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

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## Overview

#### Timeline

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

#### 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

#### Barriers

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

## Budget

Funding:	Total	FY10	FY11	FY12
DOE	\$1.8M	\$583k	\$603k	\$607k
Industry	\$0.7M	\$260k	\$223k	\$223k
University	\$0.3M	\$ 94k	\$106k	\$100k
Allocation:				
Mich Tech	\$2.3M	\$782k	\$777k	\$775k
DOE Labs	\$0.5M	\$155k	\$155k	\$155k

#### Introduction

<u>Assertion</u>: 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

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#### **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 NO<sub>2</sub>/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, NO<sub>2</sub>, HC, PM (CPF wall and cake) oxidation using experimental engine data in conjunction with high fidelity models.

• 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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Month/Year	FY10 and FY 11 Milestones	Status
Mar 2010	Task 2: Data Inventory System Report	100%
Aug 2010	Task 1: Engine / Aftertreatment Test Cell	100%
Jan 2011	Task 5: PM Loading Passive Oxidation Report	100%
Jun 2011	Task 2: SCR, CPF Sensor Estimator Model Form Report	100%
Jul 2011	Task 5: CPF Loading & Passive Oxidation Engine Test Report	100%
Oct 2011	Task 6: CPF Model Correlation (Active Regeneration) Report	100%
Jan 2012	Task 3: CPF & SCR State Estimator Strategy Report	100%
Nov 2011	Task 7: CPF Loading Maldistribution Test Plan Completion	100%
Mar 2012	Task 9: SCR Spatial Ammonia Storage Study Report	100%
Month/Year	FY12 Milestones	Status₩
Apr 2012	Task 9: SCR Storage Impact Report	90%
Apr 2012	Task 11: SCR Optimal Ammonia Storage Report	90%
Jun 2012	Task 3: Estimator Engine Test Report	75%
Jun 2012	Task 10: SCR HC Masking Test Report (Modified to aging effects)	20%
Sep 2012	Task 4: Model Adaptation Report	0%
Sep 2012	Task 6:CPF Active Regeneration Report	75%
Sep 2012	Task 7: Maldistribution Report	25%
Sept 2012	Task 8: Fuel Optimal Regeneration Report	5%
Sep 2012	Task 8: Fuel Optimal Test Report	5%
Sep 2012	Task 10: SCR HC Masking Model Report (Modified to aging effects)	20%
Sep 2012	Task 11: SCR Optimal Ammonia Storage Model Sensitivity Report	60%

**★** 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.



Cummins 2010 6.7L I6 ISB engine with ECU control and full aftertreatment system

DOC & CPF top SCR below





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#### **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 NO<sub>2</sub>/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 NO<sub>2</sub>/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 NO<sub>2</sub>/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<sub>3</sub>) 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 senor evaluations and fill gaps.

3-Year Project Technical Tasks
Task 1: Test Cell Preparation
Task 2: Baseline Estimator Model Development
Task 3: CPF and SCR State Estimation
Task 4: CPF and SCR Model Adaptation
Task 5: CPF Loading and Passive Oxidation
Task 6: CPF Active Regeneration
Task 7: CPF PM Loading Maldistribution
Task 8: CPF Fuel Optimal Regeneration
Task 9: SCR Spatial Ammonia Storage
Task 11:SCR Optimal Ammonia Storage

**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<sub>3</sub> storage have been identified at PNNL.

# Technical Accomplishments - Task 2 SCR Reduced Order Modeling

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#### Combining reactor and engine data to create a calibrated SCR engine model for state estimation strategy development Measured outlet Inlet Temp 240 – 380 °C

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.

**Experimental Studies** Cu zeolite Fe zeolite Engine studies Engine studies Data from SCR Reactor surrogate steady state ORNL using Data Supplied points with HD-FTP on CLEERS by Navistar **ISB** engine transient urea & ORNL protocol Two storage Several 1D Calibration Kinetic Models site model against parameters derived from both reactor validated by Postulated with Fe zeolite data and transient calibtations experience engine data test data Analysis

A 1D SCR model with two storage sites and 6 gas species (NO, NO<sub>2</sub>, NH<sub>3</sub> 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 NH<sub>3</sub> measurement dynamic error in engine test. T Measured outlet concentrations compared to simulation with transient test.

Inlet Temp	240 – 380 °C
SCR SV	4k – 56k hr-1



# Technical Accomplishments - Task 3 State Estimator Development



The EKF estimator

successfully estimates

and NO, NO<sub>2</sub> and NH<sub>3</sub>

storage in the SCR.

NO and  $NO_2$  in the DOC

# 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.



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# Technical Accomplishments - Task 3 CPF & SCR State Estimator Strategy

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# 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, NO<sub>2</sub>, 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  $O_2$  and NO<sub>2</sub> assisted oxidation of PM in the cake and wall will be included in the model.

# Technical Accomplishments - Task 6 CPF Active Regeneration Studies

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#### 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 incylinder 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				
Pre Exponential		Activation Energy		
1/sec		kJ/mol		
ULSD	1.84E+07	143		
B10	2.31E+07	143		
B20	3.86E+07	143		



## Technical Accomplishments - Task 7 CPF PM Loading Maldistribution

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Initial test plan developed to evaluate the Advantest system and develop a more comprehensive test matrix for Q11.



# Technical Accomplishments - Task 9 SCR Spatial Ammonia Storage Study

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- Implemented novel capillary sampling system to enable fully transient Spaci-IR measurements
- Measured spatially resolved gas concentrations and NH<sub>3</sub> storage inside an SCR catalyst under:
  - NH<sub>3</sub> saturation (no NOx)
  - standard SCR ( $NO_2/NOx = 0$ )
  - fast SCR ( $NO_2/NOx = 0.5$ )
- Standard SCR: high  $NH_3$  inventory
  - reaction zone covers most of catalyst length
  - storage sites nearly saturated within SCR reaction zone
- Fast SCR: low NH<sub>3</sub> inventory
  - reaction zone localized in front half of catalyst
  - storage sites not saturated within reaction zone
- $\mbox{-}$  Data sets will be used for validation of  $\mbox{NH}_3$  storage models

Developed transient Spaci-IR technique to measure spatially resolved NH<sub>3</sub> storage distributions



#### Collaborations

#### **Team Collaborations:**

- **ORNL** : Reactor studies for SCR spatial NH<sub>3</sub> storage behavior (using Spaci-IR for internal catalyst gas measurement) and optimal NH<sub>3</sub> 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<sub>3</sub> 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<sub>3</sub> 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**

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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. 3-Year Project Technical Tasks

Task 1: Test Cell Preparation

Task 2: Baseline Estimator Model Development

Task 3: CPF and SCR State Estimation

Task 4: CPF and SCR Model Adaptation

Task 5: CPF Loading and Passive Oxidation

Task 6: CPF Active Regeneration

Task 7: CPF PM Loading Maldistribution

Task 8: CPF Fuel Optimal Regeneration

Task 9: SCR Spatial Ammonia Storage

Task 10:SCR Spatially Resolved Aging Effect

Task 11:SCR Optimal Ammonia Storage

•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<sub>3</sub> 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<sub>3</sub> storage versus engine operation.

### 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 NO<sub>2</sub> concentrations, temperatures, exhaust flow rates, and NO<sub>2</sub>/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.

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# **Technical Back-Up Slides**

# Technical Accomplishments - Tasks 2-8 CPF Advanced Sensor Studies

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# 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

Sensor	Technology	Accomplishments	
Watlow PM	UDOC or DCPF PM Concentration	2 testing iterations completed.	
DCPF PM	DCPF PM Concentration	Working on test cell and DAQ integration.	
Pegasor PM	UDOC or DCPF PM Concentration	2nd iteration in process. 1st iteration results shown at right.	
FST PM CPF PM mass retained		3 testing interations complete. Waiting on FST updated cal.	
GE PM CPF PM mass retained		Working with GE to develop calibration and test procedure.	
Watlow Thermocouple	3 Radial Temperature Readings per Probe	Working on test cell and DAQ integration.	

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.



## Overall Project Approach – Task 2 Transient Test

#### 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.

Transient Cycle Development Proces Simplify the cycle Normalized Scale to the Remove to reduce engine ISB engine 🚔 motoring redundant engine conditions for @ 300HP sections HD-FTP cycle conditions Enigne Out 1000 100 Spd.(rpm) Load(N.m) 500 50 00 2000 50 1000

n

20

15

10

Time (min)

15

20

Speed (%) Load (%)

٥

5

10

Time (min)

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# Technical Accomplishments - Task 3 State Estimator Strategy Development

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# 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.



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# Technical Accomplishments - Task 5 CPF PM Loading and Passive Oxidation Studies

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#### **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.



## Technical Accomplishments - Task 5 CPF 1-D Model Applied to ISL Passive Oxidation Data

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# Technical Accomplishments - Task 7 CPF PM Loading Maldistribution

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#### 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 prescanned, according to Hu et al and Nishina et al.



Imamura, et al. Copyright Advantest permission granted for use.

- 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.



# Technical Accomplishments - Task 11 SCR Optimal Ammonia Storage Study

Optimal NH<sub>3</sub> 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.



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