Advanced PHEV Engine Systems and Emissions Control Modeling and Analysis

Project ID: vss041

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Overview

- **Timeline**
  - Start
    - 2005
  - Finish
    - Ongoing
- **Budget**
  - FY09 Funding
    - $700K
  - FY10 Funding
    - $350K
    - Reorganized modeling team and reduced work scope
  - FY11 Funding
    - $250K
    - Additional reorganization and reduction in 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 and emissions controls
- **Partners**
  - DOE Diesel Crosscut Team companies and CLEERS consortium of suppliers, national labs, and universities
  - Company and university participants in ACE/HCCI consortium
  - ANL, 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**
  - **Impact of engine start-stop and cold ambient**
  - **Alternative engine-aftertreatment component configurations and controls**
  - **Alternative engine and battery management strategies**
  - **Advanced combustion (HCCI, PCCI) versus conventional (SI, diesel)***
  - **Non-petroleum and bio-derived fuels***
  - **Thermal management (exhaust heat utilization for power)***

*** Reduced priority in response to budget reductions, reviewer comments**

Vehicles

Engines

Emissions Controls

Simulation Models

Relevance

2.2 Vehicle and Systems Simulation and Testing*
"VSST includes crosscutting activities not specifically tied to battery and electric of hybrid drive technologies; rather they tie all of the VTP hardware R&D together. The VSST activity comprises work in five areas: 1) **modeling and simulation**; 2) **component and systems evaluations**; 3) laboratory and field vehicle evaluations; 4) electric drive vehicle codes and standards; and 5) heavy vehicle systems optimization. This subprogram includes **all** of VTP's efforts directly related to the **planning and modeling, development, and evaluation of advanced hybrid**, electric, and **plug-in hybrid drive systems for passenger and commercial vehicles**. The subprogram also **conducts simulation studies, component evaluations**, and testing to establish needs, goals, and component/vehicle performance validation. This subprogram's funding contributes to the 21CTP and FreedomCAR and Fuel Partnership."

Evaluation of advanced hybrid technologies involves multiple critical 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).**

Bridging across OVT portfolio:

- **Links to 2011 MYPP* 2.3.1 (Combustion & Emission Control), 2.4.1 (Fuels Technology), 2.5.2 (Propulsion Materials), and 2.5.3 (High Temperature Materials)**
- **Links with industry partners: DOE Advanced Engine Crosscut Team, USCAR Advanced Combustion and Emission Control Tech Team, CLEERS partners**

***Reference: Vehicle Technologies Multi-Year Program Plan 2011-2015:**
http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/vt_mypp_2011-2015.pdf

This activity integrates a large portion of OVT's advanced engine and emissions control data and models into the systems level context

"Without aftertreatment constraints in the simulation, the model might allow engine system operation outside the emission-constrained envelope."

– National Academy of Science study on reducing fuel consumption from MD and HD vehicles (ISBN: 0-309-14983-5)

EERE VT Vehicle Systems Activities

Vehicle System Model Accountable for Emissions

EERE VT ACE and Fuels Activities

Automotive Product Component Level Model Development (Engine-Input Ready)
[capable in real engine exhaust]

Coated Catalyst (Automotive Product) Studies and Model Development
[based on controlled simulated exhaust]

Office of Science Activities

Multimode Project ($200k)
[Engine-based catalyst studies and model validation for advanced combustion modes]
Agreement 12249

Lean Gasoline Project ($200k)
[Engine-based catalyst studies and model validation for lean gasoline engines]
Agreement 9248

CLEERS Project ($500k)
[Kinetics measurement, model development, model validation]
Agreement 8746

PreCompetitive R&D Project ($200k)
[Catalyst chemistry studies for new formulations]
Agreement 8744

Other Supporting Projects:

- Pathways for Efficient Emission Controls (*Agreement 10040*)
- Neutron Imaging (*Agreement 19272*)
- NPBF Fuels Program

Milestones

- **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- Published in Int. J. Eng. Res. 2010, vol. 11, pp 137-151.**

- **FY11 Milestone: Publish transient hybrid drive cycle simulation results comparing diesel and gasoline HEV and PHEV fuel efficiencies and emissions performance with accounting of relative fuel penalties for emissions controls and intermittent engine operation during hybrid drive cycles. (September 30, 2011)- Accepted for publication in the Journal of Automotive Engineering, February 2011.**

General 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)**
  - **Validated lean NOx/PM/HC/CO aftertreatment component models**
  - **Integrated lean engines & aftertreatment**
  - **Efficiency benefits of lean vs. stoichiometric**
  - **Advanced combustion modes (HCCI, PCCI)***
  - **Conventional & bio fuels***
- **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)**
  - **Measurements and simulations of environmental compliance**
  - **Data for unconventional and bio-derived fuels***
  - **Measurements and simulations of exhaust thermal management concepts (bottoming cycles, thermo-electrics, thermo-chemical recuperation, and thermal storage)***

*** Reduced priority in response to budget reductions, reviewer comments**

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 are highly temperature dependent**

2010-2011 Accomplishments/Progress

- **Continued simulations of stoichiometric versus lean HEVs and PHEVs (risks/benefits of diesel/lean gasoline HEVs/PHEVs)**
  - **Published methodology in Journal of Automobile Engineering**
  - **Demonstrated significant efficiency advantage for urea-SCR vs. LNT NOx control in diesel PHEVs**
  - **Demonstrated impact of thermal insulation on aftertreatment catalyst performance in both gasoline and diesel HEVs**
- **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)**
- **Transferred and demonstrated 3-way catalyst model from PSAT to AUTONOMIE for stoichiometric PHEV simulations**
- **Initiated collaboration with ANL on effects of cold ambient on aftertreatment and PHEV emissions performance**
- **Developed preliminary engine maps for BMW series 1 lean-GDI vehicle**
- **Published low-order systems simulation model for predicting NOx and PM emissions from diesel engines operating in HECC modes**

Example Accomplishment Details

We generated preliminary engine maps and emissions data for the BMW DISI series 120i

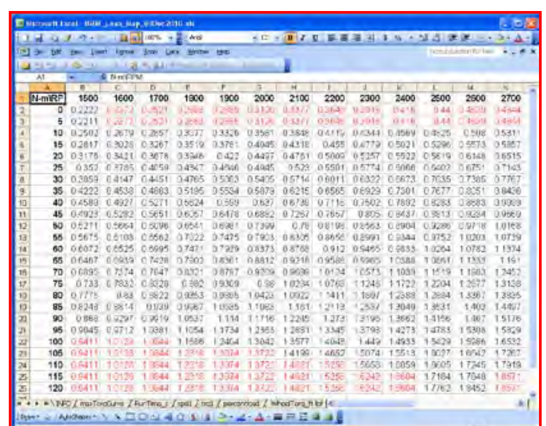
- **Chassis dyno data for BMW vehicle supplied by GM**
  - **Not HEV but serves as a model for state-of-the-art DISI engine (1.9-L) + TWC & LNT**
  - **Max engine efficiency 41%**
  - **4-15% FTP fuel economy boost over conventional gasoline**
  - **Lower PM emissions than light-duty diesel**
  - **NOx emissions > US Tier II Bin5**

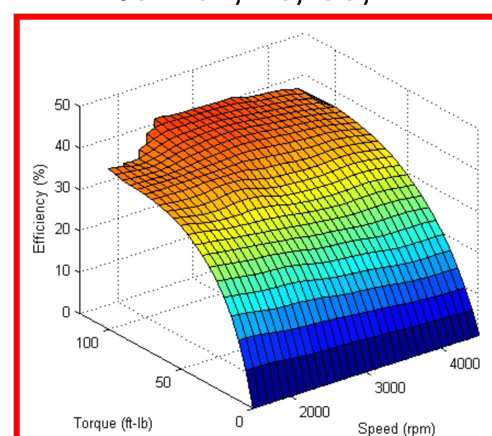
TWC/LNT data:

- **NOx reduction**
- **HC/CO reduction**

Engine map includes:

- **Fuel consumption**
- **E/O temperature**
- **E/O NOx, HC, CO, PM**

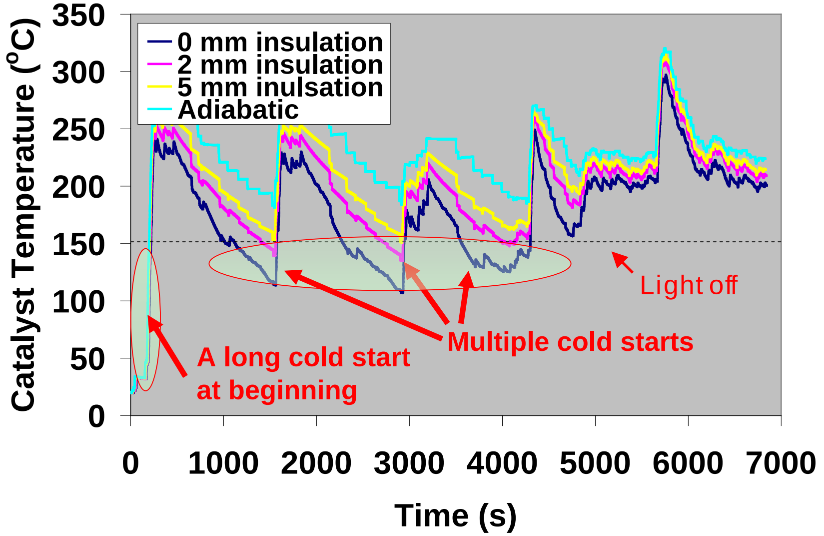




We are using our dynamic NOx component models to study effects of drive cycle transients

Example case study:

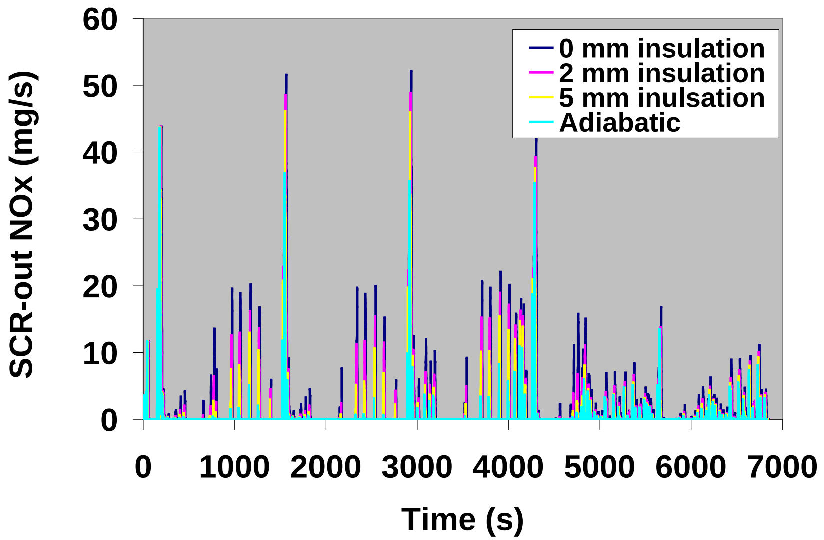
- 1542 kg, 1.5-L diesel PHEV
- 5 kWh, 24 Ah battery (full initial charge)
- 5 UDDS cycles beginning with cold start
- 2.4-L urea-SCR (Cu-ZSM-5 cat) for NOx control
- Varying level of mineral fiber cat insulation
- Non-optimized urea control



Observations:

- Insulation keeps SCR catalyst warm enough to reduce impact of cold starts
- Higher temperatures may accelerate aging
- Insulation reduces NOx and NH_3

Insulation (mm)	NOx (g/mile)	NH_3 (g/mile)
0	1.59E-01	6.84E-02
2	1.17E-01	4.83E-02
5	9.46E-02	3.48E-02
Adiabatic	6.83E-02	9.66E-03



We have been validating our DOC component model against experimental data

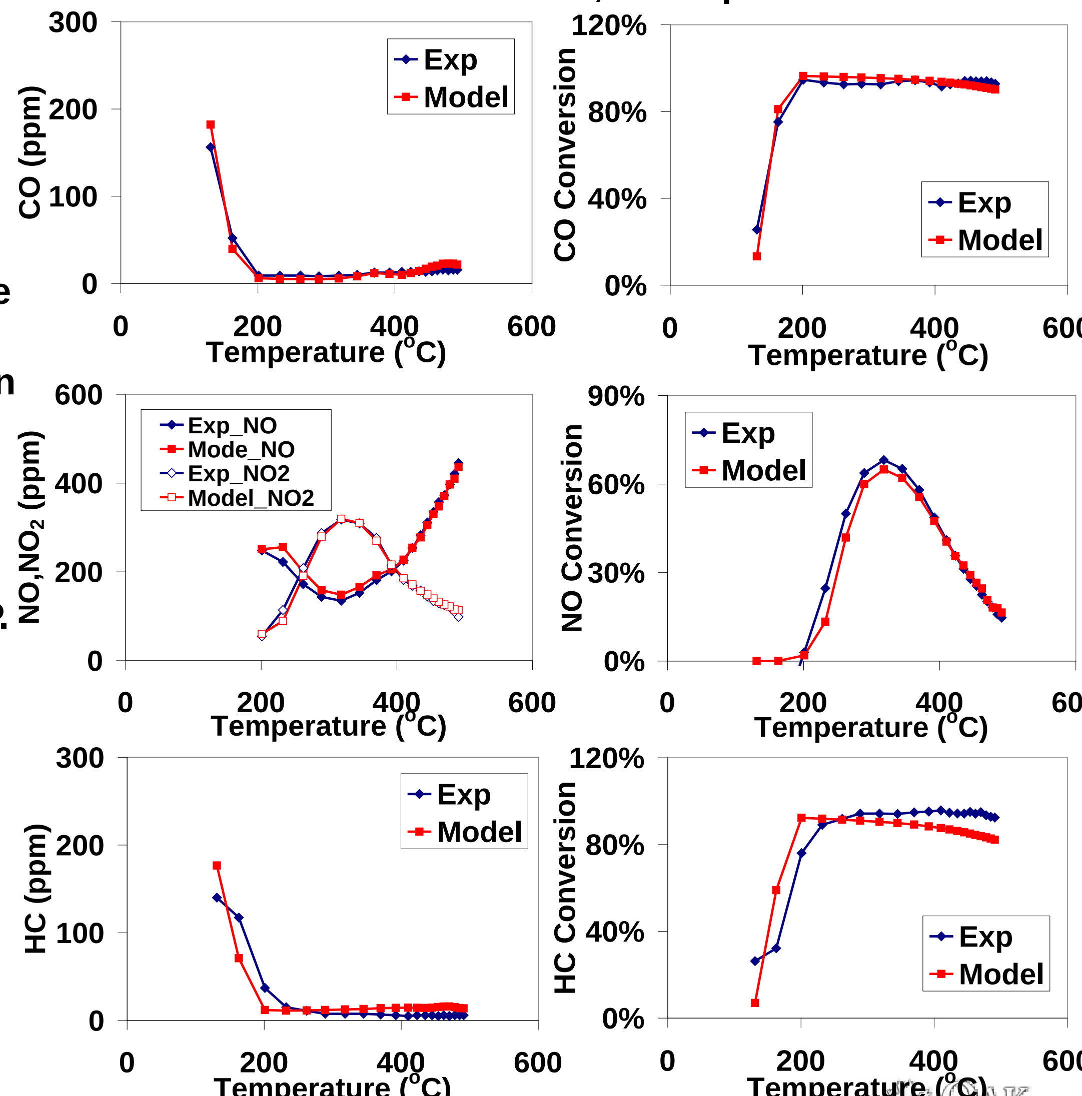
ORNL DOC model

- DOCs are critical for lean NOx, HC/CO, and particulate control
- Three global reactions: (1) CO oxidation, (2) NO oxidation, (3) HC oxidation
- Adjustable configurations needed relative to DPF, LNT, SCR aftertreatment components for simulating diesel and lean gasoline hybrids

Model validation

- Steady-state experimental engine dynamometer data from public-domain (P. Triana, Dissertation, MTU, 2005)
- 8.1L John Deere 6081H engine
- Johnson Matthey 4.9L DOC
- 5%-100% load at 1400rpm-2200rpm
- Exhaust temperature range 131-491°C

5-100% load, 1400 rpm



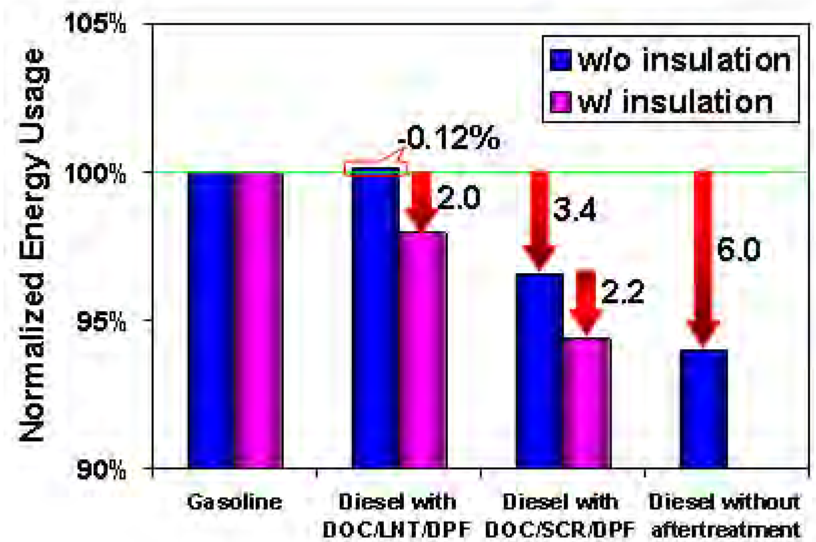
We are linking component models together to study fully integrated aftertreatment trends

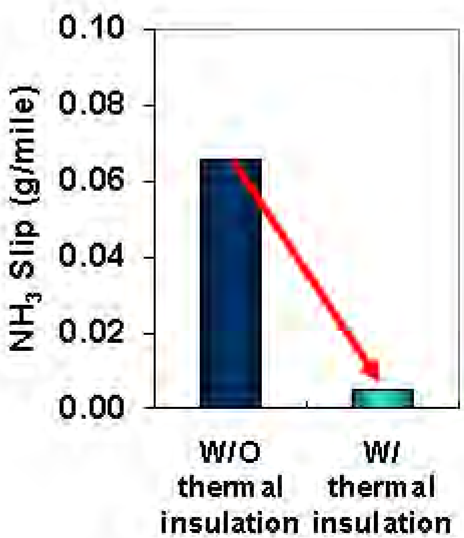
Example case study

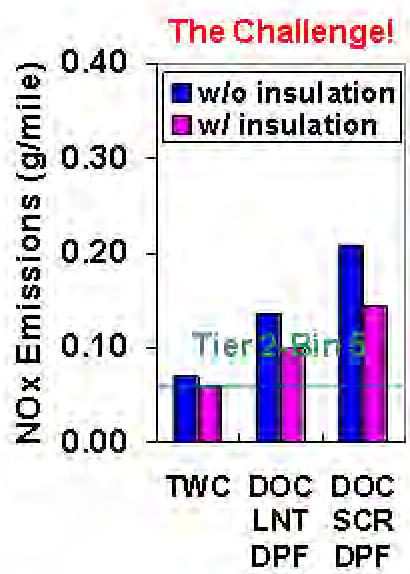
- 1450kg HEV (Gasoline vs. Diesel)
- 80 UDDS drive cycles
- 3.0mm mineral fiber insulation on catalysts
- Non-optimized NOx and PM controls

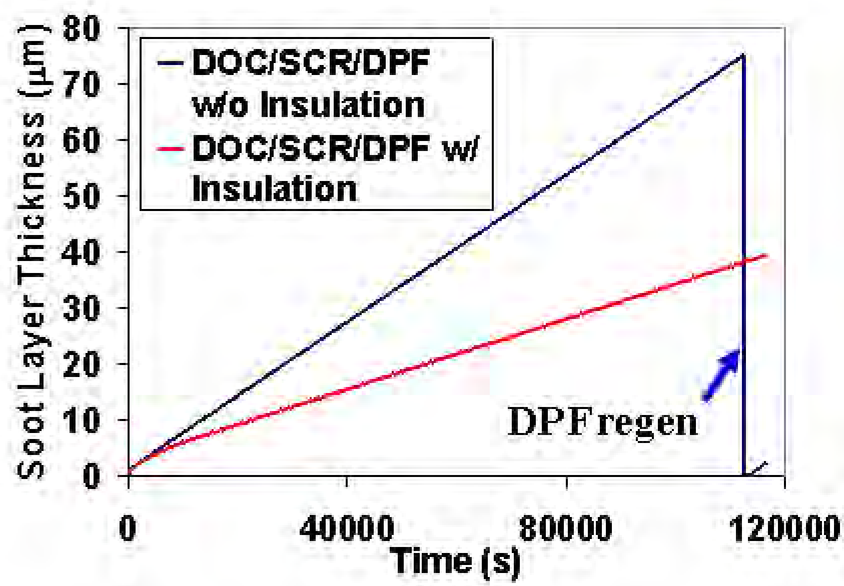
Observations

- Insulation improves fuel economy
- Enhances CDPF self regeneration
- Reduces NOx and NH_3 emissions
- May accelerate aging









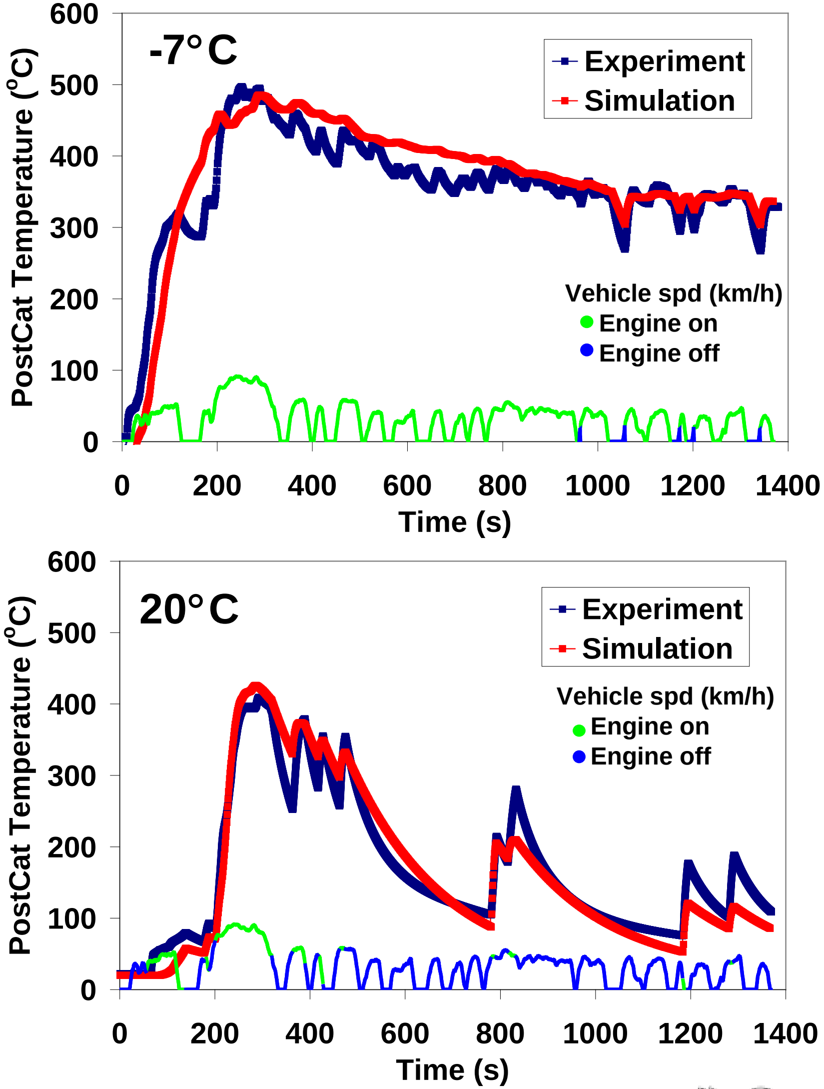
We are working with ANL to simulate cold ambient effects on HEV & PHEV TWC performance

Experimental ANL chassis data

- Hymotion PHEV Prius w/TWC (2.1-L)
- 1.5 L stoichiometric gasoline engine
- UDDS cycles with cold start (-7°C vs. 20°C ambient temperatures)
- 24 AH initial battery charge (full)

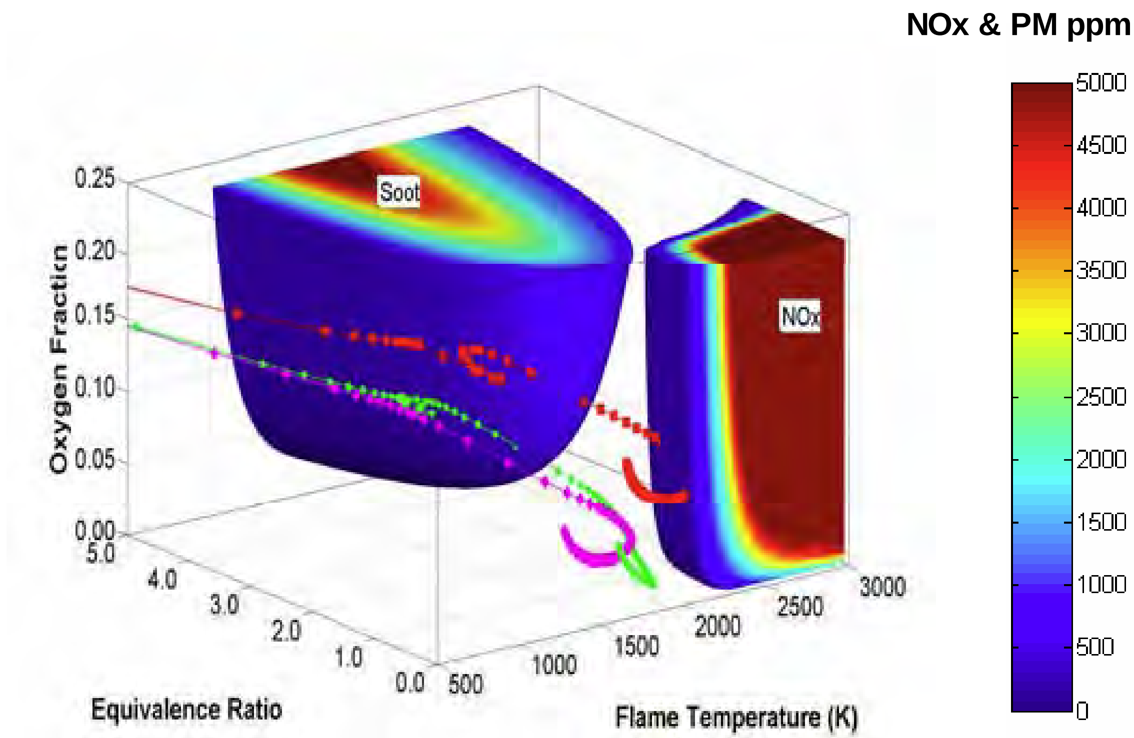
Objectives

- Validate model predictions for engine out and catalyst temperature
- Assess measured vs. predicted emissions
- Implement ANL cold-effect fuel consumption correlations
- Evaluate different engine control strategies including extreme cold ambient conditions
- At 20°C ambient, engine little utilized
- At -7°C ambient, engine heavily utilized



We also developed a component model for diesel engine advanced combustion emissions

- **Model computes 3D in-cylinder combustion trajectories correlating with NOx, PM**
- **Low-order, very fast computations suitable for systems simulations**
- **Can be used to correlate experimental data for emissions maps or predict maps when data are unavailable**
- **Compares favorably with KIVA**



Depicted Trajectories: Red symbols correspond to conventional combustion, green symbols to high dilution combustion (HDC), and pink symbols to high efficiency clean combustion (HECC).

This project integrates multiple collaborations*

- **Advanced Combustion MOU**
  - Shared data, models for advanced lean combustion modes
- **Advanced Combustion and Emission Control Team**
  - Reviews at USCAR of systems simulation results
  - Industry guidance on priorities for advanced combustion for HEVs and PHEVs
- **Advanced Engine Crosscut Team**
  - Reviews at USCAR of systems simulation results
  - Industry guidance on priorities for vehicle systems emissions controls
- **Crosscut Lean Exhaust Emission Reduction Simulation (CLEERS)**
  - Shared emissions control data and models with PNNL and SNL
  - Industry surveys on emissions control priorities
  - Supplier donated catalysts
- **Direct industry partnerships**
  - Application of tools to Arvin Meritor CRADA on HD HEVs (See poster VSS062)
  - Industry supplied engines and aftertreatment components (e.g., BMW from GM)
- **ANL**
  - Data, component models, AUTONOMIE support

***Partners include: UM, UW, SNL, ANL, PNNL, Cummins, Caterpillar, Chrysler, DDC, Ford, GE, GM, John Deere, Volvo, International, BP, Conoco Philips, ExxonMobil, Chevron, Shell, EPA, TACOM, Arvin Meritor, Umicore, Delphi, BASF, Corning, Johnson Matthey**

Proposed Future Activities*

- **Gasoline hybrid simulations**
  - Complete cold ambient transient engine/aftertreatment model verification/validation with ANL
  - Continue refinement and validation of AUTONOMIE 3-way catalyst model
  - Improve engine transients model predictions of unburned HC (cold and warm start)
  - Develop and implement HC trap simulation capability in AUTONOMIE (Supports #VSS013)
  - Demonstrate DISI gasoline HEV and PHEV simulations
- **Diesel hybrid simulations**
  - Implement lean NOx and PM aftertreatment models in AUTONOMIE
  - Continue comparisons of diesel and gasoline HEV/PHEV fuel efficiency and emissions
  - Implement hybrid vehicle simulations with advanced diesel combustion modes in AUTONOMIE
  - Evaluate more optimal control of urea-SCR and DPF operation in diesel hybrids
  - Adapt engine and aftertreatment models for HD hybrids (Supports Arvin Meritor CRADA, #VSS062)
- **Maximum efficiency genset analysis and simulation**
  - Summarize current genset efficiency limits and their thermodynamic basis
  - Identify most promising technology options for stretching genset efficiency limits
  - Develop simulation models to evaluate thermodynamic potential of most promising options
- **Coordination**
  - Continue integration of VSST activities to maximize leveraging with Combustion MOU, ACEC, AECC, CLEERS and maximize relevance to latest engine/emissions technology and industry needs

*** Activities in each category are listed in order of priority but specific plans are currently awaiting resolution of budget uncertainties**

Summary

- Published transient engine simulation methodology for HEVs and PHEVs
- Published LNT model for NOx control simulations in lean exhaust hybrids.
- Published methodology for using systems simulations to compare risk/benefits of diesel vs. conventional gasoline HEVs and PHEVs.
- Published low-order model for simulations of advanced diesel combustion.
- Demonstrated fuel efficiency advantage for urea-SCR NOx control vs. LNTs in diesel HEVs and PHEVs.
- Demonstrated benefits of thermal aftertreatment insulation for diesel HEVs and PHEVs.
- Transferred and demonstrated 3-way catalyst model in AUTONOMIE.
- Developed engine maps for BMW series 1 lean GDI vehicle.

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