Experimental Studies for CPF and SCR Model, Control System, and OBD Development for Engines Using Diesel and Biodiesel Fuels

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Michigan Technological University

16 May 2012
Project ID #ACE028
Overview

Timeline
- Start: Oct 2009
- Finish: Sep 2012
- Status: 75% Complete

Barriers
- Lack of cost effective emission control
- Lack of modeling capability for emission control and On-Board Diagnostics
- Aftertreatment durability

Partners
- Project Lead
  - Michigan Technological Univ.
- Industry
  - Cummins (Engine OEM)
  - John Deere (Engine OEM)
  - Johnson-Matthey (Catalysts)
  - Navistar (Engine OEM)
  - Watlow (Sensors)
- DOE Labs
  - Oak Ridge National Lab
  - Pacific Northwest National Lab

Budget

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<th>FY11</th>
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Assertion: Computing aftertreatment system internal states will facilitate new control strategies that satisfy emission regulations with minimal fuel penalty and will improve OBD algorithm development.

State Variables - a set of time-dependent variables whose knowledge, along with knowledge of the system’s inputs, allows one to completely compute the response of the system for all time.
Objectives

Three-Year Objectives:
• Experimentally validated reduced order models and state estimation algorithms
• Increased knowledge of biodiesel fuel blend, PM maldistribution, loading and NO2/PM ratio effects on passive regeneration, temperature effect on active regeneration, and aging for CPFs
• Increased knowledge of NH3 radial storage behavior, optimal NH3 loading, HC poisoning, and aging for SCRs
• Understand effect of sensor type / configuration on state estimation quality
• Optimal reductant strategies for SCR operation and CPF regeneration

This Year’s Objectives:
• Complete CPF maldistribution study and determine impact on CPF model and estimator and constraint on optimal CPF regeneration
• Complete advanced and conventional sensor evaluations and model development
• Complete aftertreatment component model development, and experimental validation
• Continue state estimation strategy development for CPF and complete DOC and SCR estimators.
• Complete fundamental studies to quantify CPF passive oxidation as a function of NO2/PM ratio and fuel type (ULSD and biodiesel)
• Complete fundamental studies to quantify CPF active regeneration as a function of inlet temperature and fuel type (ULSD and biodiesel) and analyze the data to determine the kinetic parameters.
• Determine kinetic models for the DOC, CPF, and SCR on the engine for CO, NO, NO2, HC, PM (CPF wall and cake) oxidation using experimental engine data in conjunction with high fidelity models.
VT Program Relevance

• A primary Advanced Combustion Engine VT program R&D direction is to

   “Develop aftertreatment technologies integrated with combustion strategies for emissions compliance and minimization of efficiency penalty”

• CPF regeneration causes a direct fuel penalty through injection and an indirect fuel penalty through decreased engine efficiency due to back pressure. SCR ammonia injection causes an indirect energy penalty due to urea usage. Closed loop control is required for both actions, but could likely be improved if estimated internal states are used in control strategies in lieu of direct, sensor output feedback.

• The state estimation strategies developed in this project are relevant to the VT program since they will:

   - Increase fuel efficiency through reductant-efficient injection strategy development
   - Permit implementation of emission control strategies on high efficiency engine’s operating on diesel or biodiesel fuel
   - Enhance aftertreatment durability through intelligent OBD strategy development
# Milestones

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<td>Task 3: CPF &amp; SCR State Estimator Strategy Report</td>
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* As of March 2012
Overall Project Approach

1. Develop fundamental knowledge in CPF PM oxidation and SCR ammonia storage to support development of reduced order models necessary for control-relevant, internal state estimation strategy design.

2. Combine engine test cell, prototype sensors, and reactor studies to validate models, verify estimator designs, and demonstrate reductant-efficient control using both diesel and biodiesel fuels.

3. Leverage team member (university, industry, national labs) expertise to efficiently execute research.

4. Two engines/aftertreatment systems 2007 ISL(8.9L) for DOC & CPF studies and 2010 ISB(6.7L) for SCR studies. The combination of unique instrumentation and experimental methods will uncover behaviors not previously seen, but relevant to state estimation.
Objective-Specific Approaches

• **CPF PM Loading and Passive Oxidation Kinetics Study:** Develop and test a new method for quantifying passive oxidation as a function of NO₂/PM ratio, temperature, and exhaust flow rate for ULSD and biodiesel fuel.
  ◦ Use existing, calibrated simulation tools to determine passive oxidation rate as a function of NO₂/PM ratio, temperature, and exhaust flow rate

• **CPF Active Regeneration Kinetics Study:** Develop test data for in-cylinder and post-turbocharger injection of diesel and biodiesel fuel as a function of CPF inlet exhaust temperatures

• **SCR Engine Kinetics Study:** Develop test data for different engine conditions (temperature, space velocity and NO₂/urea ratios)

• **SCR Spatial Storage:** Use reactor studies with an in-situ, spatial gas concentration measurement technique (Spaci-IR) to infer axial storage inside SCR samples using gas concentrations representative of engine conditions

• **Estimator Studies:** Use DOC, CPF, and SCR reduced order models for nonlinear state estimator design. Use transient engine test data to quantify performance.
Technical Accomplishments - FY12

**Tasks 2-8 CPF Advanced Sensor Studies:** Evaluation & characterization of advanced production intent sensors (PM retained, PM conc, NH$_3$) including their model development and integration into state estimation strategies.

**Task 2 SCR Reduced Order Modeling:** Utilized reactor and engine data to create a calibrated SCR model for state estimation strategy development. Completed Task 2

**Task 3 DOC, CPF & SCR State Estimator Strategy:** Reduced order models used to design state estimators for the DOC and SCR. The DOC estimator was tested with transient engine data and the SCR was tested in simulation.

**Task 5 CPF PM Loading and Passive Oxidation Studies:** CPF on-engine test procedure further developed and applied to obtain global PM oxidation rates for passive oxidation in thermal and NO$_2$ regimes. Procedure used on two engine platforms with USLD, B10 and B20 fuels. Completed PNNL PM characterization studies. Completed Task 5 reports. Additional tests to support sensor evaluations and fill gaps.

**Task 6 CPF Active Regeneration Studies:** Active regeneration test completed and engine test report submitted; work continues on the modeling of the global PM oxidation rates and determination of $\Delta P$ flow resistance.

**Task 7 CPF PM Loading Maldistribution:** Completed development of measurement methods and test plan. Phase 1 maldistribution testing nearing completion.

**Task 9 SCR Spatial Ammonia Storage:** ORNL developed a new method for spatially resolved gas species concentration measurement from which spatially resolved storage can be calculated.

**Task 11 SCR Optimal Ammonia Storage:** Review of optimal control strategies was completed and an approach to determine optimal NH$_3$ storage have been identified at PNNL.

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<table>
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<tr>
<th>3-Year Project Technical Tasks</th>
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Combining reactor and engine data to create a calibrated SCR engine model for state estimation strategy development

The research process is shown below going from an existing Fe Zeolite model, calibrated using Navistar and ORNL reactor data, to a Cu Zeolite model using engine data, as the primary focus of this project.

A 1D SCR model with two storage sites and 6 gas species (NO, NO₂, NH₃ gas and surface) was fit to both steady state and transient cycle engine data and is being used for state estimation. A sample line model is used to correct NH₃ measurement dynamic error in engine test.
Extended Kalman Filter (EKF) estimator validation and performance evaluation

The figure below illustrates the performance of DOC and SCR state estimators. The plots show DOC estimator engine evaluation results and SCR estimator simulation evaluation results.

The EKF estimator successfully estimates NO and NO₂ in the DOC and NO, NO₂ and NH₃ storage in the SCR.
A lumped parameter approach is used to model the CPF for state estimator design.

The CPF is divided into N lumped radial elements. Each element has its own flow resistance, $R_N$, and temperature, $T_{in,N}$, with heat transfer between adjacent elements, $Q_{int}$, and to the atmosphere, $Q_{amb}$. The figure below shows the two element case with an inner substrate with $R_1$ resistance surrounded by a circular outer substrate with $R_2$ resistance. Resistance of each element consists of the resistances due to the inlet channel, outlet channel, cake layer, and filter wall. Mass and energy balance equations are solved for temperature and particulate matter (PM) retained in $R_1$ and $R_2$ in addition to NO, NO₂, CO and hydrocarbon (HC) species.

A model formulation has been developed that shows that PM mass is observable. The formulation is modular allowing for N radial elements and addition of axial elements. Catalytic HC and NO oxidation as well as O₂ and NO₂ assisted oxidation of PM in the cake and wall will be included in the model.
Active regeneration experimental studies have been completed on the 2007 Cummins ISL 365 HP rating

18 tests completed on the ISL engine. PM reaction rate dependence on CPF temperature and biodiesel blends studied, with results shown below. The figure shows the experimentally determined PM reaction rate along with the model reaction rate results. The optimized model using the pre-exponential factor and activation energy for each fuel is shown by the dashed lines.

Engine tests completed with in-cylinder and exhaust HC dosing. Data analyzed and global reaction rates for three fuels (USLD, B10, B20) determined providing basis for reduced order model and estimator kinetics.

**Optimization Results**

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<th>Fuel</th>
<th>Pre Exponential (1/sec)</th>
<th>Activation Energy (kJ/mol)</th>
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<td>143</td>
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<tr>
<td>B10</td>
<td>2.31E+07</td>
<td>143</td>
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<tr>
<td>B20</td>
<td>3.86E+07</td>
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Initial test plan developed to evaluate the Advantest system and develop a more comprehensive test matrix for Q11.

Test procedure and process work completed with Cummins and Advantest. Special test CPFs fabricated by Cummins. Two of the three Phase 1 tests completed on MTU engine. Results from Test 1 scan of a filter loaded to 5 g/L is shown at right. Results show the PM load is heaviest near the outlet of the filter (6g/L) 20% higher than average PM loading.
Technical Accomplishments - Task 9
SCR Spatial Ammonia Storage Study

• Implemented novel capillary sampling system to enable fully transient Spaci-IR measurements

• Measured spatially resolved gas concentrations and NH₃ storage inside an SCR catalyst under:
  - NH₃ saturation (no NOx)
  - standard SCR (NO₂/NOx = 0)
  - fast SCR (NO₂/NOx = 0.5)

• Standard SCR: high NH₃ inventory
  - reaction zone covers most of catalyst length
  - storage sites nearly saturated within SCR reaction zone

• Fast SCR: low NH₃ inventory
  - reaction zone localized in front half of catalyst
  - storage sites not saturated within reaction zone

• Data sets will be used for validation of NH₃ storage models

Developed transient Spaci-IR technique to measure spatially resolved NH₃ storage distributions

![Graph](image)
Collaborations

Team Collaborations:

- **ORNL**: Reactor studies for SCR spatial NH$_3$ storage behavior (using Spaci-IR for internal catalyst gas measurement) and optimal NH$_3$ storage.
- **PNNL**: Acquired samples of our test engine exhaust (ULSD, B10, and B20) and performed bulk PM characterization (kinetic, nanostructural) in collaboration with Penn State University Currently developing a strategy for optimal NH$_3$ storage in SCR catalysts.
- **Cummins**: Engine/aftertreatment system support for DOC, CPF, and SCR studies.
- **Navistar**: Engine and sensor testing for DOC and CPF studies. Provided ORNL SCR Reactor Data.
- **John Deere**: Sensor model study support and DOC, CPF, and SCR model evaluation and aged component source.
- **Watlow**: Instrumentation design & installation, CPF thermal model support, and NOx and temperature sensor modeling studies. Evaluation of a prototype, wide-range PM sensor.
- **Johnson-Matthey**: Aftertreatment component model support and aged component support.

External Collaborations

- **Filter Sensor Technologies**: Installed and tested three iterations of prototype mass retained sensors
- **Advantest**: Joint effort with Cummins and Advantest; met with Advantest and developed a description of variables used in 1-D CPF high fidelity model as basis for improving output data.
- **Delphi**: Provided technical assistance for making NH$_3$ sensor operational.
- **Pegasor**: Installed and tested Pegasor particle sensor which will be used to collaborate PM concentration data and may be integrated into state estimation strategy development.
- **GE**: Developed plans for evaluating and calibrating mass retained sensor.
### Future Work

**Remainder of FY12**

- **Task 3: CPF and SCR State Estimation Engine Evaluations:** Compare trade-offs of computational complexity and accuracy for different sensor combinations. Complete engine testing of SCR and CPF estimators.

- **Task 4: CPF and SCR Model Adaptation:** Strategies for SCR and CPF devices and evaluate their performance in simulation.

- **Task 6: CPF Active Regeneration Engine Testing:** Limited testing will be conducted on B10 and B20 to confirm temperature dependence and analyze flow resistance.

- **Task 7: CPF PM Loading Maldistribution Engine Testing and Model Correlation:** Complete Phase 1 identifying critical parameters for Phase 2. Use multichannel model to determine impacts on $\Delta P$ and regeneration limitations.

- **Task 8: Fuel-Optimal CPF Regeneration Simulation & MTU Open-Loop/Closed-Loop Engine Tests:** Utilizing oxidation rates from passive and active regeneration testing, maldistribution from task 2 and engine PM/NOx maps determine constrained optimal loading/regeneration in simulated transients.

- **Task 10: Spatially Resolved SCR Aging Effects:** Conduct Spaci-IR tests using aged samples and compare NH$_3$ storage to un-aged samples.

- **Task 11: SCR Optimal Ammonia Storage Simulation Study:** Apply the optimal control strategy that was developed last year to transient engine data and calculate optimal NH$_3$ storage versus engine operation.

### 3-Year Project Technical Tasks

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Summary

- Communication and collaboration between stake-holders - universities, national labs, engine OEMs, sensor suppliers, and catalyst suppliers - is a core aspect of this project. It is expected to facilitate achievement of emission regulations with minimal fuel penalty for a wide range of engines including those operating on diesel or biodiesel fuel.

- The test cell and ISL and ISB engine installations along with sensors and lab instrumentation has been operational since July 2010 with additional sensors added in the past year.

- Development of DOC, CPF, and SCR models has continued directed toward reduced order models and estimator strategies.

- SCR reactor and engine data with a Cu-Zeolite catalyst has continued for calibration and validation of the models being developed.

- Experimental data has been collected for active regeneration with ULSD and biodiesel; and for passive oxidation with biodiesel, a report on active regeneration data was written (Oct 2011).

- Two SAE Papers on passive oxidation data under various NO₂ concentrations, temperatures, exhaust flow rates, and NO₂/PM ratios for ULSD, B10, and B20 using the new test protocol has been written and presented at the SAE International Congress April 24-26, 2012.

- A paper was written and will be presented to American Control Conference June 2012 on a Kalman filter estimator for a diesel oxidation catalyst during active regeneration of a CPF.

- This project started November 1, 2009 with a kick-off meeting held November 17, 2009 with all partners participating. A second meeting of all partners was held October 11, 2010 and a third meeting was held October 14, 2011. Phone conference calls have also taken place with all partners and with individual technical participants to foster productive collaboration.
Technical Back-Up Slides
Technical Accomplishments - Tasks 2-8
CPF Advanced Sensor Studies

Evaluation & characterization of advanced production intent sensors including their model development and integration into state estimation strategies

Advanced sensors needed for
1. State Estimator and Model Development
2. OEM Diagnostics and Control

Sensors under investigation and status

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<td>DCPF PM</td>
<td>DCPF PM Concentration</td>
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<tr>
<td>Pegasor PM</td>
<td>UDOC or DCPF PM Concentration</td>
<td>2nd iteration in process. 1st iteration results shown at right.</td>
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<tr>
<td>FST PM</td>
<td>CPF PM mass retained</td>
<td>3 testing iterations complete. Waiting on FST updated cal.</td>
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<td>GE PM</td>
<td>CPF PM mass retained</td>
<td>Working with GE to develop calibration and test procedure.</td>
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<tr>
<td>Watlow Thermocouple</td>
<td>3 Radial Temperature Readings per Probe</td>
<td>Working on test cell and DAQ integration.</td>
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New sensor technology can significantly impact state estimation and OBD. Direct sensing of PM mass retained and exhaust PM concentration could focus state estimation towards real-time optimization of CPF performance.

Pegasor PM Concentration

1st Phase Comparison

![Graph showing PM concentration comparison](image-url)
A surrogate HD-FTP transient cycle with repeatable flow rates, temperatures, and emissions was created by simplifying the HD-FTP cycle to simulate the representative transients in dyno-testcell. The transient tests were conducted on the ISB engine to obtain transient data used for both the model validation and estimator development for both the DOC and SCR.

The repeatability of the engine conditions, exhaust flow rate, temperature, and emissions was validated by comparing multiple runs of the cycle.
Sensor instrumented experimental test engine and simulation tools for estimator development

The figure below illustrates all of the sensors and ECU signals available for state estimator simulation and engine testing. Estimators calculate spatially resolved concentration and temperature states for each device.

Experimental and simulation tools have been developed that permit evaluation of different sensor combinations and algorithms for DOC, CPF, and SCR state estimation.
Experimental CPF resistance calculations completed for Passive Oxidation

Calculating the flow resistance \( \Delta P/Q_{Act} \) of the CPF provides a diagnostic check on the signals and PM loading. As the CPF PM loading increases, the resistance should steadily increase and conversely should steadily decrease during passive oxidation. If not, the signal is an indicator of problems with the volumetric flow rate \( Q_{Act} \) or pressure drop \( \Delta P \). The CPF resistance and CPF pressure drop are shown below for a Passive Oxidation test with B10 fuel.

\[
\Delta P = \Delta P_{channel} + \Delta P_{cake} + \Delta P_{substrate}
\]

\[
\frac{\Delta P}{Q_{Act}} = \text{Sum of Resistances}
\]

\[
Q_{Act} = \frac{\text{Mass Flow Rate}}{\text{Density}}
\]

\[
Q_{Act} = \text{Actual Volumetric Flow Rate (m3/sec)}
\]
During passive oxidation, the 1-D model simulates:

- **NO oxidation** in the catalyst washcoat,
- **Enhanced PM cake oxidation** due to “back-diffusion” of NO\(_2\) produced in the catalyst to PM cake layer, and
- Decrease of CPF pressure drop due to decrease in flow resistance of PM cake layer and wall (in turn due to PM mass reduction by passive oxidation)
PM distribution analysis technique, developed by Advantest, is being used with a modified CPF can to study PM distribution characteristics, in partnership with Cummins.

- According to Nishina et al., the Advantest system uses Terahertz waves to scan the substrate in the X, θ, and Z planes.
- Zhang states that terahertz waves allow for spectral analysis of an object.
- For accurate results of the localized PM concentration, the filters must be removed from the can and pre-scanned, according to Hu et al and Nishina et al.
- Two CPFs with removable cans supplied by Cummins
- Fully Instrumented
  - 31 Thermocouples
  - Emissions Sampling Ports
  - OEM ΔP and Temperature Sensors
- Faster loading times accomplished by modifying the calibration of the ISB engine.

Imamura, et al.
Copyright Advantest permission granted for use.
Optimal NH₃ storage in SCR catalysts is achieved by designing an optimal urea injection controller based on a learned non-linear SCR model and an iterative learned control approach that guarantees optimality.

Flow Chart

- Data split into training and test data for validation.
- Expectation-maximization Kalman smoothing
  - Transform inputs from \( u \) to \( v \)
  - Loop until model fits training data

Model

Given:
- Hammerstein-Weiner SCR model

Desired output
- Finite horizon
- Compute:
- Optimal urea dosing input

Controller

- Iterative Learned Control
- Given:
  - Hammerstein-Weiner SCR model
  - Desired output
  - Finite horizon
- Compute:
  - Optimal urea dosing input

Learned Model Validation

- A model learning approach to derive controllable non-linear SCR models, and an iterative learned control approach that guarantees optimality in control input were developed. The overall strategy can be implemented on-board the vehicle for real time operation.
- Learned SCR models were validated against FTP data in simulation.