
- **Barriers**
  - PHEV fuel efficiency limited by transient engine operation and emissions controls
  - Very limited transient engines and emissions models for PHEV simulations
  - PHEV optimization needs to include advanced engine combustion modes
- **Partners**
  - DOE Diesel Crosscut Team companies and CLEERS consortium of suppliers, national labs, and universities
  - Company and university participants in ACE/HCCI consortium
  - VSATT Team Participants

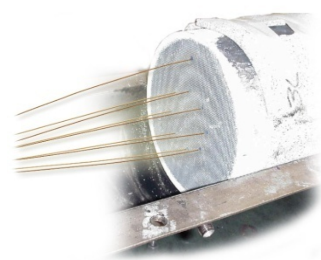
Objectives

- **Enable and demonstrate simulation of emissions and fuel efficiency for current and leading edge hybrid vehicles under fully transient drive cycle conditions**

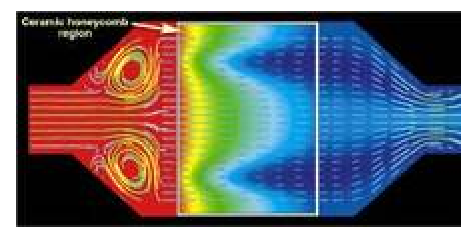
- **Apply simulation to assess fuel efficiency and emissions impact of:**
  - **Lean burn versus conventional gasoline engines**
  - **Advanced combustion (HCCI, PCCI) versus conventional combustion (SI, diesel)**
  - **Non-petroleum and bio-derived fuels**
  - **Alternative engine and emissions system control strategies**
  - **Alternative battery charging strategies**
  - **Alternative HEV and PHEV system configurations**

Vehicles

Engines



Emissions Controls



Models

Relevance

Mission
The AVTAE team's mission is to evaluate the technologies and performance characteristics of advanced automotive powertrain components and subsystems in an integrated vehicle systems context.

Objective
The prime objective of the AVTAE team activities is to evaluate VT Program targets and associated data that will enable the VT technology R&D teams to focus research on areas that will maximize the potential for fuel efficiency improvements and tailpipe emissions reduction. AVTAE accomplishes this objective through a tight union of computer modeling and simulation, integrated component testing and emulation, and laboratory and field testing of vehicles and systems.

Evaluation of advanced hybrid technologies involves multiple factors:

- **Interactions among electric powertrain, combustion engine, and aftertreatment.**
- **Integrated models suitable for full vehicle simulations and parametric studies.**
- **Validation of predictions vs. experimental data (dynamometer, full vehicle).**

Multiple OVT (inter-team) resources are available:

- **Other OVT projects & OEM collaborations (e.g., CLEERS, Engine Efficiency Colloquium at USCAR).**
- **Project evolved from AVTAE utilization of FreedomCAR advanced combustion engine data.**

Milestones

- **FY09 Milestone: Implement improved 3-way catalyst aftertreatment sub-model for simulating impact of stoichiometric biofuel engines on fuel economy and emissions of plug-in hybrids. September 30, 2009 (Completed √)**

- **FY10 Milestone: Publish methodology for simulating transient engine exhaust emissions and temperature required to account for multiple engine start-ups/shutdowns during hybrid drive cycles. September 30, 2010 (Article accepted and in press)**

Approach

- Simulate stoichiometric HEVs & PHEVs
  - Advanced gasoline & ethanol SI engines
  - Validated & refined TWC model
  - Integrated TWC & engines for leading edge hybrids
- Simulate lean HEVs & PHEVs
  - Advanced lean engines (gasoline DI, diesel)
  - Conventional & bio fuels
  - Advanced combustion modes (HCCI, PCCI)
  - Validated lean NOx/PM aftertreatment component models
  - Integrated lean engines & NOx/PM control
  - Efficiency benefits of lean vs. stoichiometric
- Generate and distribute data and simulation results
  - Public domain experimental data from lab, engine dynos, chassis dynos
  - Supplemental data from computer simulations (WAVE, GTPower, KIVA, CHEMKIN, & in-house engine & aftertreatment codes)
  - Data for unconventional and bio-derived fuels
  - Measurements and simulations of environmental compliance
  - Measurements and simulations of additional concepts (heat transfer reduction, bottoming cycles, thermo-electrics, thermo-chemical recuperation, and thermal storage)

Background

- HEVs/PHEVs can use stoichiometric or lean-burn engines
  - Stoichiometric engines
    - Heaviest emissions during cold start, transients
    - Limited data for alternative fuels
    - TWC technology still evolving (e.g., need to lower PGM)
  - Lean-burn engines
    - More fuel-efficient, focus of OEM/DOE R&D
    - Still under development
    - Limited data for alternative fuels
- TWCs not suitable for lean-NOx and PM control
  - Lean engines and controls HEVs/PHEVs only recently simulated
  - Lean emissions control technology still under development
  - Need to minimize fuel penalty without raising emissions
- Transients greatly impact fuel efficiency and emissions
  - Hybrids have unique engine on/off cycling
  - Engine efficiency varies greatly with speed and load
  - Catalytic reactions highly temperature dependent

Accomplishments/Progress

Since 2009 Review last May:

- **Published transient engine simulation methodology (engine out emissions and temperature for conventional/hybrid drive cycles)**
- **Published LNT model for systems simulation of lean HEVs and PHEVs (i.e., diesel and lean gasoline engines)**
- **Continued simulations of stoichiometric versus lean HEVs and PHEVs with lean NOx and PM controls**
  - Selected for FreedomCAR Highlight to USCAR Directors
  - Submitted publication summarizing initial results
  - Implemented urea-SCR vs. LNT NOx control in diesel PHEVs
- **Transferred 3-way catalyst model from PSAT to AUTONOMIE for stoichiometric PHEV simulations**
- **Initiated aftertreatment heat transfer impact studies on PHEV emissions performance**
- **Began detailed engine, emissions, and aftertreatment characterization of BMW series 1 lean-GDI vehicle.**

Example Details for Activities and Results

We documented our transient engine exhaust simulation approach in upcoming International Journal of Engine Research article

Example Simulation:

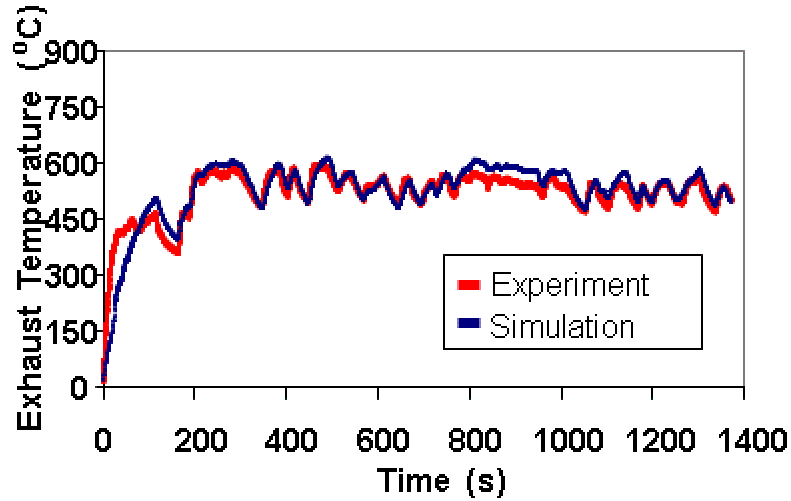
- Saab 9/5 Biopower (flex-fuel) vehicle
- 2.0 L stoichiometric engine
- LA4 cycle with cold start

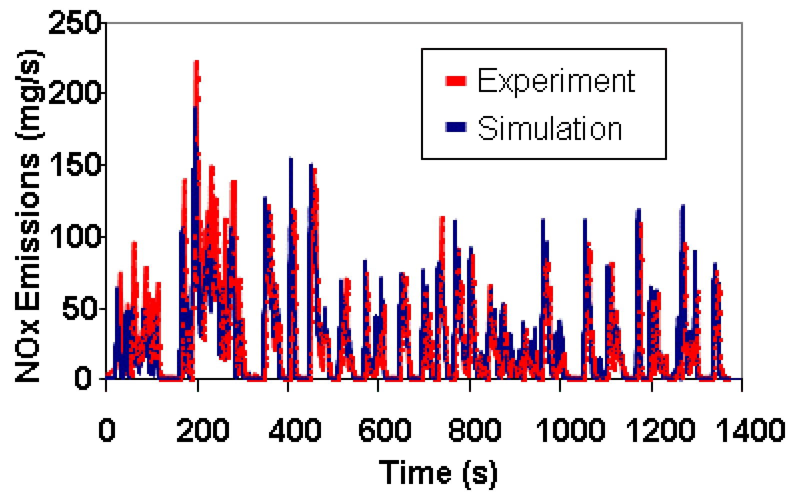
Results:

- Integrated mileage and engine-out emissions

	Fuel econ. km/L (mpg)	CO g/km (g/mi)	HC g/km (g/mi)	NO_x g/km (g/mi)
Exp	9.31 (21.9)	7.46 (12.0)	1.31 (2.1)	2.67 (4.3)
Pred	9.40 (22.1)	7.40 (11.9)	1.18 (1.9)	2.80 (4.5)

Accepted by IJER, Nov. 2009, in press.





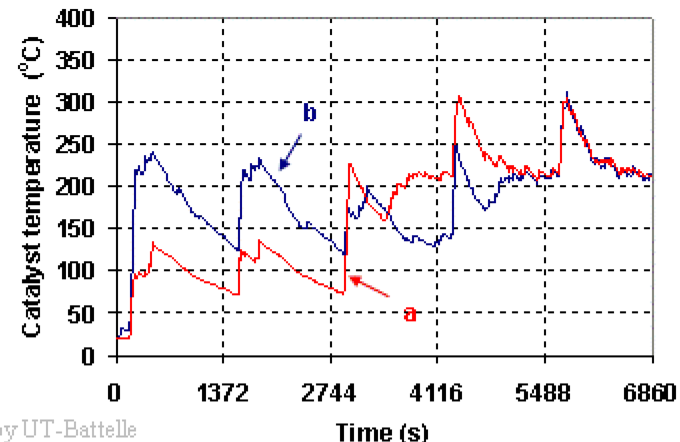
We showed transient simulation is needed to evaluate PHEV battery SOC management strategies

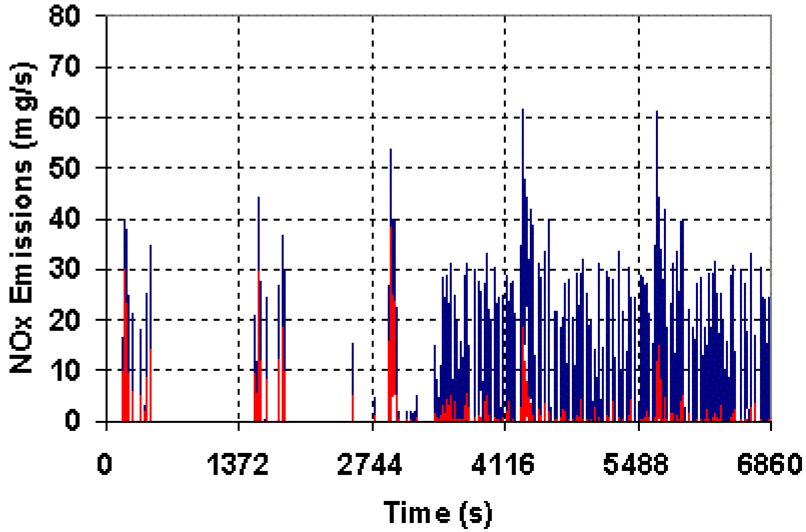
Simulation Condition

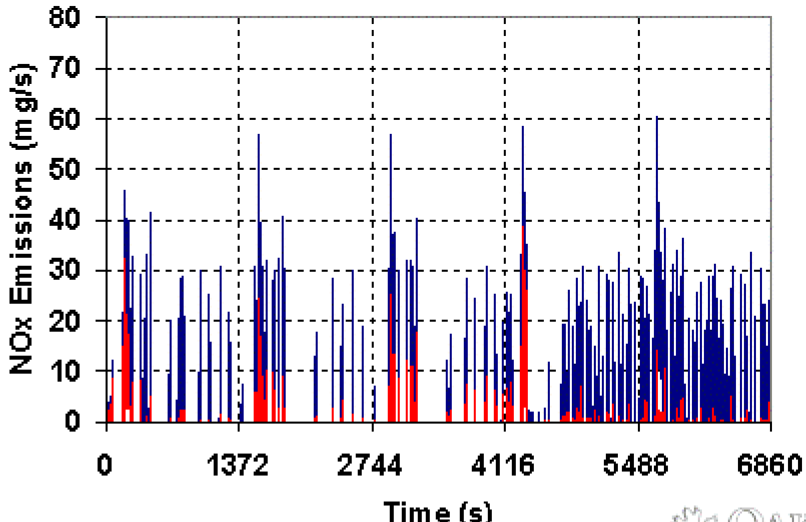
- Diesel powered 1450 kg PHEV w LNT
- 5 UDDS cycles from cold start
- 100% initial charge, 5 kWh battery
- Variable charge depletion strategies
  - Higher power threshold for engine on
  - Lower power threshold for engine on

Results

- Engine operating time: (a) 1551s vs. (b) 1483s
- Fuel economy: (a) 127.2 mpg vs. (b) 132.2 mpg
- NOx Emissions:
  - LNT out: (a) 0.08 g/mi vs. (b) 0.10 g/mi
  - Engine out: (a) 0.72 g/mi vs. (b) 0.69 g/mi







Another key issue is the impact of lean NOx controls on diesel PHEV fuel efficiency

Simulation parameters:

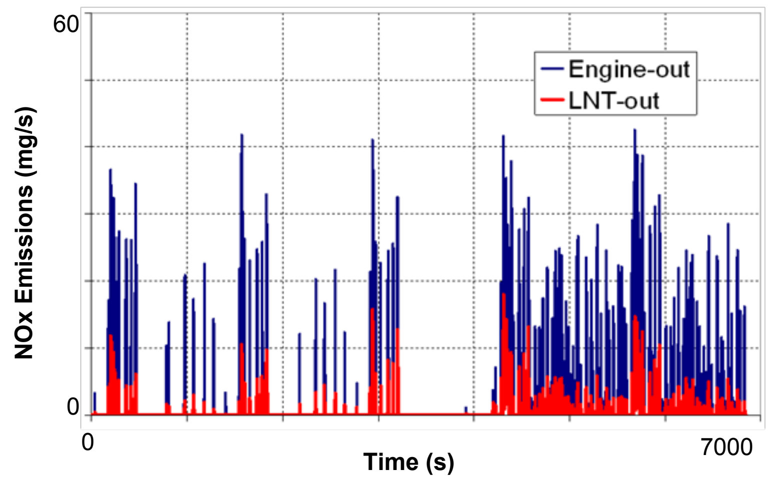
- 1450 kg vehicle
- 1.5-L engine (gasoline vs. diesel w and w/o NOx control)
- 5 kWh, 24 Ah battery (full initial charge)
- Fixed control strategy (electric until PD>threshold f(SOC))
- 5 consecutive UDDS cycles, initial cold start
- 2.4-L TWC vs. no NOx control vs. 2.2-L LNT
- No DPF

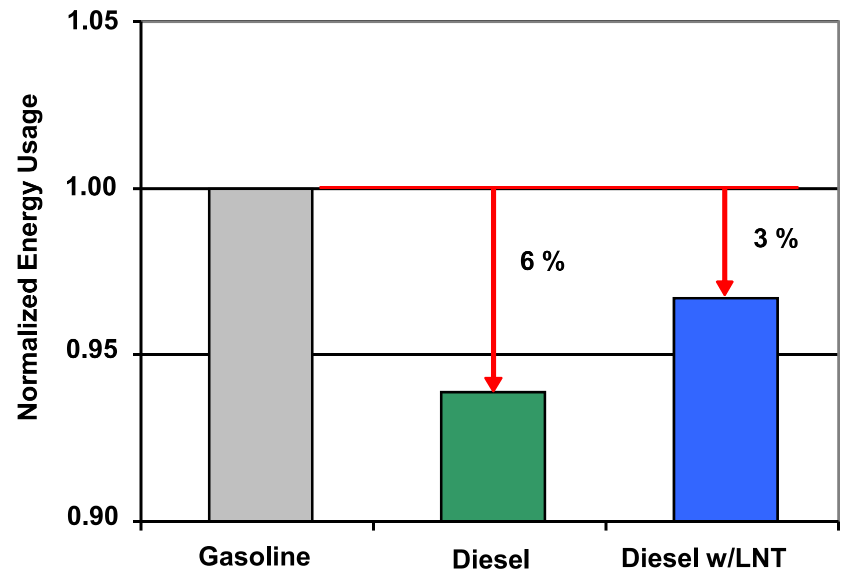
Results:

- 1st 3 cycles-charge depleting, last 2 cycles- charge sustaining
- 132.4 mpg diesel vs. 113.7 mpg gasoline
- 0.10 g/mile NOx vs. 0.11g/mile NOx
- Without LNT, diesel has 6% higher efficiency (based on LHV)
- LNT fuel penalty for diesel 3%

LNT fuel efficiency penalty has spurred interest in SCR NOx control

Diesel PHEV with LNT





We have utilized literature data to construct an initial model for SCR-NOx control

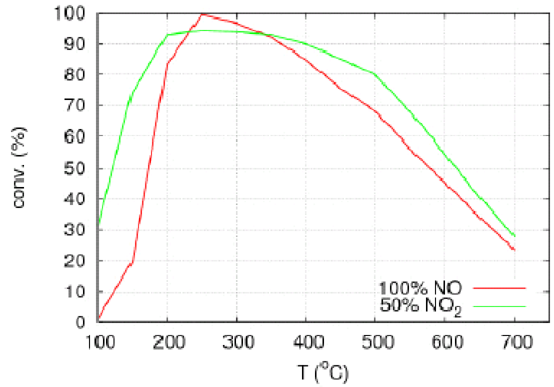
SCR model assumptions:

- 1-D transient Simulink module
- NH_3 adsorption/desorption
- NO SCR reaction
- NO_2 SCR reaction
- 'Fast' SCR reaction ($NO + NO_2$)
- NO oxidation
- NH_3 oxidation
- Currently CuZSM5 catalyst

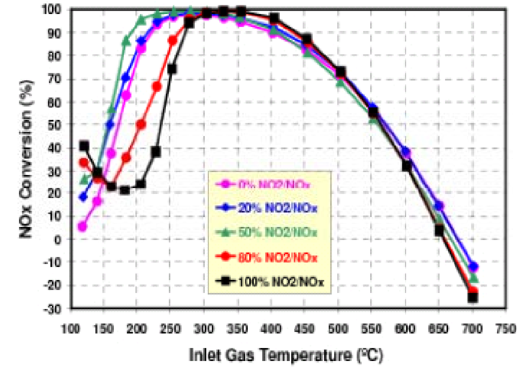
SCR vs. LNT:

- SCR uses urea for NOx reduction
- SCR does not require PGM catalyst
- No modulation of engine is required
- LNT uses fuel for NOx reduction
- LNT requires PGM catalyst
- Engine modulation may be required for catalyst regeneration

Steady State Response



ORNL Model



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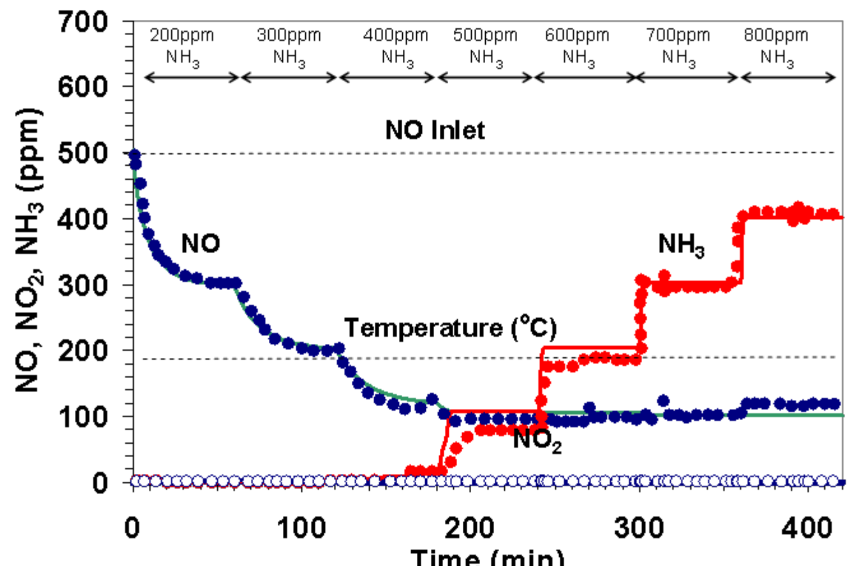
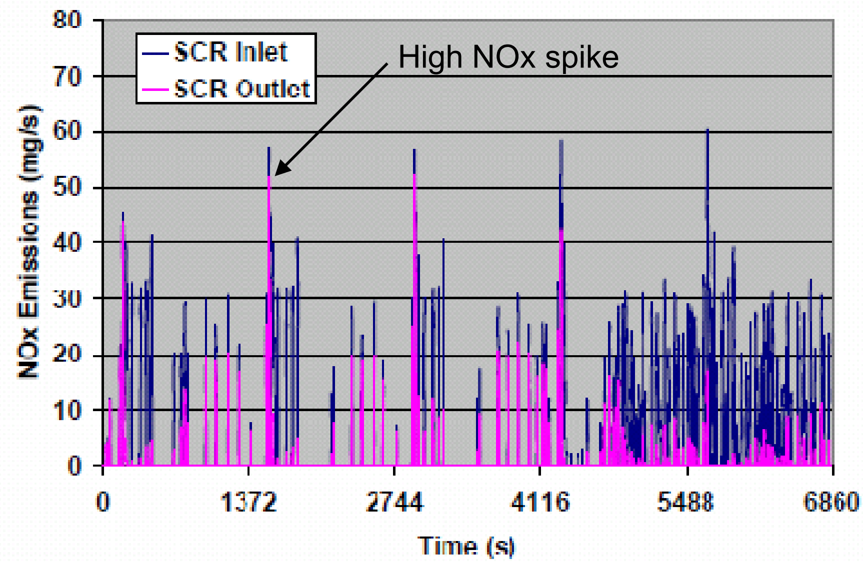


Points from experiments by Olsson et.al, Applied Catalysis B: Environmental, 81(2008), 203-217. Lines from ORNL simulation.

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

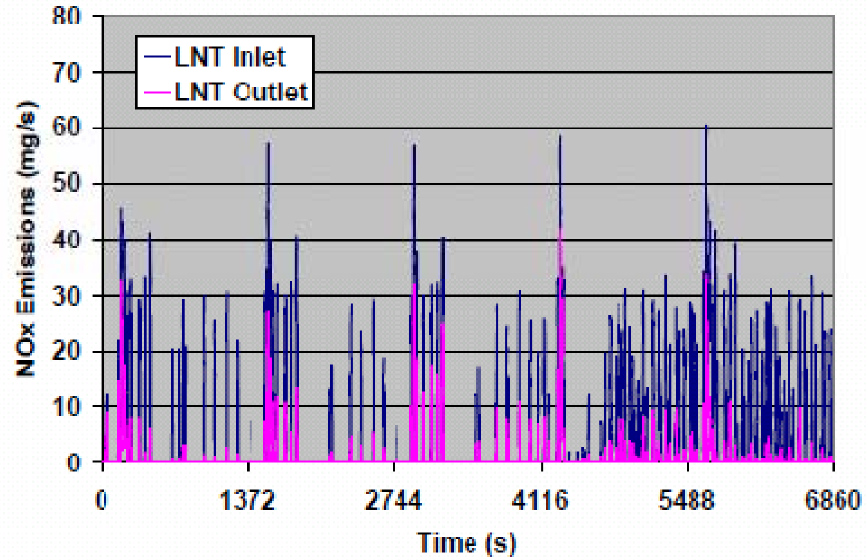
Simulation parameters:

- 1450 kg PHEV powered by 1.5-L diesel engine
- 5 kWh, 24 Ah
- 5 UDDS cycles beginning with cold start
- Initial full battery charge
- 2.4-L LNT, Urea SCR (2.4-L Cu-ZSM-5 catalyst)
- Engine fueling modulation for LNT regeneration
- Urea inj. for SCR (1:1 NH_3 to NO, non-optimal)
- No NH_3 slip control for SCR



Results:

- Tailpipe NOx: SCR = 0.16g/mile; LNT = 0.15g/mile
- SCR NOx control initially not as effective due to lack of adsorbed NH_3
- SCR generated 0.068g/mile NH_3 emissions
- Fuel economy: SCR = 136.4mpg; LNT = 133.8mpg
- 1.9% penalty in fuel efficiency for LNT vs. SCR (less LNT penalty than previous PHEV case due to less NOx removal)



We established a baseline for studying the effect of high efficiency clean combustion (HECC) in HEVs and PHEVs

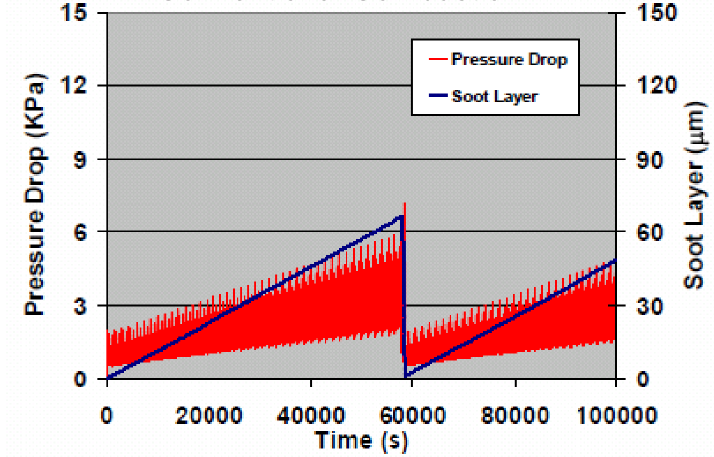
Baseline Simulation parameters:

- 1090 kg conventional passenger car
- 1.7-L Mercedes diesel engine
- Fully integrated aftertreatment with DOC, LNT, CDPF
- HECC only at low load (i.e. below 50 lb-ft, 3000 rpm)
- 80 sequential UDDS cycles
- DPF regen 600s duration when P >7.5 kPa

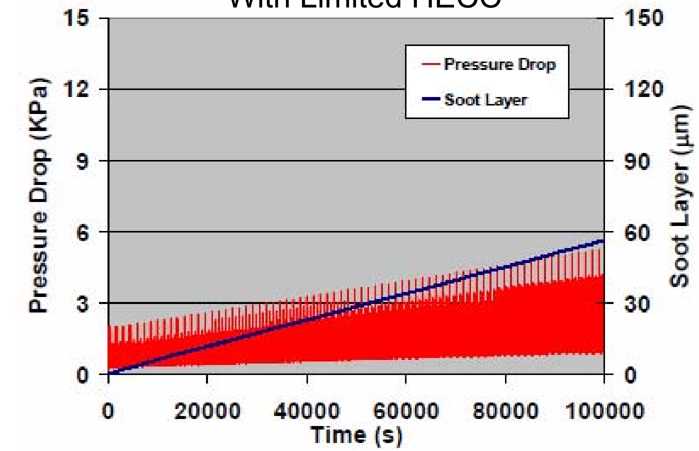
Results:

- Limited HECC boosts fuel economy by 1.8%
- Engine spends 89.4% of time in HECC range
- Improved fuel economy from reduced frequency of LNT and DPF regen
- No CDPF regens with limited HECC and one CDPF regen with conventional combustion
- HECC HEV and PHEV benefits will depend on battery charge management (strategies that allow more low-load operation will benefit more from HECC)

DPF Pressure Drop With Conventional Combustion



DPF Pressure Drop With Limited HECC



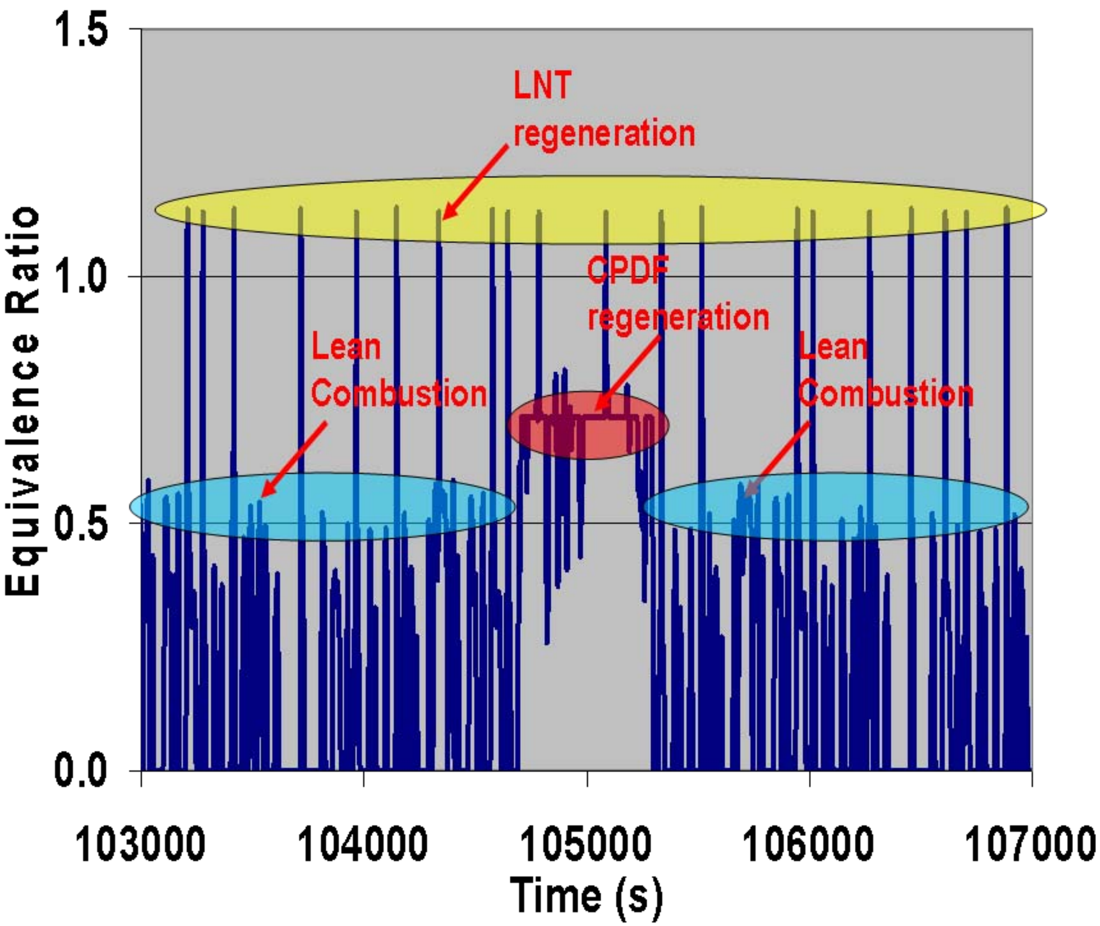
We have also begun simulating diesel HEVs with fully integrated aftertreatment

Simulation parameters:

- 1450 kg HEV
- 80 consecutive UDDS cycles, cold start
- 1.3 kWh battery, initially 65% charged
- 1.5-L diesel engine w 0.59-L DOC, 2.4-L LNT, and 1.9-L CDPF
- Non-optimized aftertreatment controls
- Conventional diesel combustion

Preliminary Results:

- 81.8 mpg
- 0.35 g NOx/mile

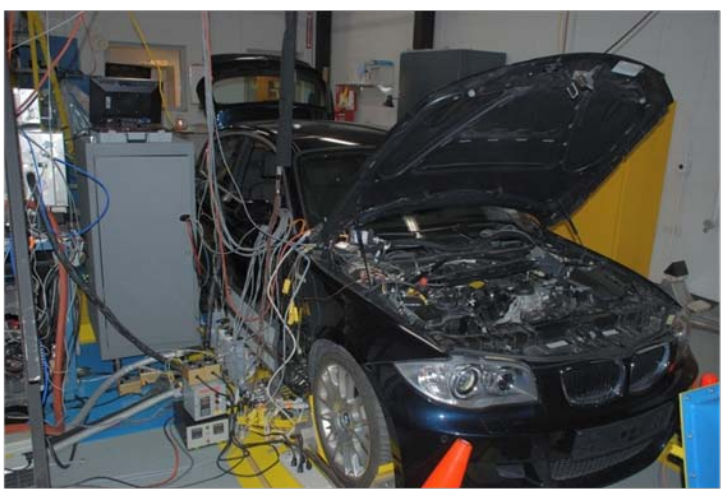


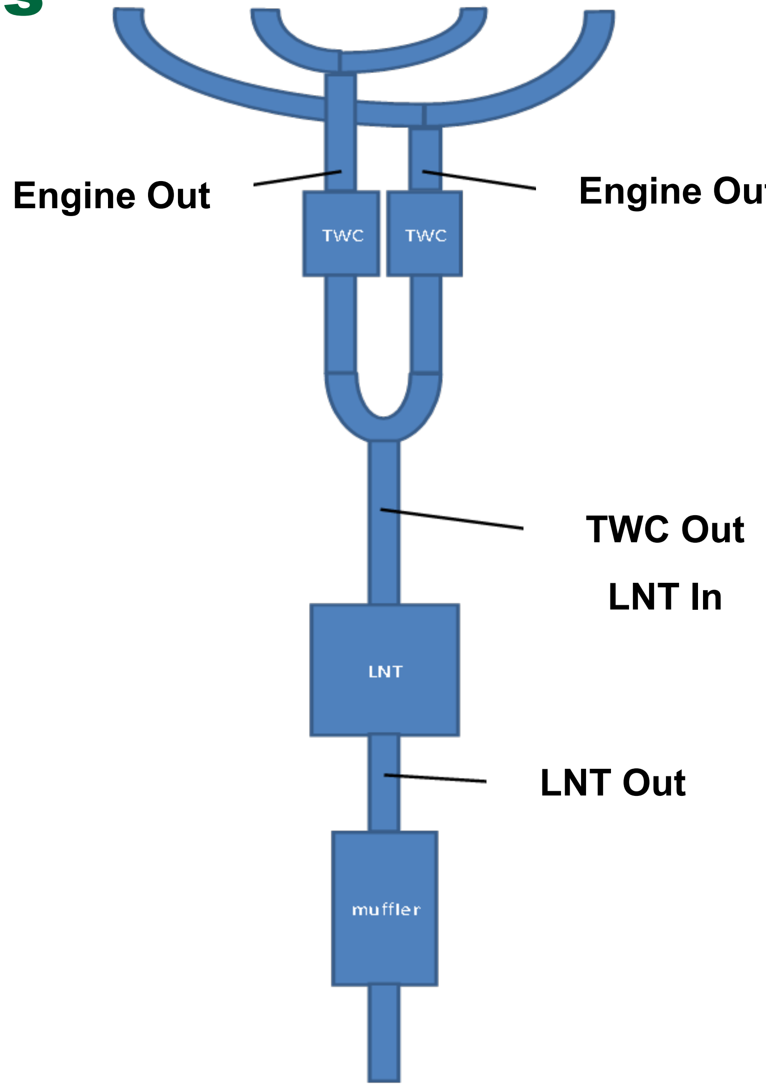
Equivalence ratio history for engine

We are compiling chassis dyno data from a BMW 1-series 120i lean GDI vehicle to validate and improve component models

- **Exhaust instrumentation at 4 locations:**
  - 5 gas analyzers
  - FTIR for transient NO, NO_2, NH_3, & HC
  - SpaciMS for transient H_2 and O_2
  - Particulate matter

- **Vehicle and engine instrumentation**
  - OBD link
  - Additional T and P sensors





Collaborations

Continuing industry feedback and data sharing via:

- Advanced Combustion Memorandum of Understanding (MOU)- Includes Cummins, Caterpillar, Chrysler, DDC, Ford, GE, GM, John Deere, Volvo, International, BP, Conoco Philips, ExxonMobil, Chevron, Shell
- Advanced Combustion and Emission Control (ACEC) Tech Team – USCAR Ford, GM, Chrysler
- DOE Diesel Crosscut Team -DDC, Cummins, Volvo, GM, Ford, Chrysler, Caterpillar, John Deere, International, EPA, TACOM
- Crosscut Lean Exhaust Emission Reduction Simulation (CLEERS) collaboration- Crosscut Team, Delphi, Umicore, Johnson Matthey, BASF, Bosch, Corning (see www.cleers.org)

Above provide opportunities for industry to test and comment on VSATT model utilization (e.g., PSAT implementation with proprietary in-house component models added as in the Delphi CRADA)

Planned Future Activities

- **Stoichiometric hybrid simulations (gasoline engines)**
  - Continue refinement and validation of 3-way catalyst model with BMW data
  - Improve engine transients model predictions of unburned HC (cold and warm start)
  - Implement/validate 3-way catalyst model in AUTONOMIE
  - Develop second generation transients model with coolant thermal storage included X
  - Evaluate potential impact of cold-start emissions 'trap' technology X
- **Lean hybrid simulation (e.g., diesel, lean gasoline engines)**
  - Continue comparisons of diesel and gasoline HEV/PHEV fuel efficiency and emissions
  - Continue refining lean NOx and PM aftertreatment models
  - Demonstrate hybrid vehicle simulations with lean HCCI and direct-injected combustion
  - Evaluate impact of PCCI/HECC diesel operation on HEV fuel efficiency and emissions
  - Expand studies of Urea-SCR and DPF control for diesel HEV X
  - Update available algorithms for engine scaling X
- **Exhaust heat recovery simulation**
  - Define and implement reference simulation for thermo-electrics impact X
  - Define and test simulation of thermo-chemical recuperation X
  - Define and test simulation of Rankine bottoming cycle X
- **Coordination**
  - Close coordination with Combustion MOU, ACEC, DCC Team, CLEERS to maintain relevance to latest engine/emissions technology and industry needs

X - Requires increased budget

Summary

- Methodology for simulating engine exhaust temperature and emissions transients in realistic drive cycles has been developed and published.
- Engine transient methodology has been demonstrated in integrated engine and aftertreatment simulations of HEVs and PHEVs.
- Fuel efficiency of diesel HEVs and PHEVs is significantly reduced by the fuel requirements for lean NOx and PM control.
- Urea-SCR lean NOx control for lean HEVs and PHEVs may have less fuel penalty than LNTs.
- Work underway to develop lean gasoline HEV and PHEV simulations.
- Extent of additional parametric studies constrained by reduced budget.

Stuart Daw
865-946-1341
dawcs@ornl.gov

Acknowledgements and Contacts

DOE Program Manager:

- ***Lee Slezak, Office of Vehicle Technologies***

ORNL Contacts:

- **David Smith[1], Stuart Daw[2], Kalyan Chakravarthy[3], Zhiming Gao[3], Dean Edwards[4], Brian West[4], Robert Wagner[4]**

- ***[1]ORNL Program Manager, Vehicle Systems***
- ***[2]Task 2a Modeling Coordination***
- ***[3]Modeling Team***
- ***[4]Engine and Vehicle Data***

PSAT and AUTONOMIE modeling team at ANL:
- **Aymeric Rousseau**