

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

John H. Johnson, P.I.

Gordon G. Parker, Co-P.I. & Presenter

Michigan Technological University

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Project ID #ACE028



Overview

Timeline

- Start: Oct 2009
- Finish: Sep 2012
- Status: 45% 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

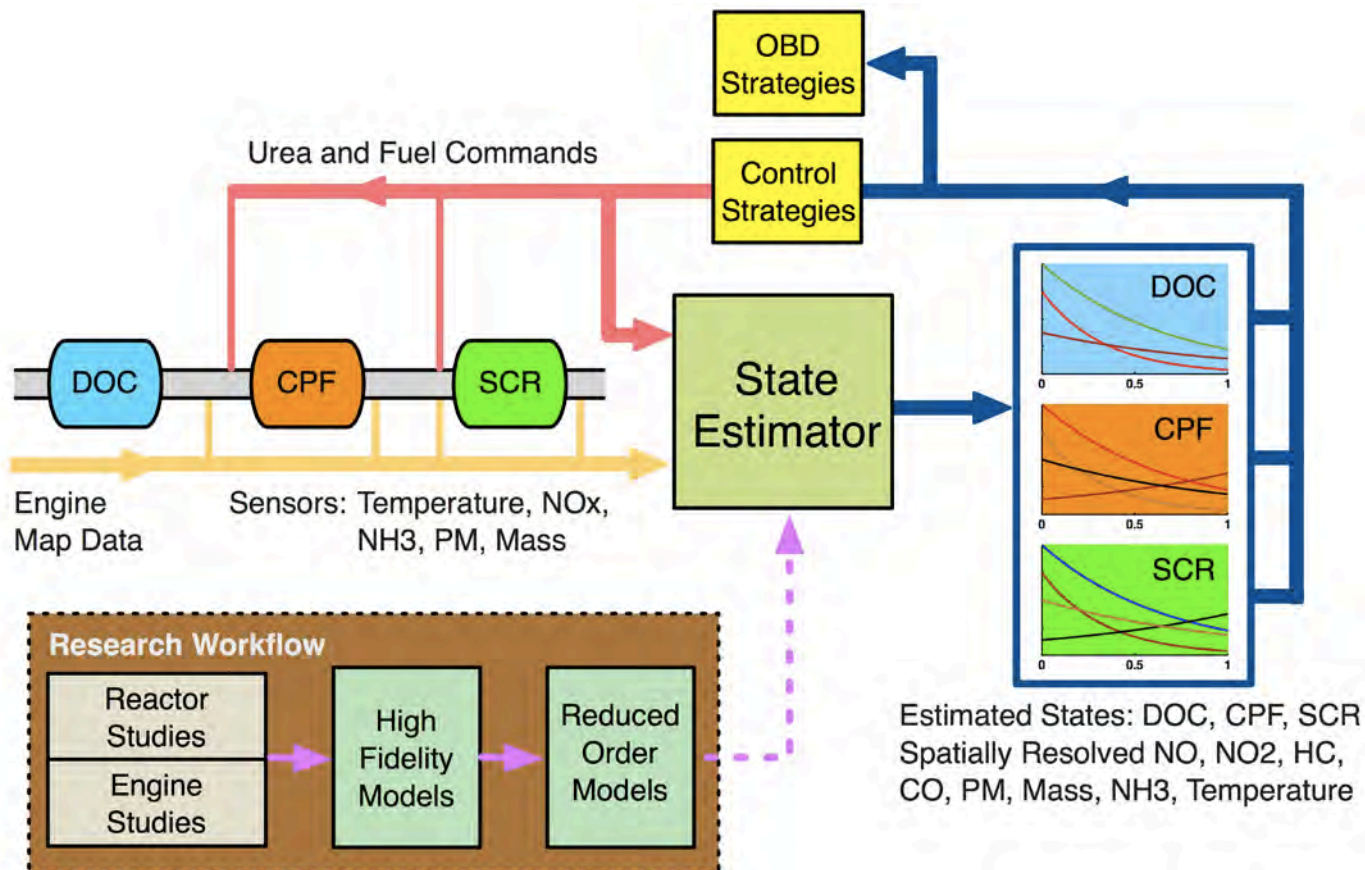
- Lack of cost effective emission control
- Lack of modeling capability for emission control and On-Board Diagnostics
- Aftertreatment durability

Budget

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

Introduction

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, 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 aftertreatment component model development, reduction, and experimental validation
- Complete advanced and conventional sensor evaluation and model development
- Start state estimation strategy development
- Perform fundamental studies to quantify CPF passive oxidation as a function of NO₂/PM ratio and fuel type (ULSD and biodiesel)
- Perform fundamental studies to quantify CPF active regeneration as a function of inlet temperature and fuel type (ULSD and biodiesel)
- Determine kinetic models for the DOC, CPF, and SCR on the engine for CO, NO, NO₂, HC, PM (CPF wall and cake) oxidation

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

Month/Year	FY10 Milestones	Status as of March
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%

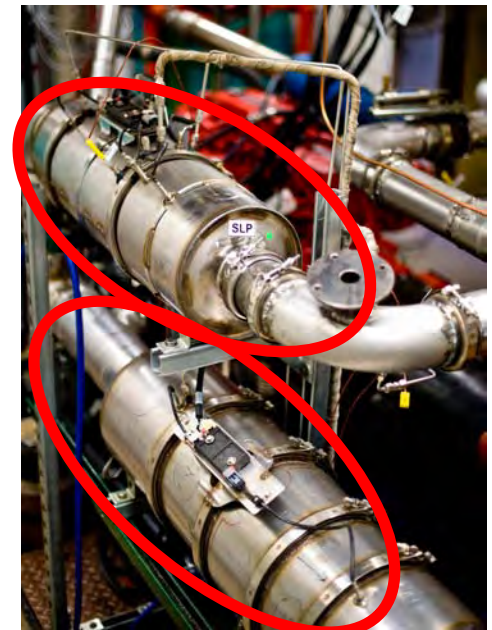
Month/Year	FY11 Milestones	Status as of March
Jun 2011	Task 2: SCR, CPF Sensor Estimator Model Form Report	65%
Jun 2011	Task 5: CPF Loading & Passive Oxidation Engine Test Report	60%
Jun 2011	Task 6: CPF Model Correlation (Active Regeneration) Report	20%
Aug 2011	Task 3: CPF & SCR State Estimator Strategy Report	65%
Sep 2011	Task 9: SCR Spatial Ammonia Storage Study Report	70%
Sep 2011	Task 7: CPF Loading Maldistribution Test Plan Completion	Not Started

Overall Project Approach

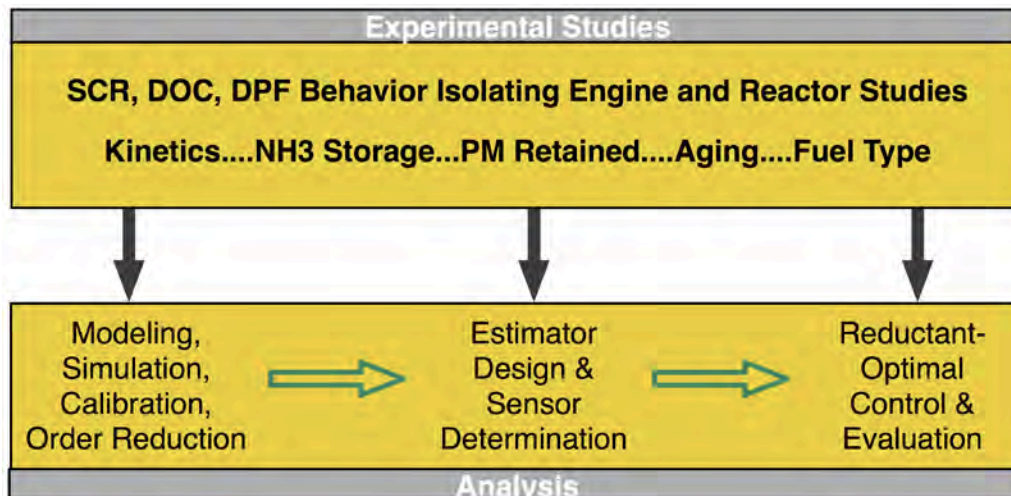
1. Develop fundamental knowledge in CPF PM oxidation and SCR ammonia storage to support development of reduced order models necessary for control-relevant, internal state estimation strategy design.
2. Combine engine test cell, prototype sensors, and reactor studies to validate models, verify estimator 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.



2010 ISB with aftertreatment system



DOC & CPF shown on top and SCR system below



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_2/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_2/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_2/urea ratios)
- **SCR Spatial Storage:** Use reactor studies with an in-situ, spatial gas concentration measurement technique (SpaciMS) to infer axial storage inside SCR samples using gas concentrations representative of engine conditions
- **Model Forms Study:** Use existing DOC, CPF, and SCR models to create reduced order models suitable for real-time, internal state estimation strategy development. Leverage partner testing to aid sensor model development

Technical Accomplishments - FY11

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Tasks 2-8 CPF Advanced Sensor Studies: Evaluation & characterization of advanced production intent sensors including their model development and integration into state estimation strategies

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

Task 2 CPF 1-Dimensional Model Development: The 1-D CPF model was developed as an initial step to a reduced order model for state estimator development.

Task 3 State Estimator Development: A nonlinear Extended Kalman Filter (EKF) state estimation strategy was applied to the surrogate DOC model using 15 axial elements.

Task 5 CPF PM Loading and Passive Oxidation Studies: New CPF on-engine test procedure developed and applied to obtain global PM oxidation rates for passive oxidation in NO₂ and thermal regimes.

Task 5 CPF Passive Regeneration Studies: High fidelity CPF model calibration to experimental data was achieved during for passive regeneration using ULSD.

Task 6 CPF Active Regeneration Studies: High fidelity CPF model calibration to experimental data was achieved during an active regeneration event using ULSD.

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 Fuel-Dependent HC Masking
Task 11: SCR Optimal Ammonia Storage

Technical Accomplishments - Tasks 2-8

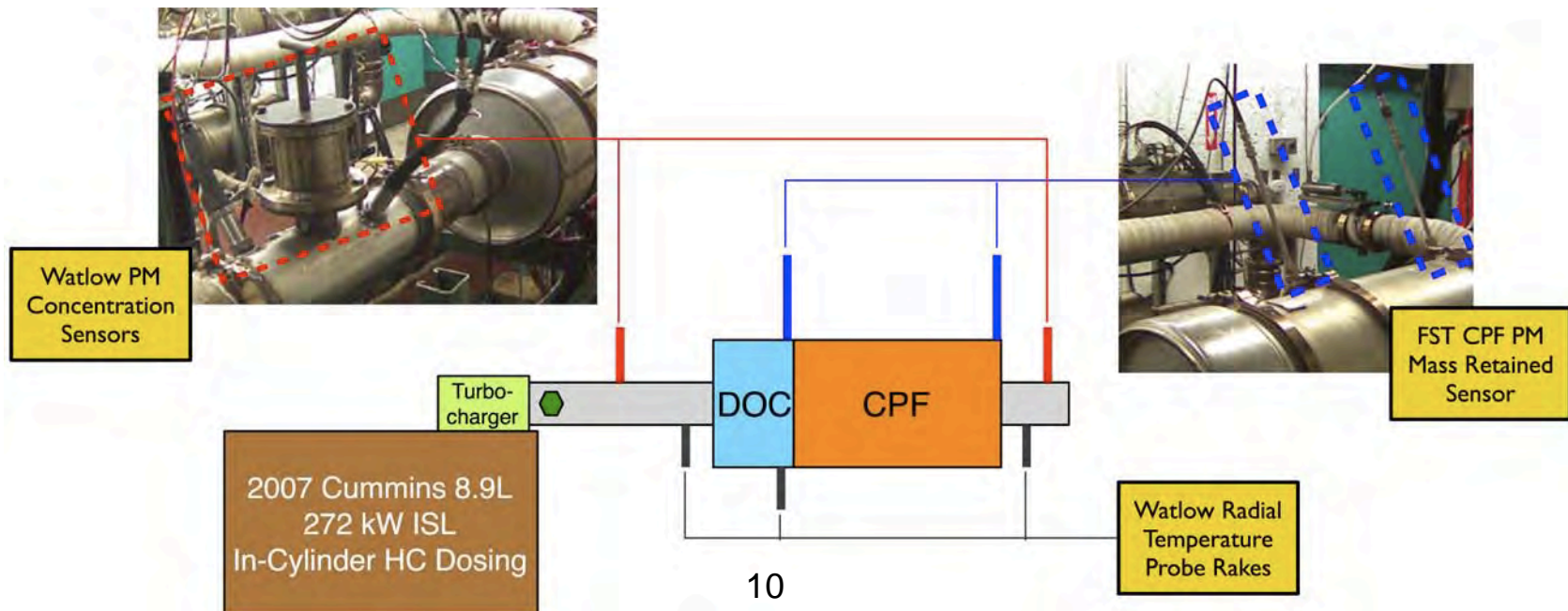
CPF Advanced Sensor Studies

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

Engine studies help focus model activities towards the most relevant phenomena for state estimator development. Sensors are a key aspect of state estimation where both sensor and CPF model fidelity is equally important for estimated state accuracy. Project visibility has enabled connections with prototype sensor developers leading to installation of (1) exhaust PM concentration sensor, (2) CPF PM mass retained sensors and (3) spatially resolved temperature probes shown below.

New sensor technology can significantly impact state estimation and OBD. Changing PM permeability makes prediction of PM mass retained difficult using only ΔP sensing. Conversely, direct sensing of PM mass retained (FST sensor) and exhaust PM concentration (Watlow sensor) could focus “state estimation” towards real-time optimization of CPF performance.



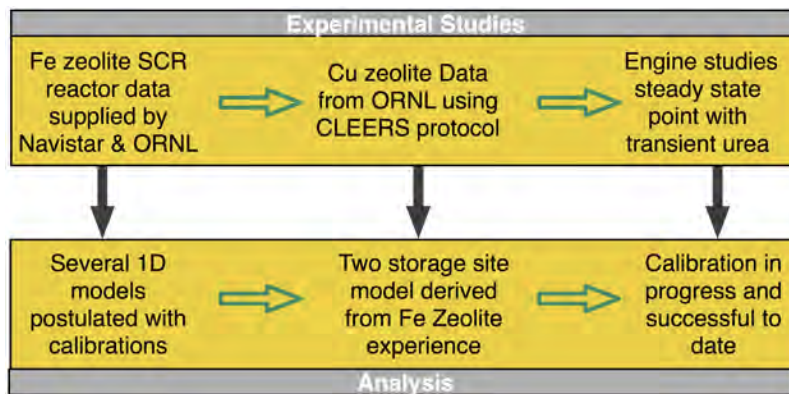
Technical Accomplishments - Task 2

SCR Reduced Order Modeling

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Combining reactor and engine data to create a calibrated SCR model for state estimation strategy development

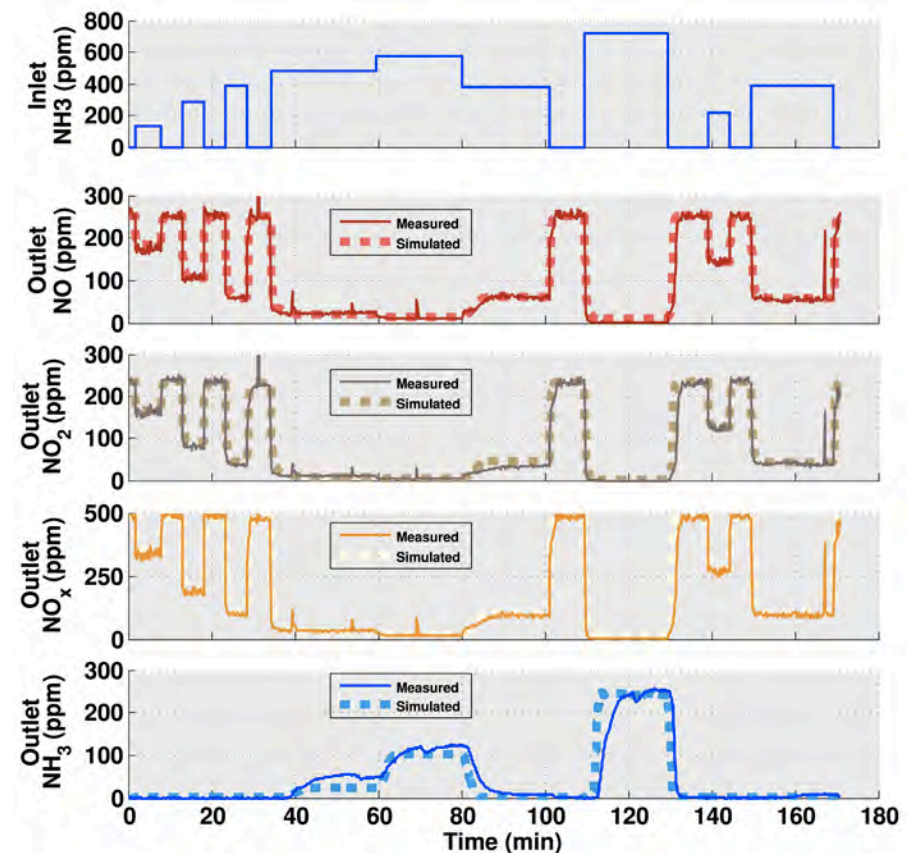
The research process is shown below going from an existing Fe Zeolite model, calibrated using Navistar and ORNL reactor data, to a Cu Zeolite model using engine data, which is the primary focus of this project.



A 1D SCR model with two storage sites and 6 gas species (NO, NO₂, NH₃ gas and surface) was fit to engine data and is suitable for state estimation use. NH₃ measurement dynamics are being explored as a source of the transient outlet NH₃ mismatch.

Measured outlet concentrations as compared to simulation data is shown below. The engine was operated at steady state while using a transient urea injection schedule.

SCR Inlet Conditions	
SV (1/hr)	21,000 +/- 300
T (deg C)	366 +/- 3
NO (ppm)	251 +/- 10
NO ₂ (ppm)	233 +/- 10
O ₂ (%)	7.79 +/- 0.25



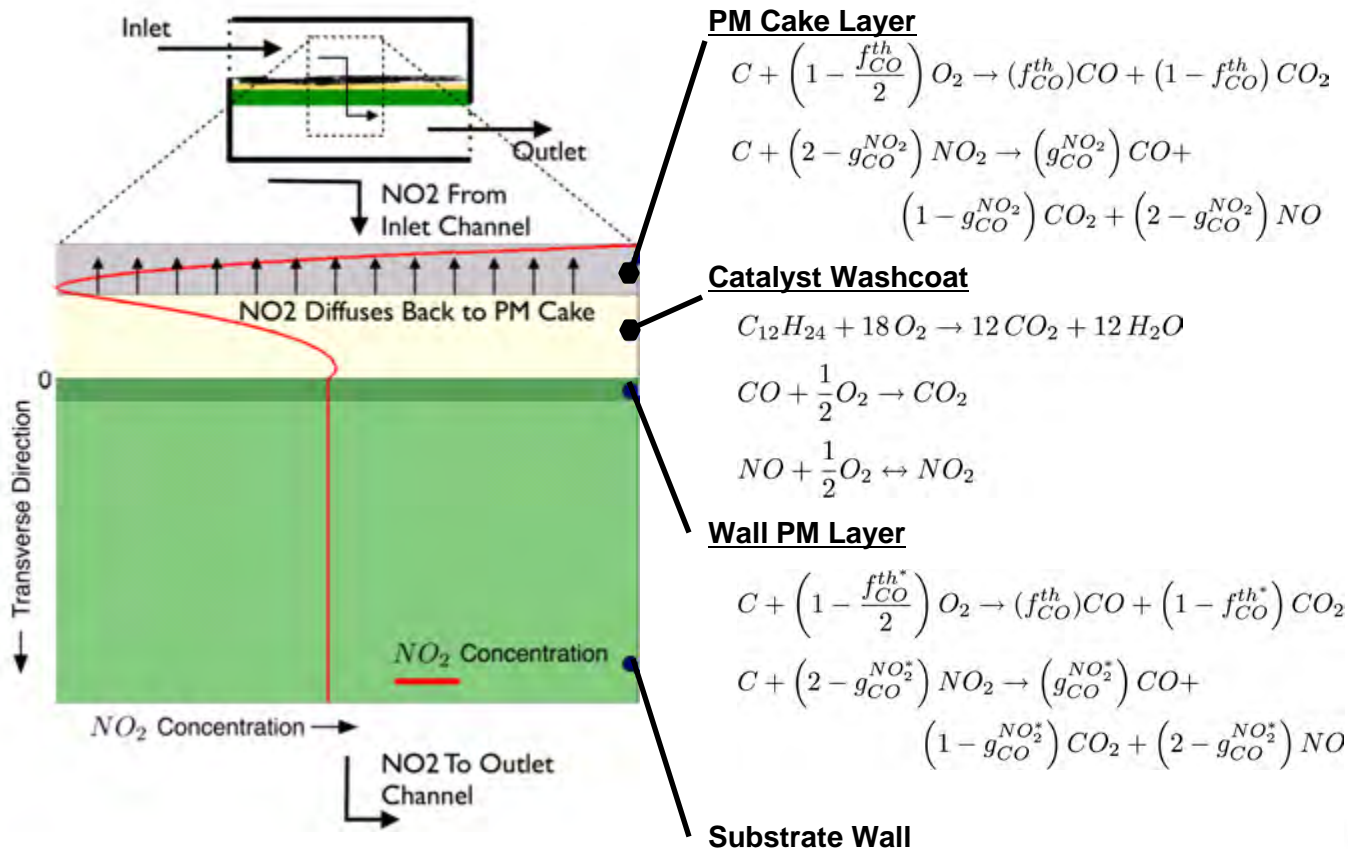
Technical Accomplishments - Task 2

CPF 1-Dimensional Model Development

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The 1-D CPF model was developed as an initial step to a reduced order model for state estimator development.

The model captures basic physical and chemical processes involving gaseous species and particulate matter inside the CPF. The phenomena modeled are summarized below.



A general math model, capturing (1) convection, diffusion, and reaction for gaseous species, (2) filtration and thermal / passive oxidation for PM can be used for predicting the performance of both surface-type and pore type catalyzed particulate filters operating in active and passive regeneration.

$f_{CO}^{th}, f_{CO}^{th*} \rightarrow$ thermal CO selectivities
 $g_{CO}^{NO_2}, g_{CO}^{NO_2*} \rightarrow$ passive CO selectivities

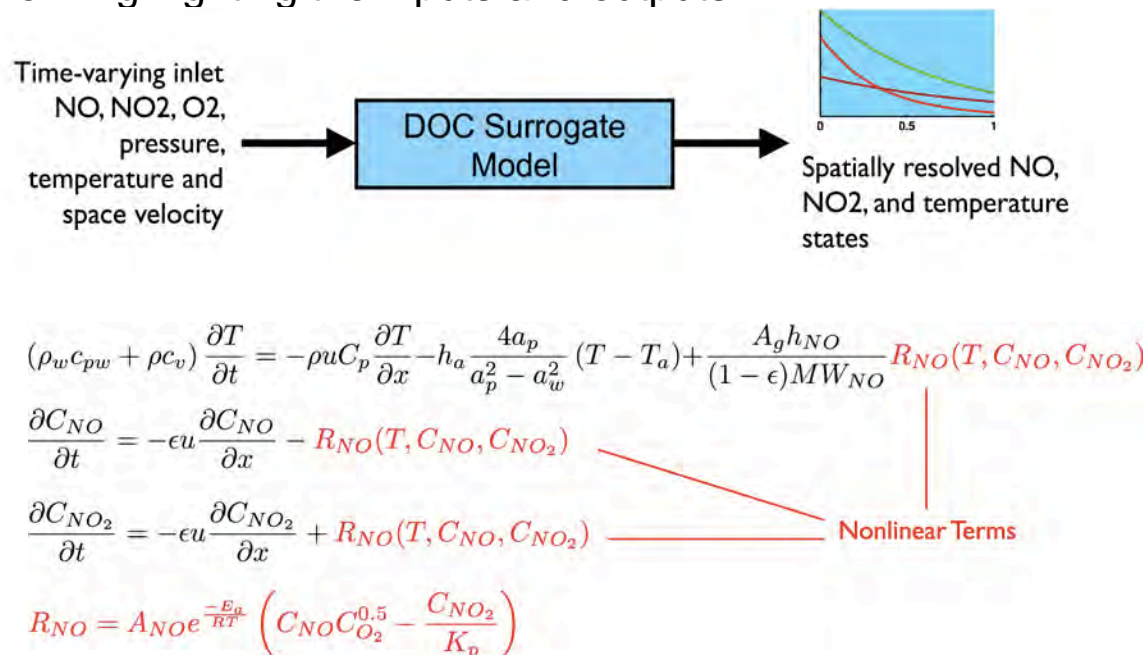
Technical Accomplishments - Task 3

State Estimator Development

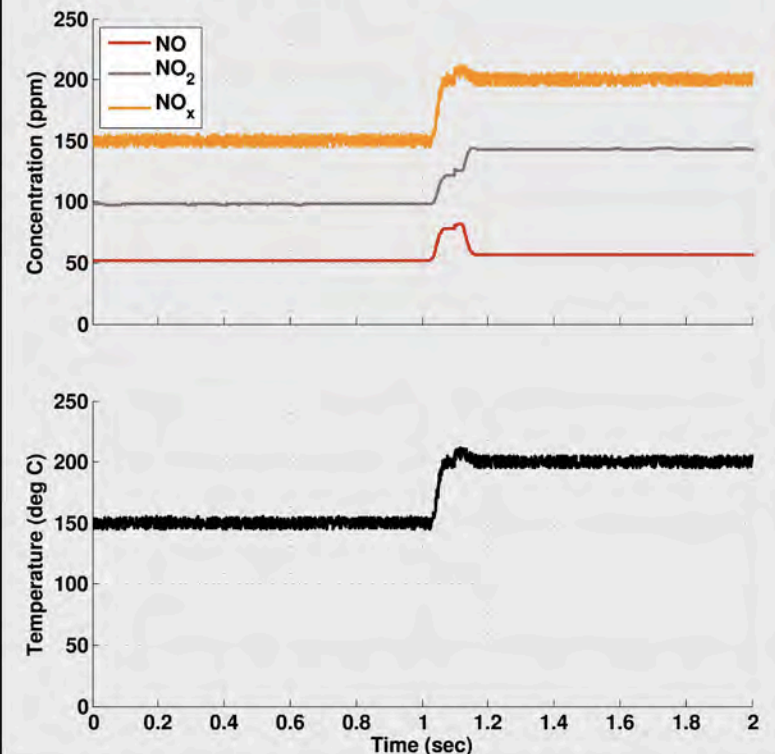
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Developed an Extended Kalman filter state estimator for a surrogate model, similar in form to a DOC and SCR.

Instead of developing state estimation strategies for a particular DOC or SCR model, a surrogate model was created that was simple, but captured the temperature and species concentration nonlinearities common to both DOC and SCR models. The surrogate model contains just the NO oxidation reaction of a DOC and its heat of reaction effect on temperature states. The model, and its equations, are shown below highlighting the inputs and outputs.



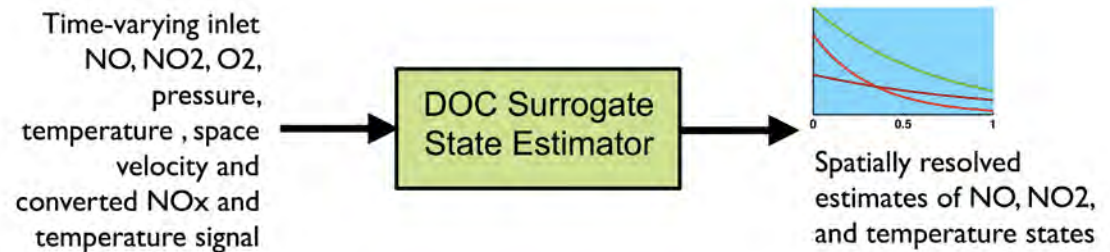
For purposes of state estimation, the simulation outputs are converted into simulated sensed NO_x and temperature. These, in conjunction with simulated inputs from engine maps, are used to “drive” the estimator. A typical set of inputs is shown below



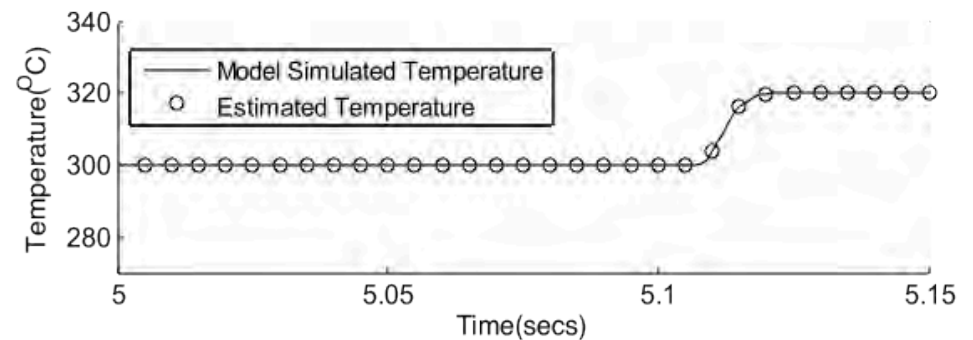
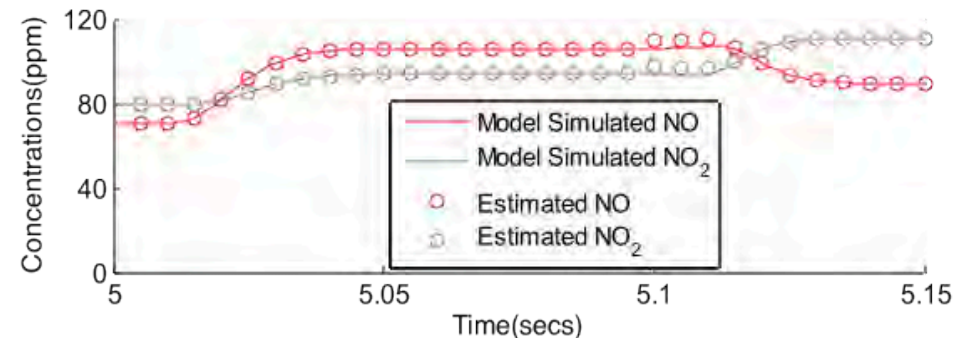
Technical Accomplishments - Task 3

State Estimator Development

A nonlinear Extended Kalman Filter (EKF) state estimation strategy was applied to the surrogate DOC model using 15 axial elements. The EKF process, illustrating the inputs and outputs, is shown at right.



The comparison between estimated and simulated states is shown at right for an element midway along the device. The axis is scaled to show the transient response of the model and the estimator. The estimated states follow the simulation with less than 0.1% error.



An Extended Kalman Filter can be successfully applied to a nonlinear aftertreatment system such as a DOC or SCR. Though this cannot be claimed for the CPF yet, that is the next target

Technical Accomplishments - Task 5

CPF PM Loading and Passive Oxidation Studies

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New CPF on-engine test procedure developed and applied to obtain global PM oxidation rates for passive oxidation in NO₂ and thermal regimes.

By conducting controlled CPF loading to target PM (e.g. 2.2g/L) and changing engine operation to target temperature, exhaust flow and PM/NO_x conditions, controlled passive oxidation tests provide PM mass oxidation rates for lumped and detailed oxidation analysis.

$$m_{stop} = \frac{Q_{exh} C_{in} \eta_f}{1000 R R_0} [1 - e^{-R R_0 t_{eff}}] + m_{start} e^{-R R_0 t_{eff}}$$

m_{stop} retained PM mass in CPF (g)

m_{start} initial PM mass in CPF (g)

Q_{exh} volumetric flow rate (std. m³/s)

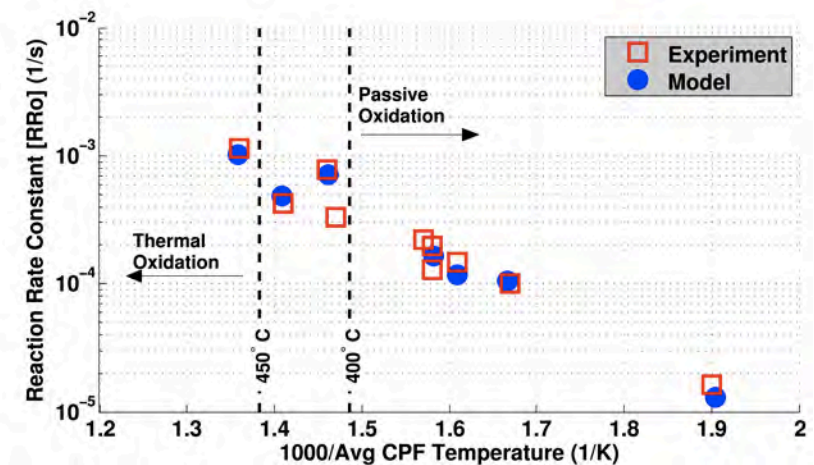
C_{in} PM concentration (mg/std. m³)

η_f filtration efficiency

$R R_0$ reaction rate (1/s)

t_{eff} time of passive oxidation (s)

	Avg CPF Temp.	Exh. Flow Rate	Exper. $R R_0$ □	Model $R R_0$ ●	NO ₂ Available Inlet	NO ₂ Consumed	NO ₂ Consumed/ NO ₂ Avail.
	°C	(kg/min)	(1/s)	(1/s)	(g)	(g)	-
2002 10.9L ISM	327	6.8	1.00E-4	1.05E-4	116	126	1.08
	348	6.8	1.48E-4	1.17E-4	104	177	1.70
	411	14.4	7.79E-4	7.13E-4	180	264	1.47
	463	16.9	11.34E-4	10.06E-4	49	239	4.84
2007 8.9L ISL	252	5.6	0.16E-4	0.13E-4	183	43	0.23
	359	7.8	1.96E-4	1.63E-4	125	208	1.66
	437	18.0	4.19E-4	4.87E-4	44	179	4.11



Experimental results show PM oxidation higher than NO₂ available at the CPF inlet indicating NO₂ production and diffusion is important over a wide range of operating conditions. MTU-1D model enhanced to account for these factors. Through calibration, NO₂ and thermal reaction rate parameters tuned. Results from PNNL PM NO₂ reactor oxidation studies will be used to further refine these rates.

Technical Accomplishments - Task 5

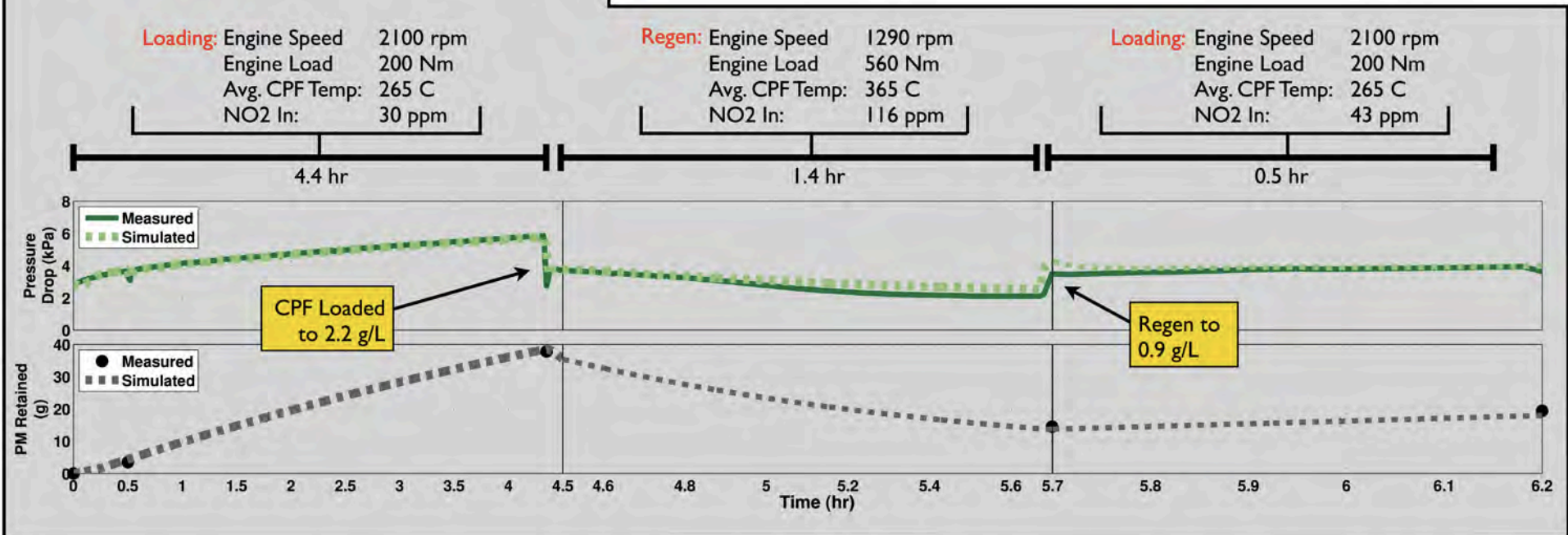
CPF Passive Regeneration Studies

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High fidelity CPF model calibration to experimental data was achieved during passive regeneration using ULSD.

The test procedure used three phases: (1) loading, (2) passive regeneration, and (3) post regeneration loading. Incorporating NO₂ back diffusion and pressure-related cake PM permeability allowed the model to be calibrated to experimental data.

Simulation using the high-fidelity model compared to experimental data of passive oxidation confirmed that diffusion of NO₂ is an important phenomenon. It increases the NO₂-assisted PM oxidation rate of the PM cake layer. This knowledge should be incorporated in the CPF reduced order model for state estimation.



Technical Accomplishments - Task 6

CPF Active Regeneration Studies

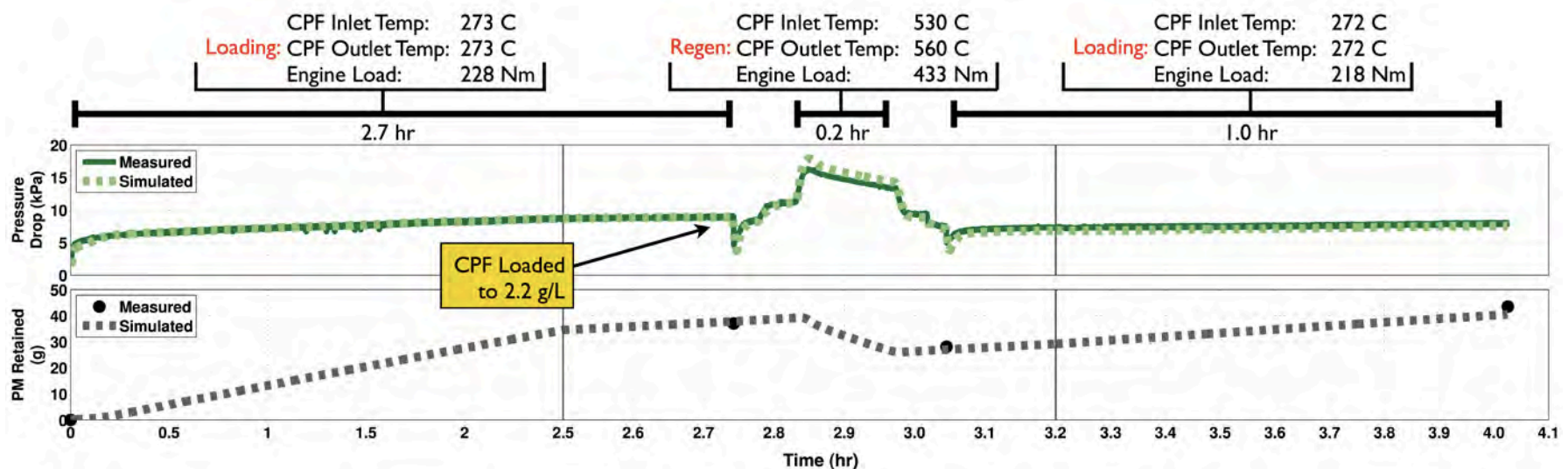
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High fidelity CPF model calibration to experimental data was achieved during active regeneration using ULSD.

Finalizing the high fidelity model, as a stepping stone to a reduced order model for state estimation, was the goal. The test procedure was finalized to include three phases: (1) loading, (2) active regeneration, and (3) post regeneration loading. Calibrating the parameters related to wall mass accumulation and oxidation were critical.

This task is continuing with focus on exhaust verses in-cylinder dosing and biodiesel blend effects on model calibration and reduced order modeling. Later tasks will address partial regeneration and PM maldistribution

It is essential that the follow-on, reduced order, state estimation model accurately predict PM in the wall. Since the CPF model requires accurate HC inlet concentrations, it is critical that the DOC model be accurate in the temperature and HC concentration range associated with active regeneration.



Collaborations

Team Collaborations:

- **ORNL** : Reactor studies for SCR spatial NH_3 storage behavior (using SpaciMS for internal catalyst gas measurement), HC masking, and optimal NH_3 storage.
- **PNNL** : CPF loading, passive oxidation, and active regeneration using SPLAT II in Michigan Tech test cell for PM morphology. Acquired samples of our test engine exhaust (ULSD) and performed PM analysis in collaboration with **Penn State University**. This will be repeated in the future with biodiesel blends.
- **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 NO_x 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 a prototype mass retained sensor into our test cell which may be integrated into state estimation strategy development

Future Work

Remainder of FY11

- Task 2: Complete Baseline Estimator Model Development** including reduced order models on SCR, CPF, and sensors suitable for estimator design.
- Task 5: Complete CPF Loading and Passive Oxidation Study** focusing on biodiesel fuels. Further testing of blends and NO₂/PM ratios for a second round of investigations will be performed based upon the results found in the previous task. The experimental results will be used to determine global oxidation rates and PM filter characterization appropriate for the MTU 1-D CPF model and control models for NO₂ and O₂ under passive operation.
- Task 6: Begin Active Regeneration Tests** at MTU and OEMs, for both ULSD and biodiesel blends and finalize model correlation.
- Task 3: Complete CPF State Estimation**, Error Quantification, Model Uncertainty studies, complete sensor suite recommendations, and begin engine testing.
- Task 9: Complete Radial Storage Spatial Distribution Experimental and Simulation Study** including models and tests. These results will then be incorporated into an SCR model structure suitable for OBD and model-based estimation and control design.
- Task 7: Begin CPF PM Loading Maldistribution** development of measurement methods and test plans.

Goals for FY12

- Task 8: Fuel-Optimal CPF Regeneration simulation and MTU Open-Loop/Closed-Loop Engine Tests.**
- Task 10: Fuel Dependent SCR HC Masking, Flow Reactor Tests.**
- Task 11: SCR Optimal Ammonia Storage Simulation Study.**
- Task 9: Spatial Distribution of Ammonia Study Estimator Impact.**
- Task 3: CPF and SCR State Estimation Engine Tests.**
- Task 4: CPF and SCR Model.**
- Task 6: CPF Active Regeneration Engine Testing with biodiesel fuels.**
- Task 7: CPF PM Loading Maldistribution Engine Testing and Model Correlation.**

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 Fuel-Dependent HC Masking
- Task 11: SCR Optimal Ammonia Storage

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.

A report on passive oxidation data under various NO_2 concentrations, temperatures, exhaust flow rates, and NO_2/PM ratios for ULSD using the new test protocol has been completed. (Jan 2011)

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 been started for calibration and validation of the models being developed.

Experimental data will be collected for active regeneration with ULSD and biodiesel, and for passive oxidation with biodiesel.

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. Phone conference calls have also taken place with all partners and with individual technical participants to foster productive collaboration.

Technical Back-Up Slides

Detailed Technical Accomplishments - FY11

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Task 1 – Developed experimental capabilities to support project experimental studies including test cell preparation, engine/aftertreatment system installation, and integration of new sensor technologies for state estimation into the existing experimental studies.

Task 2 -Continued aftertreatment component (DOC, CPF, SCR) and sensor model form studies, calibrations, and model refinement.

- Developed and disseminated detailed SCR, DOC, and CPF test plans to aid model and state estimator development.
- Developed reduced order model, the majority of the sensor effort focused on installation of prototype NO_x, PM concentration, and mass retained sensors for real-time state estimation.
- Conducted tests for a temperature probe immersion study to better understand the effects of HC injection on temperature measurement accuracy.
- Completed DOC testing and DOC temperature testing in conjunction with Watlow. *Initial testing was completed last year, but limitations on the number and types of temperature sensors indicated additional testing was required.*
- Completed SCR model of the Fe-Zeolite SCR using reactor data from ORNL .
- Continued CPF 1-D Model Development.
- Started SCR Reactor Studies using Cu-Zeolite SCR Catalyst

3-Year Project Technical Tasks

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- Task 11: SCR Optimal Ammonia Storage

Detailed Technical Accomplishments - FY11 continue

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Task 5 – Developed test plan and protocol that will allow passive oxidation rates to be determined from engine test cell data.

- Performed CPF loading, passive oxidation tests, and predictive modeling using the CPF 1-D model.
- Simulated passive oxidation test conditions on the ISM and ISL engines using CPF 1-D model the passive PM oxidation reaction rate predicted by the CPF model was used to estimate the pre-exponential factor and activation energy.
- Completed report on CPF PM loading & passive oxidation with ULSD fuel.
- Started passive oxidation tests with biodiesel fuel –B10 & B20.
- Started model based data analysis and sensitivity study.

Task 9 – Designed SCR spatial reactor test protocol to support estimator model development and spatial storage studies at ORNL. Created SCR core samples, and non-spatial testing has begun. Continued COMSOL modeling of an SCR for comparison to spatially resolved data obtained at ORNL.

Task 3 – Continued development of DOC, CPF and SCR state estimation strategy in conjunction with appropriate sensors, and postulated measured quantities. Constructed a first-cut DOC estimator using multiple spatial elements.

Task 6. CPF Active Regeneration – Developed a detailed test plan based on input from project partners including both ULSD and biodiesel fuels and identification of independent variables – work started on ULSD & biodiesel fuels.

3-Year Project Technical Tasks

Task 1: Test Cell Preparation

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Task 3: CPF and SCR State Estimation

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