After-treatment modeling for hybrid vehicles using PSAT

Zhiming Gao,
Kalyana Chakravarthy,
Stuart Daw & James Conklin

Oak Ridge National Laboratory

12 DOE-CLEERS workshop
April 28, 2009

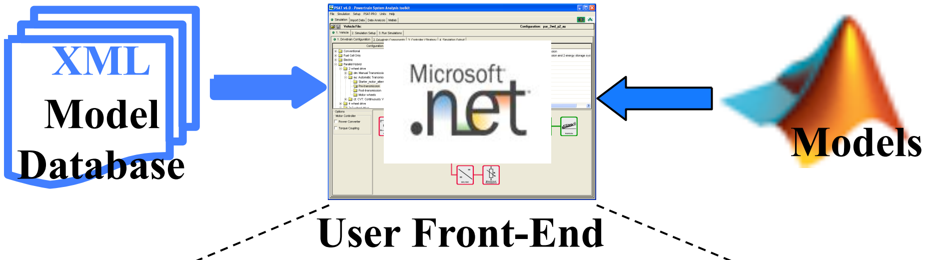
Sponsor : Lee Slezak
Vehicle Technologies Program
U.S. Department of Energy

Introduction

- What is PSAT?
  - A flexible “forward looking” simulation package for building and analyzing virtual vehicle configurations
  - Sponsored by DOE, effort led by ANL
  - Contributions from DOE laboratories and auto companies
  - not intended to be a design tool (relied mostly on experimental data/maps and not on physically based component models)
- PSAT provides a wide range of vehicle applications including light- (two- and four-wheel-drive), medium-, and heavy-duty vehicles
  - Conventional, Hybrid, Fuel cell, Electric
- PSAT provides multiple-option component model libraries
  - Major Components : Driver, Cluth/Torque converter, Engine, Exhaust aftertreatment, Energy storage, Gearbox, Fuel cell, Motor, Generator, Mechanical/Electrical accessory, Starter, Wheel axle
- Visit PSAT website: www.transportation.anl.gov/software/PSAT/index.html

PSAT construct

- User-friendly graphical user interface written in C#
- Component modules written in Matlab, Simulink, State Flow
- Model database managed by XML
- Users define components

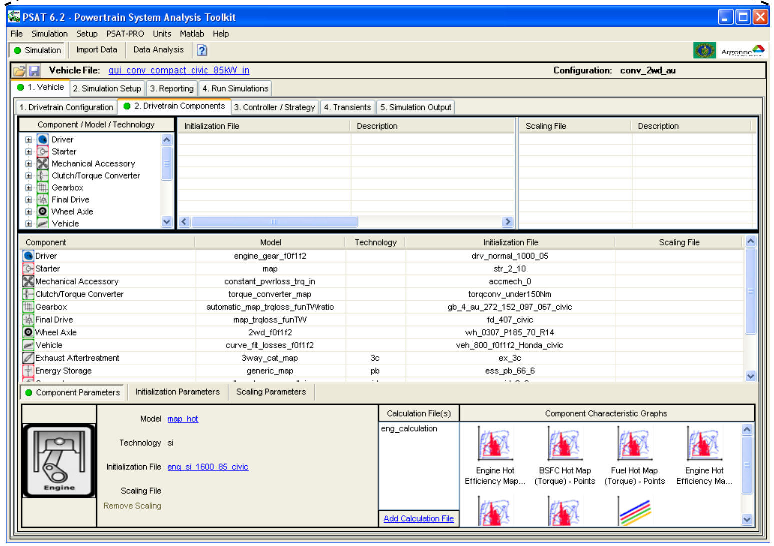


Vehicle Configuration

Powertrain Components

Driving, braking & shifting

Simulation Setup and Run



Vehicle File: gui_conv_compact_civic_85kW_in

Configuration: conv_2wd_au

Component	Model	Technology	Initialization File	Scaling File
Driver	engine_gear_f0f1f2		drv_normal_1000_05	
Starter	map		str_2_10	
Mechanical Accessory	constant_pwrloss_trq_in		accmech_0	
Clutch/Torque Converter	torque_converter_map		torqconv_under150Nm	
Gearbox	automatic_map_trqloss_funTWratio		gb_4_au_272_152_097_067_civic	
Final Drive	map_trqloss_funTW		fd_407_civic	
Wheel Axle	2wd_f0f1f2		wh_0307_P185_70_R14	
Vehicle	curve_fit_losses_f0f1f2		veh_800_f0f1f2_Honda_civic	
Exhaust Aftertreatment	3way_cat_map	3c	ex_3c	
Energy Storage	generic_map	pb	ess_pb_66_6	

Model map_hot

Technology si

Initialization File eng_si_1600_85_civic

Scaling File

Calculation File(s)

eng_calculation

User Define Components

Variable Solver Options

Post Analysis & Simulation Output options

Save & Reload Data

PSAT GUI

PSAT uses

- System integration
  - Compatability (catalyst sizing, battery capacity)
  - Active control : engine on/off in hybrid vehicles, start/stop regeneration of LNT/ DPF
  - Costs (fuel penalty associated with regeneration, pressure drop effect on engine load)
- Comparative studies
  - Lean burn vs. conventional gasoline engines
  - Advanced (HCCI, PCCI, MKI) vs. conventional combustion (SI, diesel)
  - Different hybrid configurations (series, parallel, split)
  - Petroleum vs. bio-fuels

ORNL contribution to PSAT

- Objective : develop engine maps and emissions control device models for simulating the performance of conventional, advanced hybrid and plug-in hybrid vehicles operating with gasoline, diesel and alternative fuels
  - Engine maps (steady state)
  - Transient engine warm-up model
  - Map based oxycat model (no NO-NO2 interconversion)
  - Lean NOx trap (LNT) model
  - 3-way catalyst (TWC) model
  - Diesel particulate filter (DPF) model
- Approach
  - Physically based models to deal with transients (move away from pseudo-steady state assumptions wherever possible)
  - Generate/utilize public domain lab, engine dynamometer data for building maps and models
  - Fill gaps in experimental data using predictions from computational tools such as WAVE, GT-Power or in-house software

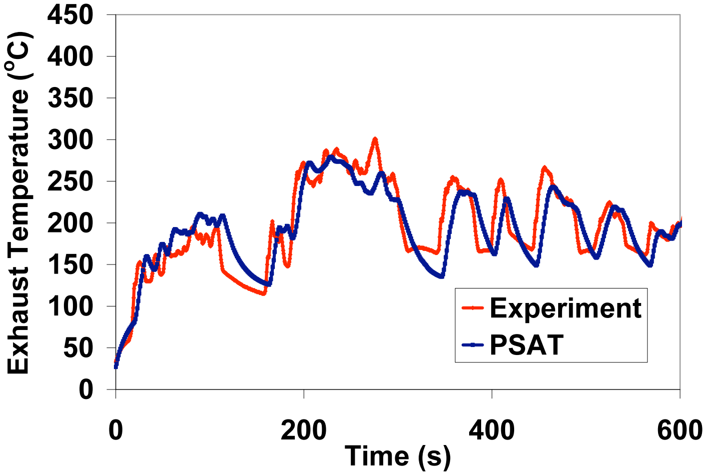
Present study:compare diesel & SI hybrid vehicles

- SI engines
  - Stoichiometric combustion => higher exhaust T
  - Most emissions during cold start but faster light-off
  - 3-way catalyst technology mature but still evolving (low precious metal catalysts, dual catalysts systems)
- Diesel engines
  - Burn very lean => lower exhaust temperature
  - More efficient than SI engines (mainly due to higher compression ratio)
  - Aftertreatment is a significant challenge, technologies still evolving
  - Unconventional modes (HCCI, PCCI, MKI etc.) are possible in addition to conventional mode of combustion
  - Fuels costs associated with aftertreatment (DPF pressure drop, regeneration of DPF and LNT)
- Hybrid vehicle pose some aftertreatment problems
  - Engine may switch on and off several times during a drive cycle
  - Smaller engine size => lower exhaust temperature

Engine warm-up model

Simulation parameters:

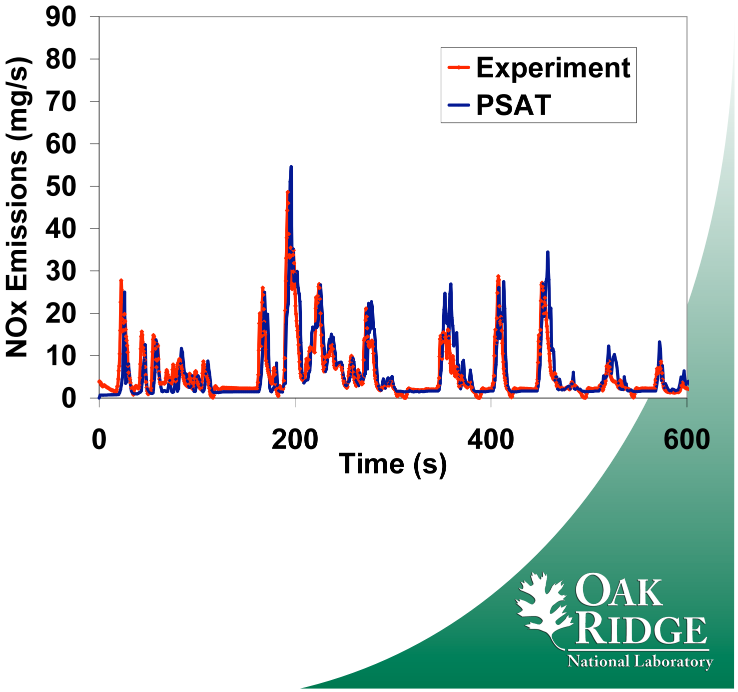
- Mercedes 1.7L diesel engine (A170 compact car)
- UDDS cycle with cold start



Results:

- Integrated mileage and engine-out emissions

	Mileage (mpg)	CO (g/mi)	HC (g/mi)	NOx (g/mi)	PM (g/mi)
Experiment	40.3	2.28	0.54	0.74	0.14
Simulation	40.4	2.29	0.54	0.89	0.12



Successfully handles cold/warm start transients for both gasoline and diesel engines.

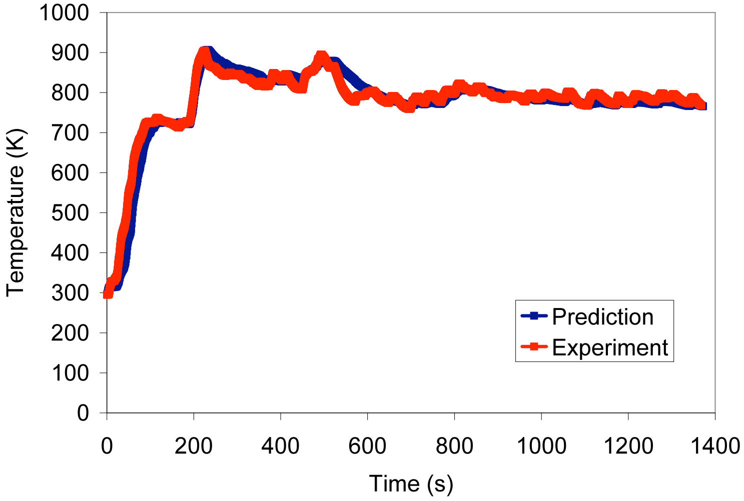
TWC model : sample results

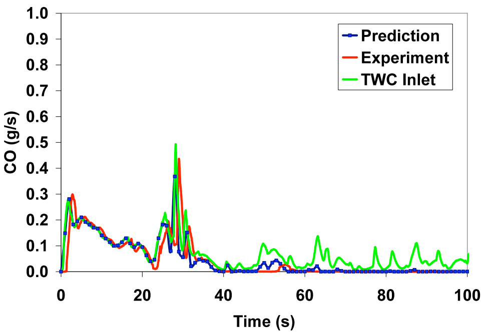
Model validation conditions:

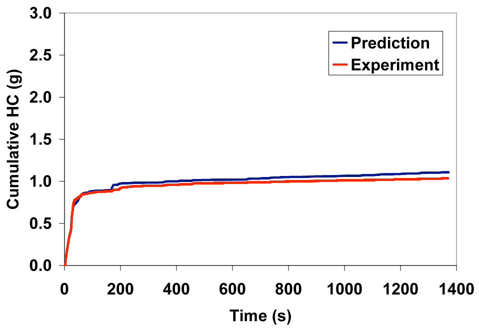
- Data for a gasoline engine from vehicle tests (supplied by an OEM)
- UDDS cycle with a cold start

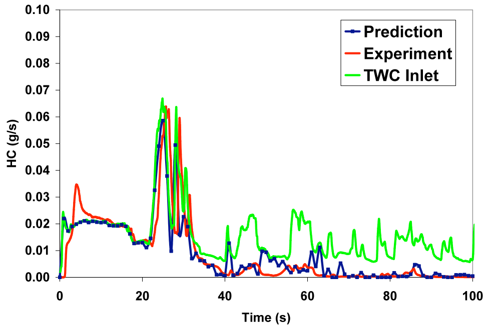
Integrated emissions:

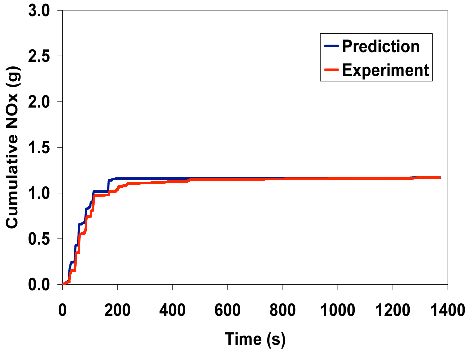
- CO (g/mi): 0.833 (exp) vs. 0.836 (model)
- NOx (g/mi): 0.156 (exp) vs. 0.157 (model)
- HC (g/mi): 0.139 (test) vs. 0.148 (model)

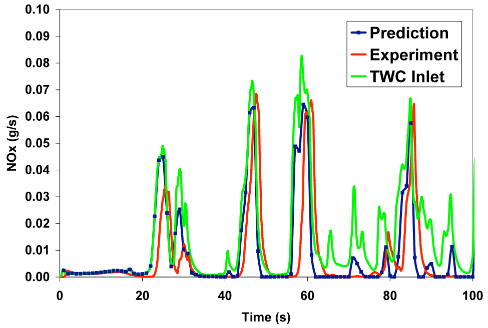


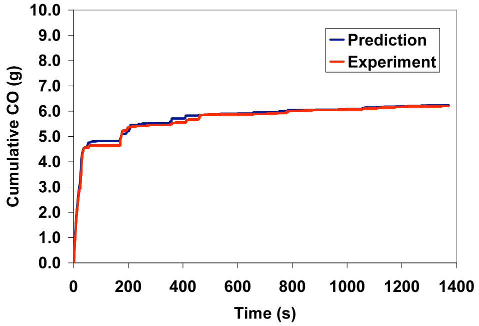








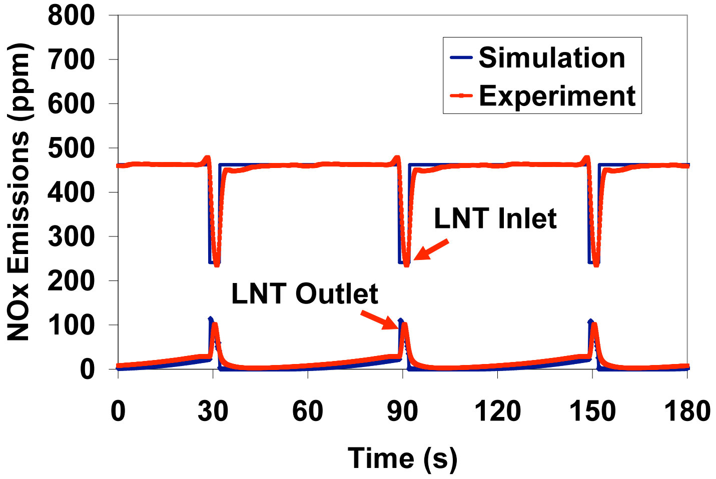




LNT model : sample results

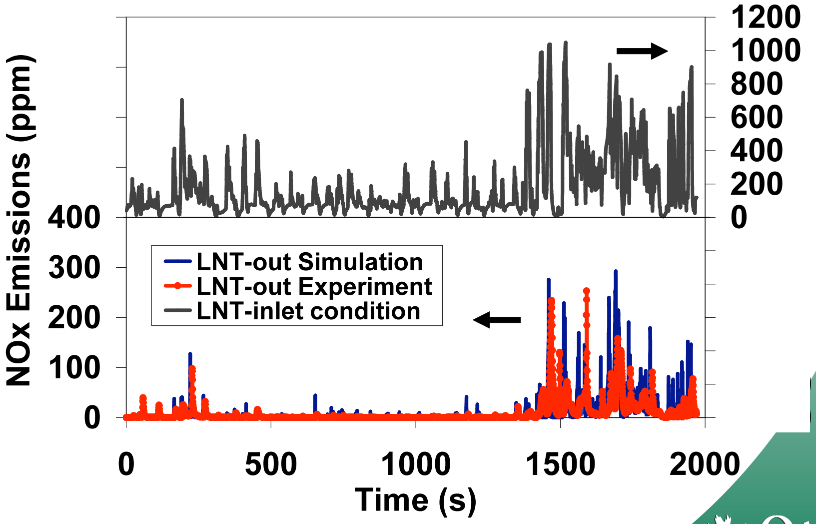
Features :

- transient 1-D model
- 14 reactions account for o2 storage, NO oxidation, NOx storage (nitrite/nitrate form), release and reduction of NOx with CO (+ H2) & Hcs
- shrinking core model for NOx storage (based on Olsson & Blint, Ind. Eng. Chem. Res., 2005
- caibrated originally using data generated for a Umicore catalyst using CLEERS experimental protocol, chemical kinetic rates in the version used for this study were adjusted to match with engine test data
- aging submodel based on exp. data (fresh catalyst is used here)



validation :

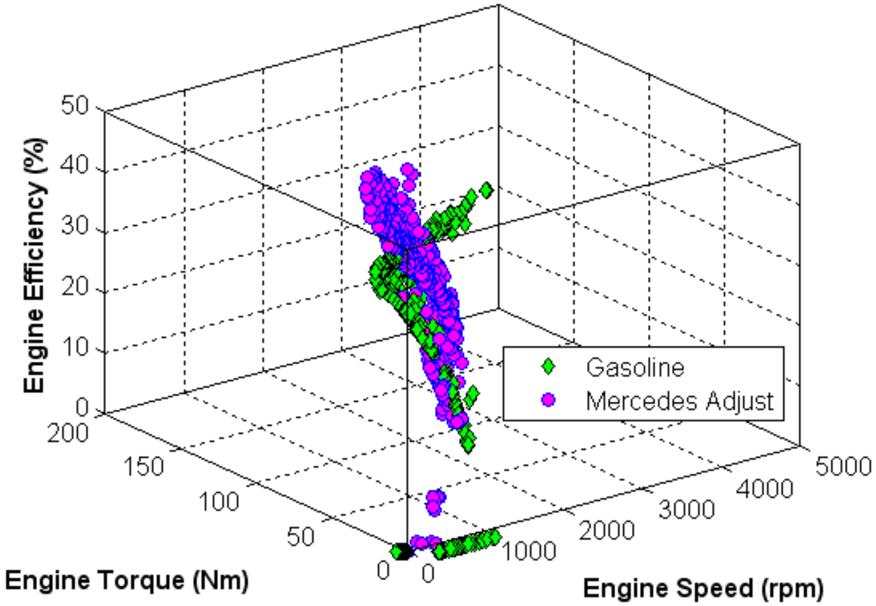
- Data from tests using Mercedes 1.7L engine
- steady state cycling (57s lean, 3s rich)
- Combined UDDS+US06 drive cycle
  - LNT-out NOx: 0.046g/mi (model) vs. 0.035g/mi (test)
  - NOx Reduction: 94.1% (model) vs. 95.5% (test)



Gasoline vs. diesel HEVs comparison indicates large diesel fuel economy benefit

Simulation parameters:

- **Prius HEV, 28% serial- 72% parallel**
- **Hot start UDDS cycle**
- **1.3 kWhr battery charge (65%)**
- **1.5 L stoichiometric gasoline engine with Atkinson cycle (map available in PSAT), TWC**
- **1.5 L diesel engine (performance scaled down from a 1.7 L Mercedes A170 map), no NOx/ PM control**



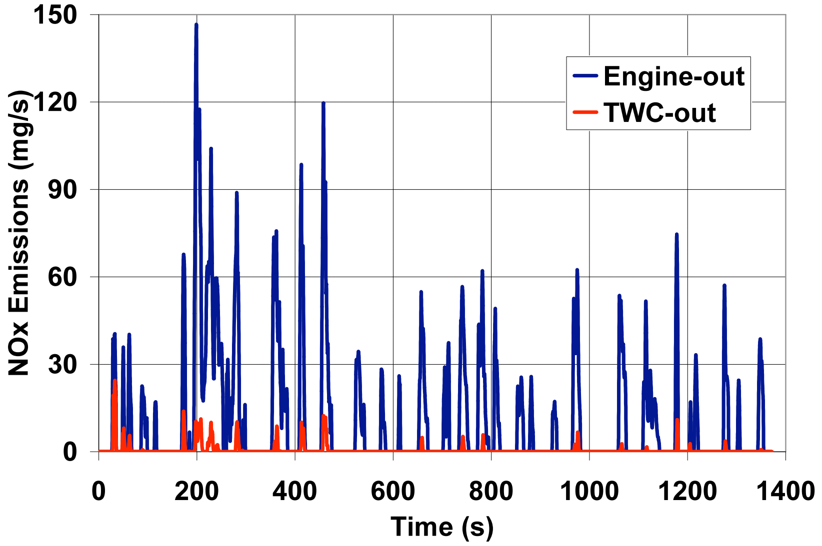
Results:

- **84.2 mpg diesel vs. 70.7 mpg gasoline (SAE 2007-01-0281 reports 71.2 mpg for Prius)**
- **Max engine efficiency: 41% diesel vs. 37% gasoline**
- **Cycle average engine efficiency: 36% diesel vs. 34% gasoline**
- **Diesel (without aftertreatment) has 19% better MPG, 5.4% better energy efficiency***
- ***Better mpg in case of diesel is partly due to higher density of diesel compared to gasoline**

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

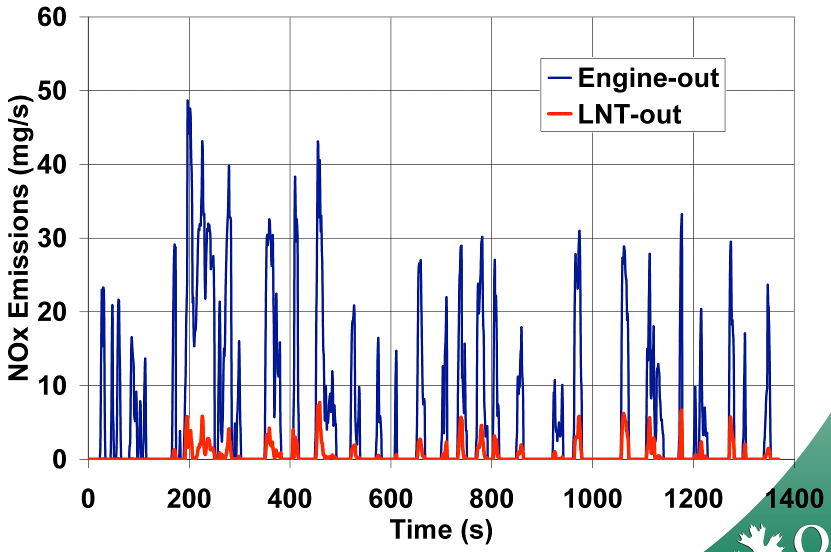
Simulation parameters:

- Prius HEV
- Hot start UDDS drive cycle
- 1.3 kWhr battery charge (65%)
- 1.5-L gasoline and diesel engines
- 2.2-L TWC and 2.2-L LNT



Results:

- 81.6 mpg diesel vs. 70.7 mpg gasoline
- Regen pulse adjusted till cumulative NOx emissions fall below regulated limit
- NOx emissions : 0.09 g/mile from LNT vs. 0.10g/mile from TWC
- 92% NOx reduction (LNT) vs. 96% NOx reduction (TWC)
- LNT fuel penalty for diesel 3.1%
- With LNT, diesel efficiency advantage is just over 2%



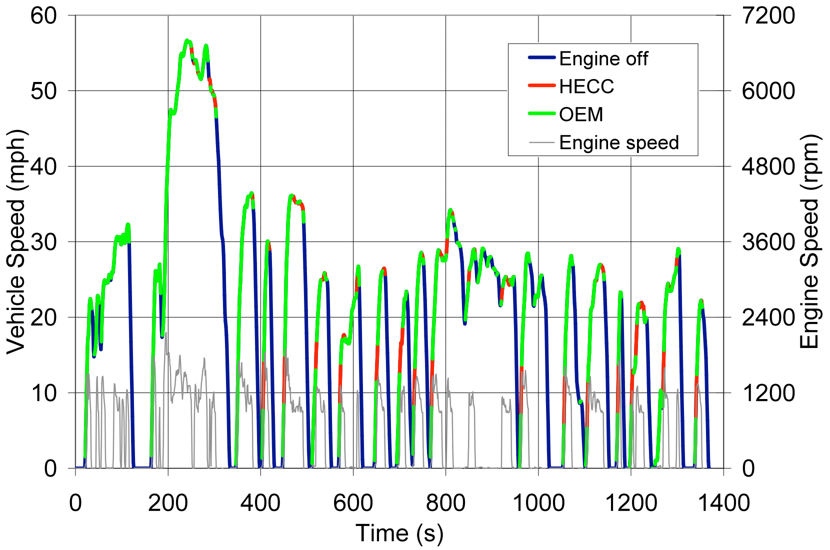
Current High Efficiency Clean Combustion (HECC) only has modest HEV efficiency benefit

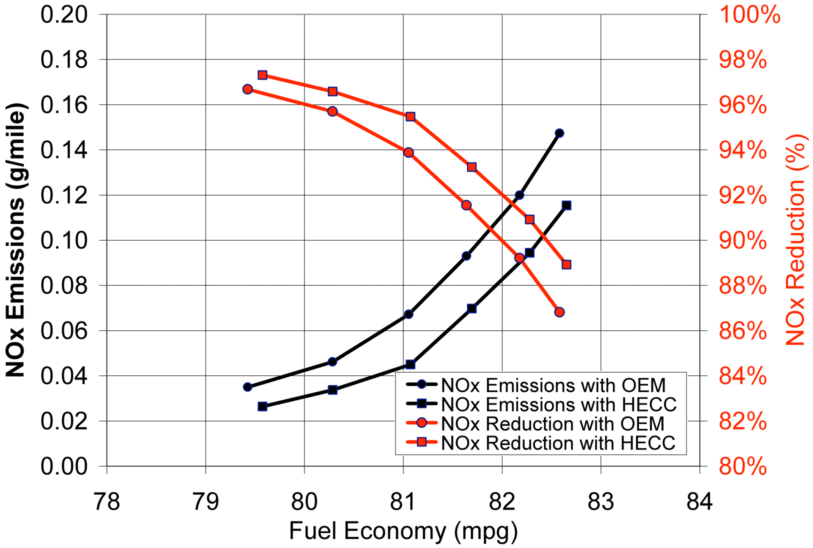
Simulation parameters:

- Prius HEV
- Hot start UDDS drive cycle (1372s and 7.45mile)
- 1.3 kWhr battery charge (65%)
- 1.5-L diesel HECC-capable engine
- 2.2-L LNT NOx control
- Variable regeneration duration (3-8s)

Results:

- HECC boosts fuel economy around 0.8% (82.3 vs. 81.6 mpg)
- HECC benefit limited by small operating range:
  - Engine is on for 560s
  - Engine in HECC model for 120s (20% total engine on time)
- Demonstrates need for increasing HECC range (currently being worked on)





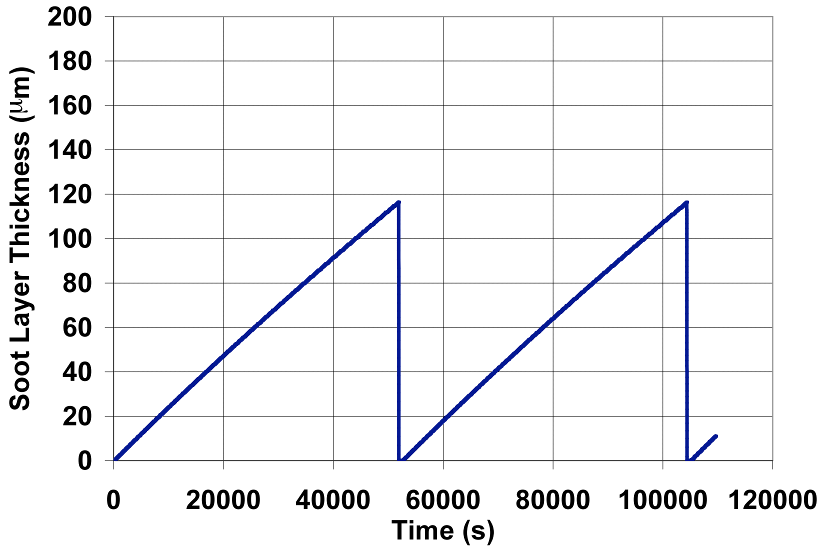
DPF particulate control also has a big impact on diesel HEV efficiency

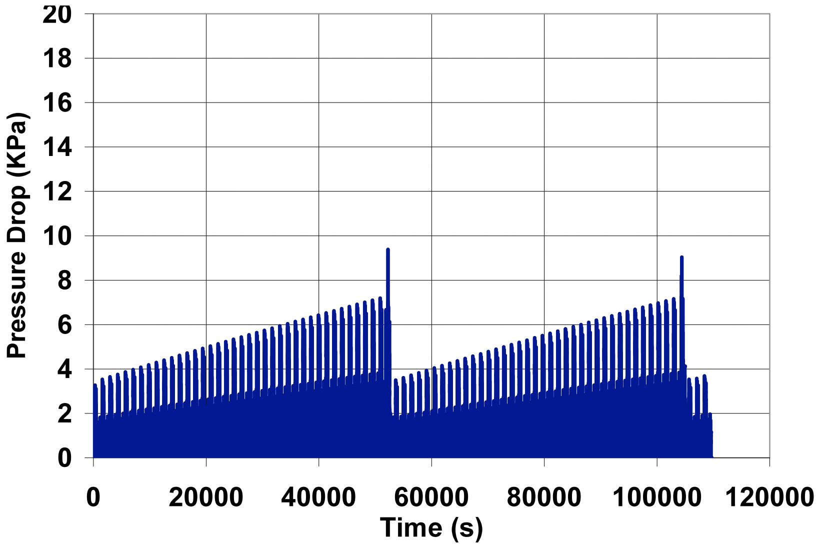
Simulation condition:

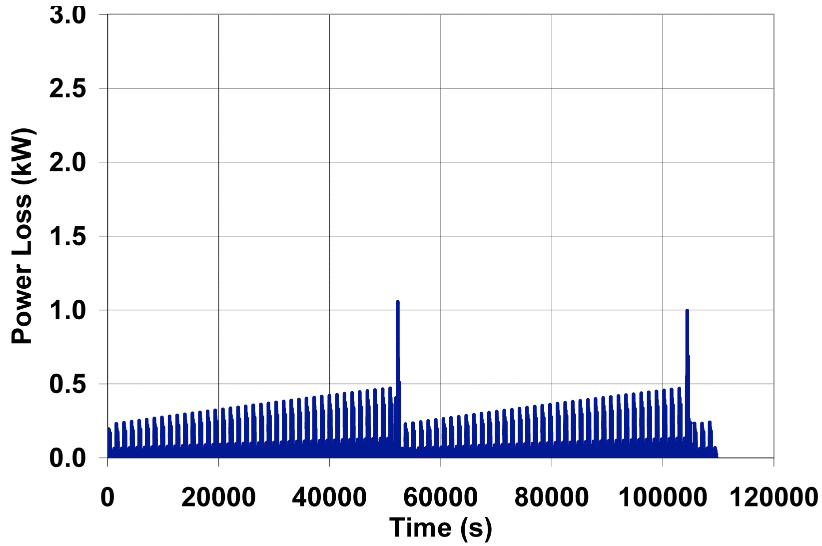
- 80 consecutive UDDS drive cycles on Prius
- Cold start and 1.2kWh battery charge
- 1.5-L diesel engine
- 2.1 L Non-catalytic DPF
- DPF controlled regen for 600s (SAE 2007-01-3997)
- regen approximately every 40 cycles (15 hours)

Results:

- Overall (80 cycle) fuel penalty for DPF 2.9%
- Penalty from regen fueling boost and DPF pressure drop







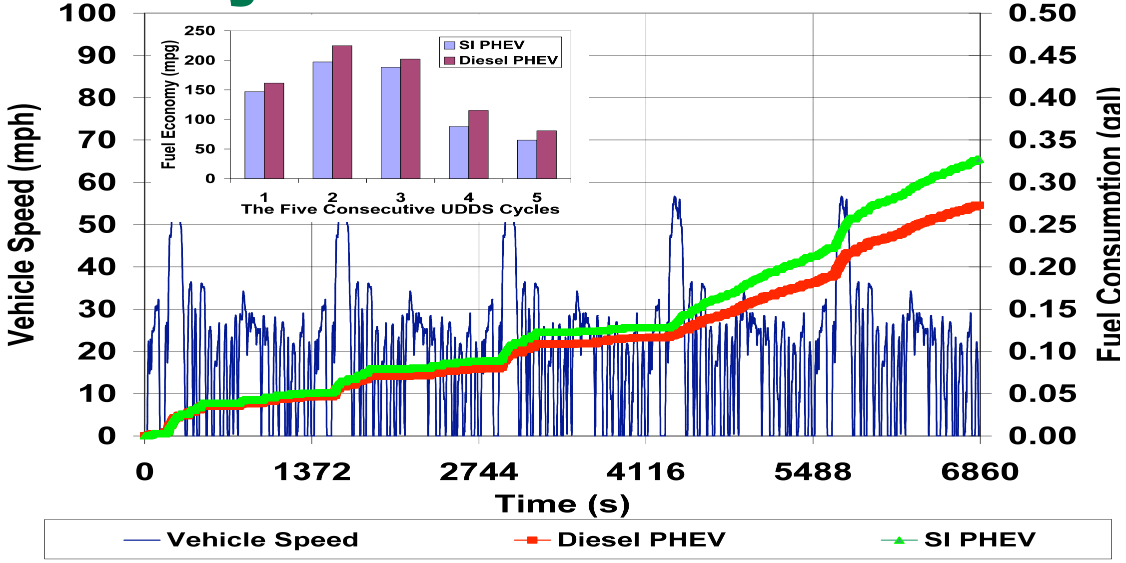
PHEV baseline comparison indicates large potential diesel efficiency benefit similar to HEV

Simulation condition:

- **Prius PHEV**
- **5 consecutive UDDS cycles**
- **Cold start, 5 kWh charge (100%)**
- **1.5-L gasoline engine w TWC**
- **1.5-L diesel engine w no NOx/PM control**

Results:

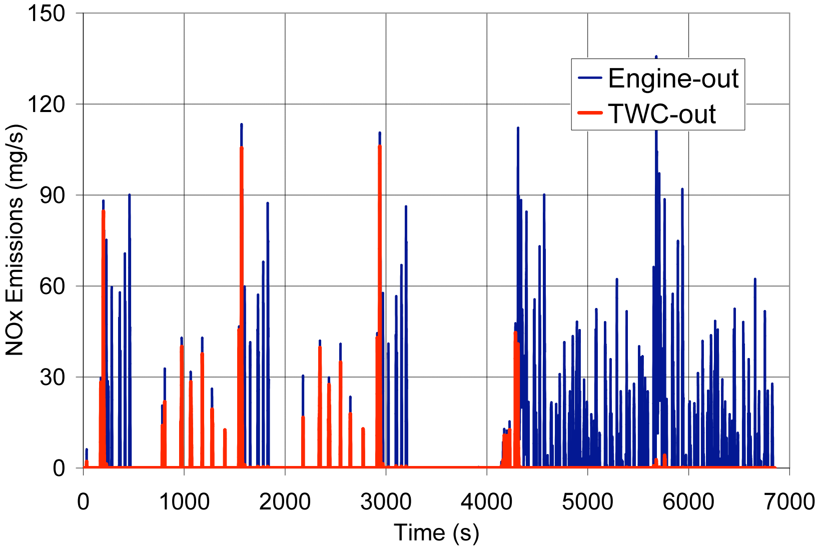
- Overall 19.9% better mpg for diesel (6% higher energy efficiency)



UDDS Cycle number		1	2	3	4	5	Total
Fuel economy (mpg)	Gasoline	147.1 (148*)	197.2 (200*)	188.2 (187*)	88.1 (74*)	65.0 (66*)	113.8 (108.9*)
	Diesel	161.3	224.7	202.0	115.2	80.9	136.5
Battery energy consumption (kWh)	Gasoline	0.74 (0.93*)	0.95 (0.96*)	0.92 (0.94*)	0.47 (0.23*)	0.03 (-0.12*)	3.11 (2.94*)
	Diesel	0.72	0.93	0.87	0.54	0.02	3.08

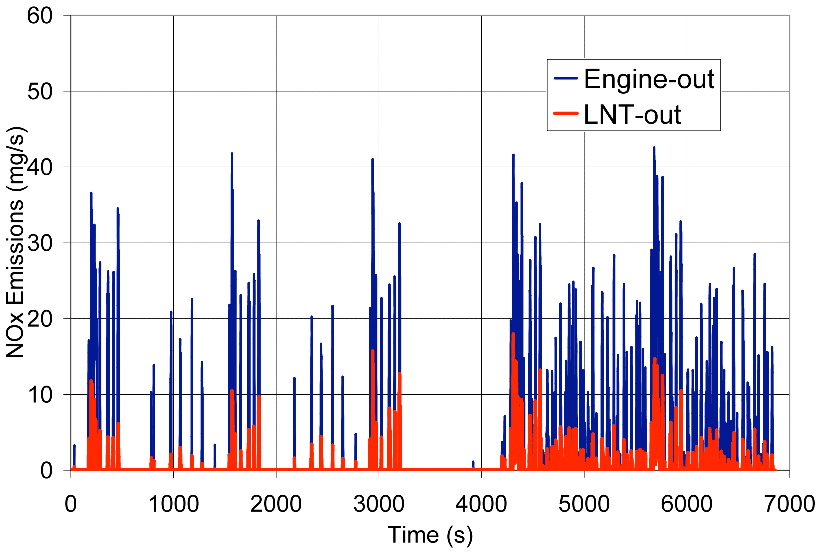
*** data from SAE 2007-01-0283**

However, NOx control also significantly impacts expected diesel PHEV efficiency



Simulation condition:

- Prius PHEV
- 5 UDDS drive cycles
- Cold start, 5 kWhr initial charge (100%)
- 1.5-L stoichiometric gasoline engine w TWC
- 1.5-L diesel engine with LNT



Results:

- Diesel mpg drops from 136.5 to 132.4 (3% LNT fuel penalty)
- Diesel still 3% better than gasoline
- Regen pulse width increased till NOx emissions drop to 0.11g/mile

Summary

- Systems simulations indicate that diesel engines offer significant potential fuel efficiency advantages for HEVs and PHEVs, but these advantages are likely to be reduced (or perhaps even eliminated) by fuel penalties associated with lean NOx and PM controls
- Use of both LNT and DPF may result in SI engine based hybrid vehicle being more efficient
- Studies are needed to determine if urea-SCR (or LNT-SCR combination) based lean NOx control may be a better option for lean HEVs and PHEVs.
- Comparative studies are needed for HEVs and PHEVs powered by lean gasoline engines vs. diesel engines.

Significance

- **Current HEV and PHEV systems typically involve frequent engine idling and/or restarts which can have large impact on emissions**
  - **Our engine and aftertreatment models are physically-based**
    - **a significant departure from the modus operandi of PSAT**
    - **can deal arbitrary transients and respond to to any input drive cycle**
    - **qualitatively respond appropriately even if quantitative predictions are off**
    - **validation against experimental data is done whenever possible**
- **Unexpected results while comparing diesel vs gasoline hybrids**
  - **efficiency advantages of diesel diminish significantly due to after-treatment requirements, an observation that merits further scrutiny of results**

Planned Future Activities

- Stoichiometric hybrid simulation (e.g., Prius-type engines)
  - develop second generation transient model with coolant thermal storage included
- Lean hybrid simulations (e.g., VW Rabbit, GM 1.9L engine)
  - continue comparison of diesel and SI HEV fuel efficiency and emissions
  - evaluate urea-SCR, LNT-SCR combinations for NOx control
  - expanded PCCI (HECC) regimes of operation (might increase efficiency)
- Further development of engine scaling methodology
- Exhaust heat recovery
  - Rankine bottoming cycles
  - thermo-electric device sub-model