VSS041 Advanced Light-Duty Engine Systems and Emissions Control Modeling and Analysis

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Lead, Vehicle and Systems Simulation and Testing (VSST)

Office of Vehicle Technologies

US Department of Energy

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY

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OVERVIEW

Timeline • Project start date: Oct. 2011 • Project end date: Continuing • Just started	**Barriers*** • Risk aversion • Cost • Constant advances in technology • Computational models, design, and simulation methodologies **from 2011-2015 VTP MYPP*

Budget (DOE share)
 	
• New project, no FY11 funding
• FY12 funding: $200K
	Partners
	
	• Argonne National Laboratory
	• USDRIVE Advanced Combustion and Emissions Control Technical Team
	• DOE Advanced Engine Crosscut Team
	• CLEERS Collaborators
	• Oak Ridge National Laboratory
	  – Fuels, Engines, & Emissions Research Center
	  – Vehicle Systems Integration (VSI) Laboratory

OBJECTIVE: Reduce petroleum consumption for light-duty (LD) vehicles through advanced powertrain hybridization

"WHY"

- **Hybrid powertrains offer potentially large reductions in fuel consumption, criteria pollutants and green house gas emissions.**
- **The most fuel efficient LD combustion engines utilize advanced lean-burn technology (diesel or lean gasoline), which requires lean exhaust aftertreatment.**
- **LD powertrain hybridization requires globally optimizing the fully integrated aftertreatment , engine, and battery systems to meet efficiency targets and satisfy emissions constraints**

"HOW"

- **Develop and validate accurate component models for simulating integrated engine, battery, and aftertreatment systems in LD passenger vehicles.**
- **Evaluate the merits of specific alternative hybrid engine-battery-aftertreatment configurations and control strategies under realistic LD drive cycle conditions.**
- **Use the results to identify promising paths for improving LD drive-cycle energy efficiency, fuel mileage and emissions.**

Integrated vehicle simulation is essential for proper development, evaluation, and validation of emerging high risk, long term advanced transportation technologies.

RELEVANCE (1): Targets VT 2011-15 Multi-Year Program Plan*

- Supports LD hybrid simulation with advanced powertrains and emissions constraints:
  - Models for advanced LD diesel and lean gasoline combustion engines.
  - Models for advanced emissions controls components.
  - Methodologies for integrating engine and emission components under transient drive cycle conditions.
- Directly supports 3 VSST cross-cutting activities:
  - Modeling and simulation; component & systems evaluations; passenger vehicle systems optimization.
- Indirectly supports VSST laboratory and field vehicle evaluations.
- Addresses the following VSST Barriers:
  - Risk aversion: Develop, guide, and verify passenger hybrid system concepts through integration of model-based simulation and analysis with experimental measurements.
  - Cost: Utilize facilities and core technical expertise at ORNL VSI laboratory + data and models from other OVT projects and CLEERS to leverage resources.
  - Constant advances in technology: Emphasize advanced LD combustion engine and lean aftertreatment technologies for reducing petroleum consumption and meeting increasingly stringent emissions regulations.
  - Computational models, design, and simulation methodologies: Combine fundamental physics and chemistry with best available lab and dynamometer data to maximize accuracy of simulations.

*http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/vt_mypp_2011-2015.pdf

RELEVANCE (2): Bridges multiple R&D areas in both the Office of Vehicle Technologies and Office of Science

EERE VT Vehicle Systems Activities

Vehicle System Models Accountable for Emissions

EERE VT ACE, Fuels, and VSS 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

Industry Access to Specialized Tools and Data

Basic Combustion and Surface Chemistry Measurement and Modeling
[CRF, CNMS, HTML, EMSL]

PreCompetitive R&D
[Catalyst chemistry studies for new formulations]

CLEERS
[Kinetics measurement, model development, model validation]

Diesel Emissions R&D
[Engine-based catalyst studies and model validation for advanced diesel engines]

Advanced Combustion R&D
[Engine-based combustion mode and stretch efficiency analysis and demonstration]

Other Supporting Projects:

- Advanced LD Engines and Emissions Modeling
- Pathways for Efficient Emission Controls
- Neutron Imaging
- NPBF Fuels Program

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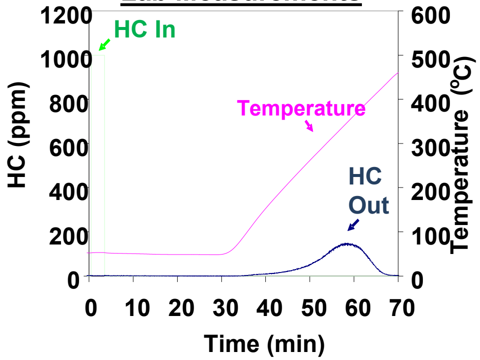
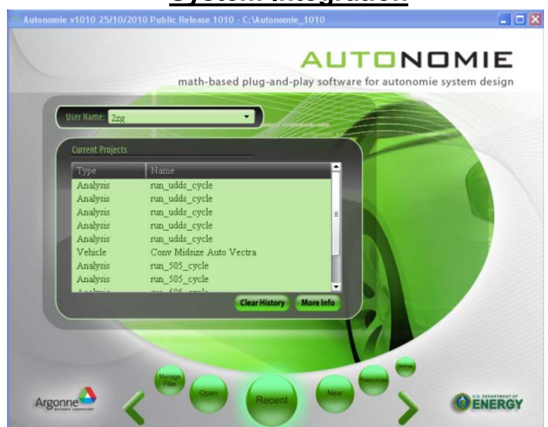
APPROACH: Develop , implement, & exercise key component models

- **Engine components**
  - Steady-state and transient LD engine maps from dyno measurements and models for advanced combustion
- **Aftertreatment components**
  - Update previous models (LNT, SCR, DOC, DPF, and TWC), develop new models (e.g., passive adsorbers).
- **Advanced LD hybrid hardware configurations and control options.**

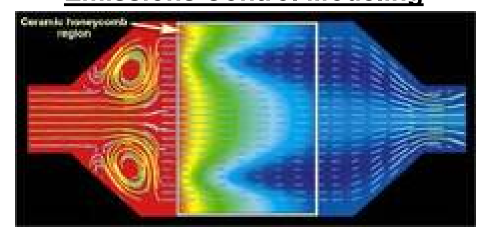
Lab Measurements



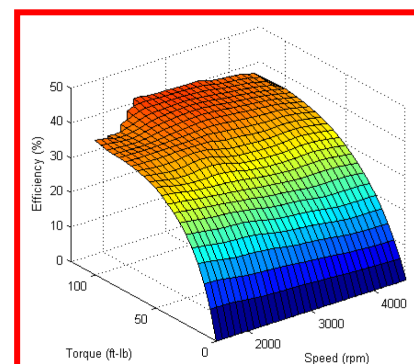
System Integration



Emissions Control Modeling



Dynamometer Measurements



Combustion Engine Modeling

Vehicle Simulation

FY2012 MILESTONES

- **Provide ANL partners with recommended engine and aftertreatment measurements for conventional Ford Fusion passenger car (September 30, 2012).** ✓
- **Develop and demonstrate initial model for passive trapping of hydrocarbon emissions (September 30, 2012).** ✓

Ford Fusion Dynamometer Measurements

Prius HEV and PHEV Simulations

Detailed tracking of critical transients

- Engine-out NOx, HC, CO, CO_2, O_2, and temperature
- TWC inlet and outlet emissions and temperatures
- TWC monolith temperatures
- Tailpipe-out emissions and temperature
- Engine and radiator coolant temperatures and flows

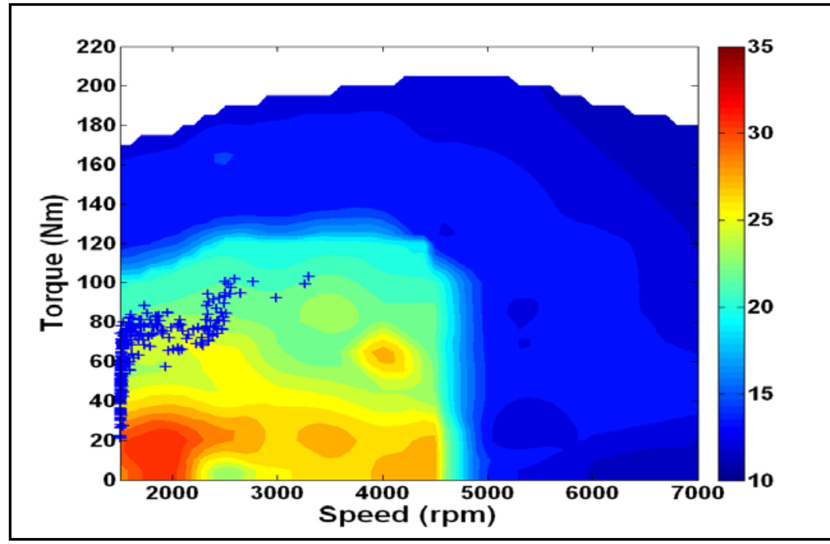
Model for passive transient adsorber

- Initial parameters for HC sorbent from lab data
- Sensitivity analysis and trends for NO adsorber
- Adsorber design impact
- Identification of future key experimental data needs
- Comparative HEV and PHEV simulations

ACCOMPLISHMENT (1): Refined LD lean-GDI engine maps from BMW

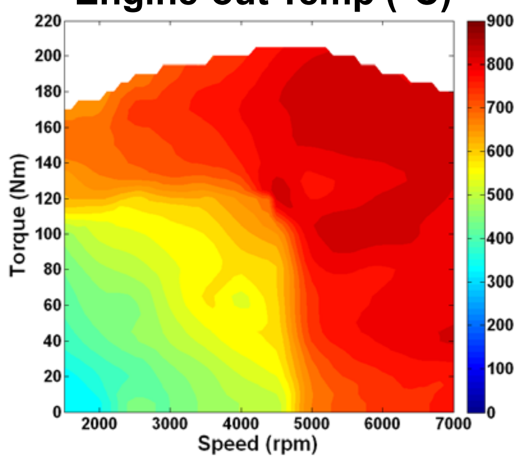
- **BMW Chassis dyno data**
  - Advanced 2.0-L, LD GDI engine
  - 4-15% FTP fuel economy boost over conventional (max BTE 41%)
  - Lower PM emissions than LD diesel
  - NOx emissions > US Tier II Bin5
- **LD lean-GDI engine maps**
  - Maps for lean ,rich, stoichoimetric modes
  - Fuel rate, engine out T, CO, HC, NOx, & PM
  - Steady-state & transient parameters

Simulated UDDS Air/Fuel Ratio for GDI HEV

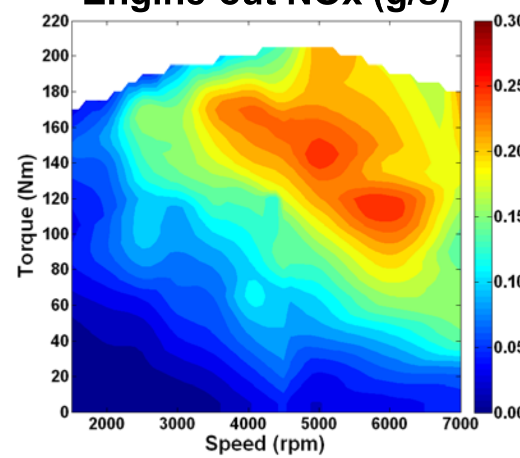


Chassis Measurements

Engine-out Temp (°C)



Engine-out NOx (g/s)



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ACCOMPLISHMENT (2): Continued updating LNT aftertreatment device model based on BMW catalyst data

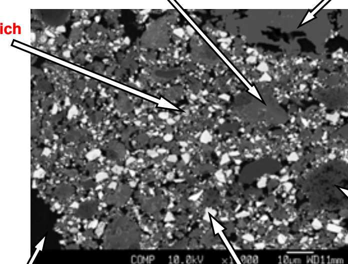
Experiments

- **Bench reactor evaluation**
  CLEERS protocol
- **Specialized measurements**
  SpaciMS, transient response
  Microscopy, DRIFTS

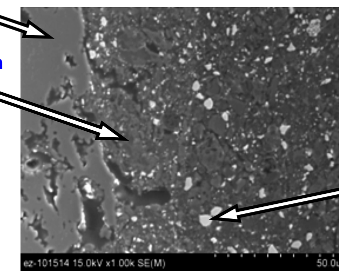
Automated bench reactor for CLEERS catalyst calibration

New calibrations for lean GDI LNT model

Current parameters based on CLEERS 2004 Umicore reference



New parameters based on BMW 2008 catalyst reference



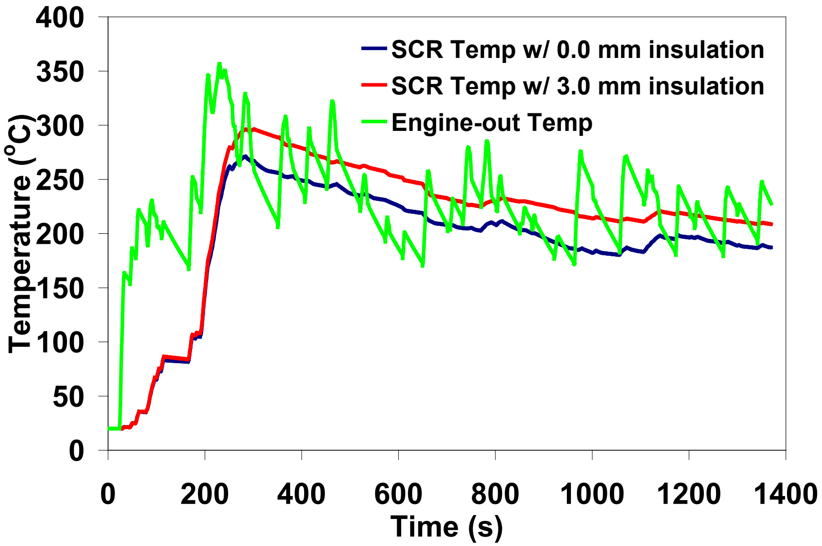
Simulation

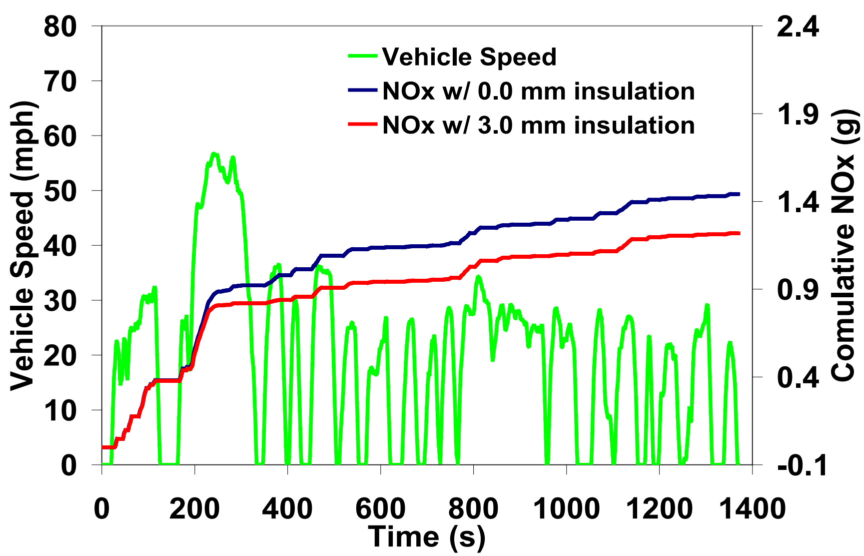
- **Revise LNT model parameters based on improved BMW formulation**
- **Improve prediction of NH_3 and N_2O when data available**
  - **Increasing constraints on NH_3 & N_2O**
  - **Potential aftertreatment device interactions**

ACCOMPLISHMENT (3): Implemented LD SCR device model in Autonomie

- **Example case study:**
  - 1450 kg, 1.5-L diesel-powered HEV
  - 1.3 kWh, 6.5 Ah battery (w/ 70% charge)
  - 1 UDDS cycle beginning with 20°C start
  - 0.59-L DOC for CO/HC control and NO oxidation
  - 2.4-L urea-SCR NOx cat (commercial Cu-ZSM-5)
  - Varying insulation on both DOC and SCR
  - Non-optimized urea control
- **Observations:**
  - Thermal insulation keeps SCR catalyst warm to reduce impact of cold starts
  - Insulation reduces NOx and lowers fuel demand for cold start.

Insulation (mm)	NOx (g/mile)
0	1.94E-01
1	1.86E-01
3	1.64E-02
5	1.57E-02





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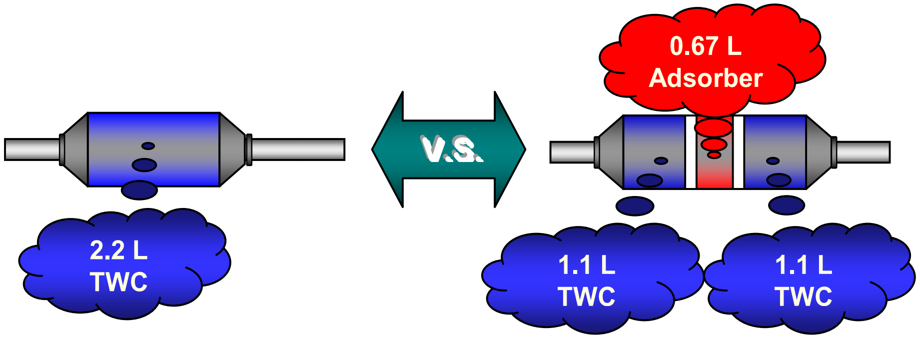
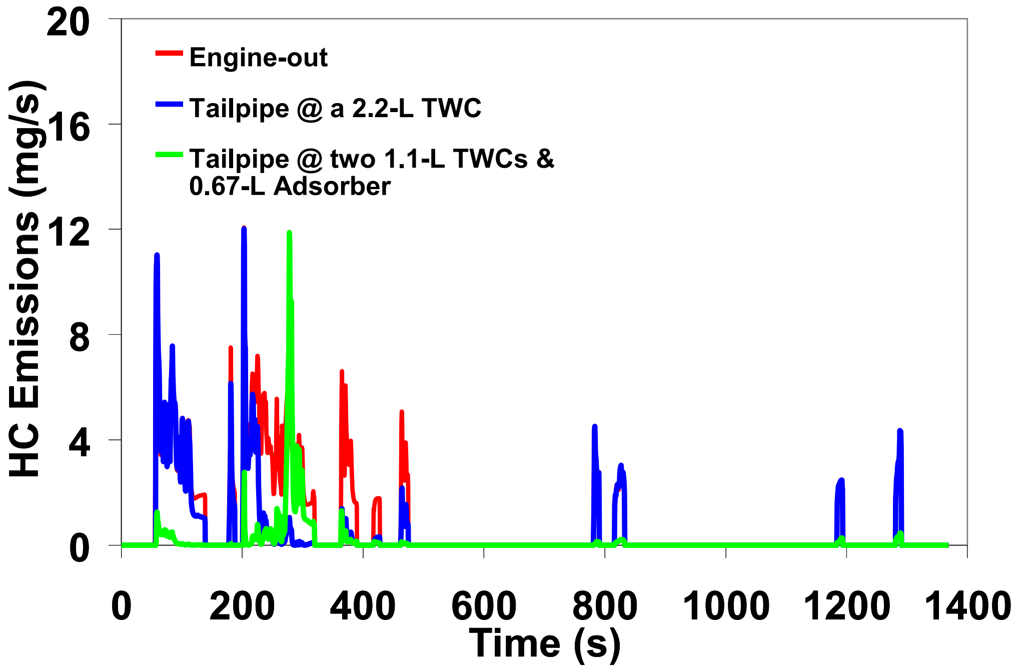
ACCOMPLISHMENT (4): Developed and exercised adsorber device model for LD hybrids*

- Example case study:
  - 1542 kg PHEV powered by 1.5-L gas engine
  - 5 kWh, 24 Ah battery for PHEV
  - UDDS cycle, cold start at 20°C
  - TWC with & without HC adsorber
- Observations:
  - Adsorber substantially reduces HC emissions by trapping them until TWC is hot
  - HC desorption begins at 250°C, peaks at 350°C
  - Benefits for PHEV > similar HEV (reflects more frequent PHEV restarts)
  - No fuel penalty or change in engine operation
  - Adsorber materials much cheaper than TWC





*Article accepted for publication in Journal of Automobile Engineering

COLLABORATION AND COORDINATION

- **ANL and Vehicle Systems Tech Team**
  - Advanced HD Engine Systems and Emissions Control Modeling and Analysis Task (VSS089)
  - Advanced Technology Vehicle Lab Benchmarking at ANL (VSS031)
  - Autonomous Intelligent Electric Vehicles at ORNL (VSS092)
  - PHEV Engine Control and Energy Management Strategy at ORNL (VSS013)
- **CLEERS Collaboration**
  - Multiple engine OEMs, emissions controls suppliers, universities, national labs (ACE022)
  - DOE Advanced Engine Crosscut Team (AECT)
  - USDRIVE Advanced Combustion and Emissions Control Tech Team (ACEC)
- **Other Related ORNL Activities**
  - Neutron Imaging of Advanced Engine Technologies (ACE052)
  - Emissions Control for Lean Gasoline Engines (ACE033)
  - Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes (ACE015)
  - High Efficiency Clean Combustion in Multi-Cylinder Light-Duty Engines (ACE016)
  - High Efficiency Engine Systems Development and Evaluation (ACE017)
  - Non-Petroleum-Based Fuels: Effects on Emissions Control Technologies (FT007)
  - Gasoline-like Fuel Effects on Advanced Combustion Regimes (FT008)

PROPOSED FUTURE WORK

- **FY2012**
  - **Continue development of representative LD engine maps (emissions and exhaust T)**
    - **Transient mode parameterization**
    - **Implementation in Autonomie**
  - **Update and refine urea-SCR and LNT component models based on most recent catalyst data**
    - **Impact of catalyst changes on HEV and PHEV drive cycle performance**
    - **LD urea-spray component model**
  - **Continue refinement of passive adsorber and TWC device models**
    - **Identify and implement updated NOx sorbent parameters**
    - **Update TWC model parameters and evaluate with ANL Fusion measurements**
    - **Implement and demonstrate adsorber and TWC functionality in Autonomie**
- **FY2013**
  - **Refine transient engine maps for ANL Fusion, ORNL advanced combustion engines**
  - **Evaluate fuel efficiency and emissions for alternative aftertreatment-drive train configurations**
  - **Support emissions modeling for HEV and PHEV controls optimization**
  - **Add models for exhaust heat recuperation/stretch efficiency components**

SUMMARY: Advanced LD engine systems and emissions modeling provides critical information for developing fuel-efficient, emissions-constrained passenger powertrain technologies

- Successful implementation of advanced passenger powertrain technologies requires a system level understanding of the complex interactions among energy generation, storage, utilization, and parasitic losses.
- Simulation of advanced passenger powertrain efficiency and emissions involves several key issues:
  - Accurate representation of most advanced engine and emissions control components.
  - Development and evaluation of optimized supervisory control and advanced propulsion strategies.
  - Data from full prototypes with transient and thermal conditions consistent with real world drive cycles.
  - Detailed analysis of component-to-component interactions.
  - Experimental validation of simulation predictions to minimize uncertainties.
- Simulation has an important role in component development, characterization, and commercialization:
  - Pathway to rapid development and commercialization of high efficiency vehicle technologies for LD vehicles.
  - Supports OEMs and suppliers in accelerating component and system discovery and refinement.

ACKOWLEDGEMENTS

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