Michigan Tech Final Technical Report

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

Award Number: DE-EE0000204

Recipient: Michigan Technological University
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Report Number: DOE-2013-MTU-01-FINAL

Date of Report: July 29, 2013

Reporting Period: October 1, 2009 – April 30, 2013

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1. Executive Summary

The research carried out on this project developed experimentally validated Diesel Oxidation Catalyst (DOC), Diesel Particulate Filter (DPF), and Selective Catalytic Reduction (SCR) high-fidelity models that served as the basis for the reduced order models used for internal state estimation. The high-fidelity and reduced order/estimator codes were evaluated by the industrial partners with feedback to MTU that improved the codes. Ammonia, particulate matter (PM) mass retained, PM concentration, and NO_x sensors were evaluated and used in conjunction with the estimator codes. The data collected from PM experiments were used to develop the PM kinetics using the high-fidelity DPF code for both NO₂ assisted oxidation and thermal oxidation for Ultra Low Sulfur Fuel (ULSF), and B10 and B20 biodiesel fuels. Nine SAE papers were presented and this technology transfer process should provide the basis for industry to improve the OBD and control of urea injection and fuel injection for active regeneration of the PM in the DPF using the computational techniques developed. This knowledge will provide industry the ability to reduce the emissions and fuel consumption from vehicles in the field. Four MS and three PhD Mechanical Engineering students were supported on this project and their thesis research provided them with expertise in experimental, modeling, and controls in aftertreatment systems.

2. Introduction

The primary objective of this project was the development of estimation strategies for the internal states of diesel particulate filters and selective catalytic reduction catalysts (SCRs). This will permit advanced control and on-board diagnostic strategy development that will result in attaining emission regulations in an energy efficient manner. Studying the effects of sensor type and combinations and state estimate quality is an inherent aspect of the estimator design process. State estimate quality is ultimately limited by the accuracy of the device and sensor models. Thus, two additional phases of this work focus on developing SCR and CPF models in specific, high-impact areas. The CPF research includes particulate matter maldistribution, particulate matter (PM) loading and passive regeneration over large NO_x /PM ranges for engines using both diesel and biodiesel-diesel fuel blends, and optimal active regeneration. The SCR research will examine ammonia distribution, optimal ammonia loading, and hydrocarbon poisoning as a function of engine and fuel type.

The overall goal for this project was energy efficient emission control for heavy-duty diesel engines and the development of accurate methods for OBD. Energy efficiency impacts associated with emission control can be classified as direct or indirect. Diesel particulate filters (DPFs) have two direct fuel penalty effects. First, active regeneration, to oxidize accumulated particulate matter (PM), can result in a fuel penalty. Second, inefficient regeneration control strategies can cause unnecessary exhaust backpressure, and potentially large fuel penalties due to inefficient engine operation. The inability to identify and adapt control strategies to aging or compromised components is a secondary fuel penalty scenario. Taken to the extreme, this falls into the category of the need for on-board diagnostics (OBD).

Selective catalytic reduction devices (SCRs) are used to reduce exhaust NO_x levels through reaction with ammonia. The typical ammonia delivery mechanism is through injection of liquid urea. The fuel penalty associated with inefficient SCR operation arises from over injection of urea. This requires more frequent resupply and wastes the energy required for urea production and distribution. Excessive ammonia slippage, an unregulated toxic emission, is a side outcome of this scenario and should be minimized through proper control and OBD strategy implementation.

Exploration of biodiesel effects on DPF and SCR functionality, with particular attention to control system impact, is another aspect of this study. The results of this research could have significant indirect fuel efficiency impact not only in proper functioning of DPFs and SCRs on engines using biodiesel, but also in reducing the U.S. reliance on diesel fuel which comes from foreign crude.

Although SCR and DPF devices have fundamentally different objectives, there is commonality in the model requirements from an OBD/controls perspective. This motivates the benefit for considering both DPFs and SCRs in the same research project. Diesel oxidation catalysts (DOCs) were also included since they react the exhaust species coming from the engine, which feeds into the DPF.

The objective of the proposed research was to develop experimentally validated DPF and SCR models with real-time internal state estimation strategies that support future OBD, advanced control system, and system optimization objectives for DOC-DPF-SCR aftertreatment systems that minimize the energy penalty of meeting emission regulations.

To make optimal use of these devices in current and advanced engine and vehicle technologies there must exist: (1) internal state estimation strategies (2) methods to quantify state uncertainty, (3)

adaptation to aging, and (4) fundamental and applied knowledge of the effects of alternative fuels. The proposed research project addresses these issues while also providing fundamental knowledge that will support aftertreatment development and control activities for low NO_x diesel engines. The expected results of this project are:

1. Recommendations for DPF and SCR estimator strategies suitable for advanced control and OBD strategy development and a measure of their accuracy
2. Evaluation of sensor type and combinations and how they affect DPF and SCR state estimation
3. Recommendations on methods to perform online SCR and DPF model adaptation in the presence of off nominal catalyst/sensor operation
4. Demonstration of how a wide range of NO_x/PM ratio and biodiesel impacts DPF loading, passive oxidation and active regeneration
5. Demonstration of how DPF regeneration affects PM loading maldistribution
6. Recommendations for fuel-optimal DPF regeneration
7. Recommendations of the amount of spatial variability in ammonia storage in an SCR and how to accommodate it for estimation and control design
8. Demonstration of diesel and biodiesel HC poisoning of SCR catalysts
9. Recommendations of optimal ammonia storage targets for SCR urea injection control

The program objectives were achieved through the following tasks:

Task 1: Project management and planning, including incorporating sensors into the engine test cell

Task 2: Baseline estimator model development and form studies, including DOC, CPF, SCR, and sensor models

Task 3: DOC, CPF, and SCR State Estimation

Task 4: CPF and SCR Model Adaptation

Task 5: CPF loading & passive oxidation study including execution of ISB 365 and B10, and ISL 425 ULSD and B20 fuel tests and modeling

Task 6: CPF active regeneration test analysis and modeling

Task 7: CPF PM Loading Maldistribution

Task 8: Fuel-Optimal CPF Regeneration

Task 9: Spatial distribution of ammonia study including modifying experimental protocol and continued flow reactor experiments on SCR catalyst core samples by ORNL

Task 10: Fuel Dependent SCR HC Masking

Task 11: SCR Optimal Ammonia Storage

Details regarding the goals and accomplishments are discussed in the next section organized by the tasks in the project statement of work. Ancillary results including: publications and inventions, website, technology/techniques transfer, licensing agreements are provided in the Ancillary Results section.

3. Goals and Accomplishments

The tasks that were proposed for the project are listed below with a subsection devoted to each that briefly describes the goals for this project and what was accomplished.

3.1 Task 1. Project Management and Planning

Goal 1: Integration of industry and laboratory partner collaboration throughout the project.

This was achieved through several teleconferences with team members and with suppliers focusing on specific technical issues and by yearly team meetings along with the distribution of quarterly reports and copies of all technical papers prior to their publication. The last 8 months of the project involved four of the partners using MTU DOC and SCR codes with their data and models. This effort resulted in MTU developing second versions of the codes that were significantly improved.

Goal 2: Technical, financial, and reporting oversight processes.

Weekly team meetings were held to identify the elements of each project task in detail and to develop plans for completing tasks and deliverable reporting. Quarterly reports and this Final Report were prepared.

3.2 Task 2. Baseline Estimator Model Development

Goal 1: Design and deploy a data inventory system making project data available to team members and the aftertreatment community. This was completed during Q2.

Goal 2: Continue aftertreatment component (DOC, CPF, SCR) and sensor model studies. Progress towards this goal continued along multiple paths (1) sensor model development and (2) SCR, CPF, DOC reduced order model development. These activities are summarized below.

The objective was to develop an estimator form suitable for DOC, CPF and SCR state estimation. A reduced order DOC model was used to develop the base line estimator form. A computationally efficient DOC state estimator predicts the DOC internal states that cannot be directly measured and is valuable for OBD and controls. The DOC estimator is important to predict the exhaust gas states entering the CPF in a DOC-CPF-SCR aftertreatment configuration. The states affected by the DOC that are critical for the performance of the CPF and SCR systems are

- *NO & NO₂ exhaust gas states to accurately predict passive oxidation of PM in the CPF and for urea injection control for the SCR.*
- *During active regeneration, the DOC is used to achieve an exhaust temperature exotherm by oxidizing the injected diesel fuel that results in HC slip into the CPF and an increased CPF inlet temperature (550-600°C) to promote CPF PM oxidation.*

To develop the baseline estimator, a high fidelity DOC model was developed based on engine experimental data [1]. The high fidelity model was then used as a basis to develop a reduced order DOC model and estimator [2].

DOC High Fidelity Model Development

DOC engine experiments under various conditions including steady state, active regeneration and transient conditions were performed in an engine test cell with a 2010 Cummins ISB engine [3]. A high fidelity DOC model simulating the mass transfer, heat and energy transfer and DOC chemical reactions associated with inhibition effects [1] was calibrated to the engine experimental data. Three DOC space velocities, low, medium, and high, and DOC inlet temperatures from 230 to 500 °C were tested under steady state conditions. The steady state data were used for identifying the kinetic parameters including pre-exponential factors and activation energies for the DOC reactions. The DOC experiments under the active regeneration conditions were performed to measure the DOC performance under different space velocities and different target DOC outlet temperatures. The data collected under these conditions were used for identifying the inhibition parameters associated with high HC concentrations under active regeneration conditions. The model parameters identified from the engine data including pre-exponential factor and activation energy for the DOC reactions and the inhibition parameters associated with HC are shown in Table 1. The DOC transient data collected from a surrogate HD-FPT cycle were used for determining the heat transfer coefficients and validating the model performance under transient conditions. The results showed that the calibrated high fidelity DOC model is able to simulate the DOC performance and provide inputs to the CPF and SCR.

Table 1: DOC Kinetic parameters used to simulate active regeneration data

	CO Oxidation		HC Oxidation		NO Oxidation	
A_i	894000		10000		715000	
$E_{ai}(\text{kJ/gmol})$	39.0		25.0		46.4	
Inhibition	$A_{a,j}$	$\Delta H_{a,j}$	$A_{a,j}$	$\Delta H_{a,j}$	$A_{a,j}$	$\Delta H_{a,j}$
$j=1$	0	7990.0	0	7990.0	0	7990
$j=2$	7.0E+07	75000.0	20.5	3000.0	6.8E+08	75000
$j=3$	0	96534.0	0	96534.0	0	96534
$j=4$	0	31036.0	0	31036.0	0	31036
$j=5$	0	0	0	0	0	0

Base line DOC Estimator Development

A high-fidelity DOC model capable of capturing the nonlinear behavior of the DOC described in references [3, 1] was used as a basis to develop the reduced order model. The reduced order model employs bulk phase energy balance equations and reactions instead of separate gas phase and surface phase reactions and energy balance equations. This reduces the complexity and reduces the simulation time and computational requirements to simulate the DOC. A 1-D, single channel representation was developed using Matlab/Simulink®.

An extended Kalman filter (EKF) state estimator, based on an N axial element DOC model, was developed. The estimator uses the inlet mass flow rate, temperature, pressure, CO, NO, NO₂, C₃H₆ and O₂ concentrations from the ECU maps along with the downstream NO_x and temperature measurements to estimate the CO, NO, NO₂, C₃H₆ and temperature states in the catalyst. The parameters needed for the estimator and their measurement location and source of measurement are shown in Figure 1. The estimator results were compared to the experimental data collected from the surrogate HD-FTP tests.

Figure 1: Schematic showing the inputs to the estimator from the sensors and ECU Maps

Figure 2: Comparison of the DOC outlet NO₂/NO_x ratios and temperatures with the estimator in closed loop

Figure 2 shows the comparison of the DOC outlet NO₂/NO_x ratio for a closed loop estimator. The DOC outlet temperature closely follows the response of the measured DOC outlet temperature with less than 0.1% error. With the accurate temperature estimate, the estimator agrees with the measured DOC outlet NO₂/NO_x ratio for most parts of the test with a maximum error of 26%. The improved temperature estimate from the closed loop estimator results in reduced error (maximum error reduced from 50 to 26%) in the NO₂ concentration estimate compared to the open loop estimator at the DOC outlet during the surrogate FTP cycle test. This effort shows that Kalman Filter based state estimation could be suitable for nonlinear systems such as a DOC, CPF and SCR.

3.3 Task 3. DOC, CPF and SCR State Estimation

Goal 1: The goal of this research is to develop both nonlinear and linear state estimation strategies for both SCR and DPF devices. Development of “device health” outputs, as a function of real-time estimated states and nominal-operation states is an objective. Proving stability and quantifying the accuracy of these methods will be a primary objective. Finally, developing rational metrics for comparing trade-offs of computational complexity and accuracy will be developed.

The objective of this research was to develop estimators for DPF and SCR state estimation. The SCR state estimator is based on the high fidelity model in reference [4, 5]. The DPF state estimator is based on the high fidelity model in reference [6]

SCR High Fidelity Model Development

A high fidelity multi-step global kinetic SCR model is important for studying the kinetics of the SCR reactions and provides a basis for developing the SCR reduced order model and state estimator. The performance of the SCR models and state estimator are highly dependent on the kinetic model parameters. SCR reactor and engine experimental studies and model calibration to experimental data are necessary for developing the SCR high fidelity model and identifying the model parameters.

The high fidelity SCR model was developed from an existing model calibrated to Fe-zeolite reactor data [7]. The model was modified for Cu-zeolite SCR by changing the mass transfer correlations and adding necessary reactions. The model considers of a 1-D single channel of the SCR catalyst which was axially divided into a series of axial elements. The model contains equations describing the mass transfer, heat transfer and a series of SCR chemical reactions. It simulates the species concentrations in both the gas phase and surface phase for NO, NO₂, NH₃ and N₂O gas and wall temperatures, as well as the NH₃ storage along the axial distance of the channel.

The experimental data supporting the high fidelity SCR model development and calibration were collected from a flow reactor setup. The reactor experiments and the model calibration to reactor data were discussed in reference [4]. The core SCR samples tested in the reactor were taken from a 2010 Cummins ISB engine catalyst. An isothermal test protocol designed to separate the effects of different SCR reactions, was tested for three space velocities (60k, 90k and 120k hr⁻¹) and temperatures from 200 to 425 °C. The model was calibrated to the data through both manual calibration and running optimization functions to determine the optimal set of parameters which gave the least error between model simulation and the experimental measurements. The calibrated model is able to simulate the axially resolved concentrations of NO, NO₂, NH₃ and N₂O in both the gas and surface phases as well as the NH₃ storage.

The reactor experiments were important for studying the SCR kinetics and developing the SCR model. However, the SCR engine experiments are necessary to study the SCR performance in engine applications and the SCR model calibrated to engine data is valuable for developing the SCR state estimator. The reactor testing environment is simplified compared to engine exhaust conditions by using synthetic exhaust flow generated from gas cylinders and injecting gaseous NH₃ instead of liquid urea water solution. With more complex exposure conditions including urea decomposition and nonuniform gaseous concentration distribution, the SCR performs differently in engine exhaust environments. In order to study the SCR performance in engine exhaust conditions and develop a model calibration based on engine data, the SCR engine experiments under both steady state and transient conditions were tested on a 2010 Cummins ISB engine and the model was calibrated to the engine experimental data [5].

The model calibration developed from the reactor data was used as a basis when calibrating the model to engine data. The calibrated model is able to simulate the SCR performance under both steady state and transient conditions with reasonable errors.

The identified model parameters from the SCR engine data were given in reference [5] and were compared to the model parameters identified from the reactor data. Differences in the kinetic parameters were observed between the two calibrations, indicating that the SCR performs differently in engine exhaust environments than the reactor environments. The more complex engine exhaust conditions were considered to be the reason causing the differences. A combined experimental and simulation study was carried out to study the NH_3 non uniformity effects on the SCR performance and the kinetic model parameters. The results showed that the NH_3 maldistribution at the SCR inlet was obvious in engine tests, resulting in lower NO_x conversion efficiency and higher NH_3 slip. It also contributed to the differences between the SCR model calibrations for the reactor and engine data [8]. However, the high fidelity SCR model calibrated to the engine data accounts for the complex exhaust environments and is suitable to be used as a basis for developing the state estimator.

SCR Estimator Development

A reduced order SCR model, capable of capturing some of the nonlinear behaviors of the high-fidelity SCR model [4] was developed. The reduced order model employs bulk phase energy balance equations and reactions instead of separate gas phase and surface phase reactions. The reduced order model was used as the basis for the development of the state estimator, also reduces the computational requirement to simulate the SCR.

Two nonlinear versions of a Kalman Filter, EKF and Unscented Kalman Filter (UKF) were developed using a five element SCR model. The internal states of the estimators are compared with the simulated states. The results of this study are included in the report [9] submitted to the DOE. Based on the results for the cases studied, it was concluded that both EKF and UKF based state estimators estimate the states in the SCR with less than 1% error and EKF estimation strategy needs less computational resources and is accurate enough for the purpose of state estimation in the SCR. An EKF estimator [10] was developed with the NH_3 storage on site 1 and site 2 as the states in the estimator and NO_x and/or NH_3 sensors at the SCR outlet as the measurements.

Figure 3 shows a schematic of the SCR estimator with all the inputs needed. The SCR estimator uses the exhaust mass flow rate, NH_3 , NO , NO_2 and O_2 concentrations from the engine maps along with the temperature and the NO and NO_2 concentrations upstream (NO_x sensor upstream or NO and NO_2 out of the CPF from a model) of the SCR and NH_3 and/or NO_x sensor downstream of the SCR to estimate the states of the SCR. The models for NO_x and NH_3 sensors were developed using the data acquired with the available NO_x and NH_3 sensors. The NO_x sensor model is based on the sensor model in reference [11].

Figure 3: Schematic of the SCR estimator with the inputs

The estimator was simulated on the surrogate FTP cycle with both NO_x and NH₃ sensors at the SCR outlet and Figure 4 shows a comparison of the SCR outlet NO, NO₂, and NH₃ concentrations. From the figure it can be observed that the estimator simulates the SCR outlet NH₃ concentration with a maximum error of +/-26 ppm and ±75 ppm for the NO and NO₂ concentration, respectively.

Figure 4: Comparison of the SCR outlet NO, NO₂, and NH₃ concentration for the FTP cycle with the estimator in closed loop- With NO_x and NH₃ sensor

The effect of the NO_x and NH_3 sensors on the state estimation quality was evaluated using the surrogate FTP cycle [10]. The results showed that the NH_3 sensor has a more significant effect on the performance of the estimator. The estimator had the best performance with both the NO_x and NH_3 sensors and the worst performance with just the NO_x sensor while the estimator with just the NH_3 sensor was in the middle.

CPF High Fidelity Model Development

A 1-dimensional numerical model of the CPF (called CPF high-fidelity model) was developed at MTU [6] and calibrated to experimental data [12] from passive oxidation [13] and active regeneration [14,15] experiments. A reduced order model [16] was developed based on the framework of the CPF high-fidelity model as part of the efforts towards this research, which then formed the basis for the development of an EKF-based state estimator designed to predict and/or adjust the internal states of variables (the PM mass retained in the cake and wall of the CPF) associated with the CPF such that certain estimated outputs (for example, the total pressure drop across the CPF) simulate the experimental measurements of the same output variable.

The CPF high fidelity model simulates flow, filtration, oxidation, mass and heat transfer processes related to the particulate matter (PM) and exhaust gas species as the exhaust gas mixture passes through a geometry that is considered to be represented by a single inlet channel, substrate wall and outlet channel. Flow of exhaust gas through the CPF is assumed to be compressible laminar flow at quasi-steady state. Mass and momentum conservation equations for the exhaust gas mixture flowing through control volumes in the inlet channel, substrate wall and outlet channel are accordingly developed and solved for to obtain the velocity of flow at all locations within the CPF. In a similar manner, energy balance of control volumes constructed in the inlet channel, substrate wall and outlet channel are solved sequentially to obtain the temperature of the exhaust gas mixture at all locations in the CPF. The energy balance in the inlet channel and outlet channel are considered as quasi-steady state while the wall energy balance is considered to be transient. Gaseous species concentrations are also solved for by considering the mass balance of individual gaseous chemical species ($\text{C}_{12}\text{H}_{24}$, O_2 , CO_2 , H_2O , CO , NO and NO_2) in the inlet channel, substrate wall and outlet channel control volumes. All chemical reactions involving gaseous chemical species are considered to be occurring in the catalyst washcoat layer which is located on/in the substrate wall. These reactions cause a proportional change in the concentrations of species involved in those reactions as reactants or products. The chemical reactions considered in the CPF high-fidelity model are $\text{C}_{12}\text{H}_{24}$ oxidation, CO oxidation and NO oxidation/ NO_2 reduction. PM is considered to be elemental carbon and is carried into the CPF by the exhaust gas mixture as it flows through the CPF. Deposition of PM first occurs in the substrate wall and transitions to being deposited as a PM cake layer when a certain threshold of substrate wall permeability (called “transition permeability”) has been reached. Oxidation of the filtered PM occurs through thermal (oxidation of C with O_2 to form CO and CO_2) and passive (oxidation of C with NO_2 to form CO , CO_2 and NO) mechanisms both in the substrate wall and PM cake layer. The pressure drop across the CPF is also calculated in the CPF high-fidelity model by calculating the absolute pressure field in the CPF utilizing the axial momentum conservation equation and assuming that the pressure at the outlet of the CPF (and hence the outlet side of the outlet channel) at any point in time is known and equal to the barometric pressure measured at that same point in time during the experiment when the system is a DOC-CPF.

Calibration of the filtration, PM kinetics and gaseous kinetic parameters used as inputs for the CPF high-fidelity model is crucial to getting an accurate quantitative description of the processes occurring during different operating conditions that the CPF is subjected to. Experimental data from both passive oxidation experiments and active regeneration experiments were analyzed and used as inputs to the CPF model to calibrate the input parameters to the CPF model. The process of calibration and the results obtained are detailed in reference [12]. The results obtained from optimization of PM kinetics were used (with appropriate conversion factors) as a starting point for calibration of the reduced order model (as explained below) in order to aid in the estimation of the internal states of PM mass retained in the cake and wall during engine conditions that the CPF undergoes.

CPF Estimator Development

The CPF estimator uses a reduced-order version of the 1-D model. The lumped model is derived from the high fidelity model in reference [6]. The states of the lumped model are reduced from 24 in the high fidelity model to 3: the substrate temperature and the mass retained in the substrate wall and cake layer. The lumped model simulates the filtration and oxidation of PM in the PM cake and substrate wall, oxidation of NO, CO and HC's, energy balance equations for temperature and pressure drop across the CPF. The reduced order model simulates oxidation of PM through NO₂ and O₂. The oxidation reactions for CO, NO and HC is assumed to be instantaneous. The outlet temperature in the lumped model is assumed to be equal to the substrate temperature and the heat transfer is calculated to the packing, can, and ambient. The total pressure drop is calculated to be the sum of the average of the inlet and outlet channel pressure drops, as well as the pressure drop of the substrate wall and cake layer.

The reduced order model was used to develop an extended Kalman filter for state estimation. Figure 5 shows a schematic of the SCR estimator with all the inputs needed for the simulation. The estimator uses the species concentrations from the DOC estimator, the exhaust mass flow rate and PM concentration from the ECU, and the inlet gas temperature sensor to calculate the a priori state estimate (substrate temperature and mass in the cake layer and substrate wall). It then uses the measured pressure drop, along with information from numerical state and output Jacobian calculations, to correct the prior state estimate such that the error between the measured pressured drop and the lumped model calculated pressure drop is reduced. The estimator primarily adjusts the mass retained in the cake layer and wall because the substrate temperature has little effect on the pressure drop error. A PM sensor is shown in the figure because it is currently being explored.

Figure 5: CPF Reduced Order Model and Estimator Data Flow Schematic

The parameters from the higher order model were used as the starting point for simulating the reduced order model and estimator. Some of the parameters needed to be tuned within an order of magnitude due to the simplifications made. The values used in each test case compared to the higher order model can be found in Table 2. A comparison of the key performance criteria (pressure drop and PM retained) between reduced order and higher order model using these modified parameters is shown in Table 2.

Table 2: Filtration and gaseous species reaction kinetics from calibration of high-fidelity CPF model and resulting reduced order model kinetics

Parameter	Units	High Fidelity	Reduced Order
		AR-ULSD-1	AR-ULSD-1
FILTRATION			
$k_{s,0}$	$[m^2]$	1.19×10^{-13}	1.19×10^{-13}
k_{trans}	$[m^2]$	8.00×10^{-13}	8.00×10^{-13}
$C_{1,ppw}$	$[1/m^3]$	2.20	2.20
$C_{2,ppw}$	$[kg/m^3]$	1.5	1.5
$\alpha_{p,0}$	$[.]$	0.05	0.05
$k_{p,0}$	$[m^2]$	7.00×10^{-15}	7×10^{-15}
$\rho_{p,0}$	$[kg/m^3]$	104	104
A_η	$[.]$	0.937	0.937
GASEOUS KINETICS			
A_{HC}	$[m^3/kmol.s]$	6.00×10^8	
Ea_{HC}	$[J/kmol]$	4.35×10^7	
A_{CO}	$[m^3/kmol.s]$	3.00×10^8	
Ea_{CO}	$[J/kmol]$	3.90×10^7	
A_{NO2}	$[m^{3/2}/kmol^{1/2}.s]$	1.50×10^7	
Ea_{NO2}	$[J/kmol]$	3.00×10^7	
PM KINETICS			
$A_{NO_2,cake}$	$[m/s]$	0.3	0.3
$Ea_{NO_2,cake}$	$[kJ/gmol]$	74.1	74.1
$A_{NO_2,wall}$	$[m/s]$	1.5	1.5
$Ea_{NO_2,wall}$	$[kJ/gmol]$	74.1	74.1
$A_{th,cake}$	$[m/s]$	0.65	0.65
$Ea_{th,cake}$	$[kJ/gmol]$	139	
$A_{th,wall}$	$[m/s]$	0.97	0.97
$Ea_{th,wall}$	$[kJ/gmol]$	139	

The pressure drop performance of the reduced order model compared to the higher order model is shown in Figure 6. This is used to validate the calibration of the model used for the estimator. There are nine curves: red circles for experimental pressure drop every 250 s, four green curves for the high fidelity (hifi) model, and four blue curves for the reduced order model (rom). The solid green and blue lines represent the total pressure drop, the dashed line represents the pressure drop across the substrate wall, the dot-dashed line represents the pressure drop across a channel, and the dotted line represents the pressure drop across the cake layer.

Figure 6: Pressure drop comparison between higher order model, reduced order model, and experimental data using parameters found in Table 1 for AR-ULSD-1

The mass balance performance of the reduced order model compared to the higher order model is shown in Figure 7. This is also used to validate the calibration of the model used in the estimator. There are nine curves: red circles for experimental PM retained, four green lines for the high fidelity model (hifi), and four blue lines for the reduced order model (rom). The dashed green and blue lines represent the inlet PM, the solid line represents the total PM retained, the dot-dashed represents the outlet PM, and the dotted line represents the PM oxidized (including both thermal and NO_2 assisted oxidation).

Figure 7: PM retained comparison between higher order model, reduced order model, and experimental data using parameters found in Table 2 for AR-ULSD-1

Figure 8 shows the PM retained performance of the reduced order model compared to the higher order model divided into components. This is also used to validate the calibration of the model used in the estimator. There are seven curves: red circles for experimental PM retained, three green lines for the high fidelity model (hifi), and three blue lines for the reduced order model (rom). The solid green and blue lines represent the total PM retained, the dashed line represents the PM retained in the cake, and the dot-dashed represents the PM retained in the wall.

Figure 8: PM Retained comparison between the higher order model, reduced order model, and experimental data using parameters found in Table 1 for AR-ULSD-1

The EKF provides an improved estimate of the pressure drop. The case used to test the model and estimator was Test 1, an active regeneration test case with ULSD fuel type [15]. Figures 9-10 show the results of the model and estimator superimposed on the measured test results.

Figure 9 shows the pressure drop performance of the estimator for Test 1. This is one of the performance criteria for the estimator. It contains nine curves, similar to Figure 6 where the green curves are for the estimated values and the blue curves are the reduced order model. At around 2 and 3 hours, there are points where the pressure drop decreases sharply. This is when the estimator is turned back on after large pressure drop changes (including in the noise) and is reconverging.

Figure 9: Comparison of the reduced order model, EKF estimator, and experimentally measured pressure drop across the CPF for AR-ULSD-1

Figure 10 shows the PM retained performance of the estimator for Test 1. This is another performance criterion for the estimator. The figure contains ten curves similar to Figure 8, where the green curves are the estimated values and the blue curves are the reduced order model results. The estimator behaves as expected: since the model pressure drop is higher compared to the experimental values during loading, the estimator decreases the mass retained in the wall to reduce the pressure drop error.

Figure 10: Comparison of the reduced order model, EKF estimator, and experimentally measured total PM retained for AR-ULSD-1

To summarize, a reduced order CPF model was developed using the sub-models from a higher order model. The reduced order model was calibrated starting with the higher order model parameters, and tuned manually to achieve a proper fit. An extended Kalman filter was developed using the reduced order model. The reduced order model fits the experimental data well, and the estimator improves the estimate of the PM mass and the pressure drop. Detailed CPF estimator results can be found in the estimator engine test report [16]

3.4 Task 4. DPF and SCR Model Adaptation

Goal 1: Using aged and failed data from engine OEM's to the estimation models will be identified, this will provide a quantitative bound on the parameters, and may provide correlations between device health and parameter vectors.

Goal 2: The correlations will be used to determine if parameter vectors can be used for deterministic health predictions of both the SCR and DPF.

During its life span, an SCR or a DOC experience changes in their performance characteristics. For the model adaptation study the reduced order SCR model and estimator [10] were used. In an SCR, NH_3 storage capacity and activation energies for NO_x reduction are some of the parameters that can change with time. To estimate these parameters periodically, a nonlinear batch mode least squares estimator can be used, and for real time estimation an extended Kalman Filter (EKF) can be used. To use the nonlinear least squares approach for onboard diagnostics (OBD,) the estimator must be implemented on

the ECU of an engine. To do this, periodically the time history of the inputs from the sensors and estimators would be stored in the ECU and used for the estimation.

A nonlinear least squares estimator was developed to estimate the activation energy using the NO_x sensor located at the SCR outlet. The least squares estimator uses the NO_x sensor measurements at the SCR outlet along with the inputs to the SCR (SCR inlet NO , NO_2 , NH_3 , O_2 concentrations, exhaust mass flow rate and SCR inlet temperature) to estimate the activation energies in the SCR. The results show that the least squares estimator is able to estimate the activation energies based on the NO_x sensor signal. The EKF SCR estimator in reference [10] was modified to estimate the activation energies for fast SCR, standard SCR 1, standard SCR 2 and slow SCR reactions. The SCR estimator can estimate the NO , NO_2 , NH_3 , temperature and NH_3 storage states in the SCR based on NO_x and/or NH_3 sensor measurements at the SCR outlet. The EKF estimator was simulated on the surrogate FTP experimental data. The results show that the EKF estimator is able to reduce the error between the simulated and estimated NO_x sensor signals, but is unable to estimate the activation energies. The EKF estimator cannot differentiate between the error in the states and the error in the parameters. A detailed report on the model adaptation study was submitted to the DOE [17].

3.5 Task 5. CPF Passive Oxidation Kinetics Study

Goal 1: Develop a test plan that minimizes the test load while maximizing the information for use in future model development. This goal was completed Q1.

Goal 2: Being able to model the passive, NO_2 oxidation of accumulated PM in the CPF is critical to creating accurate state estimation strategies. Understanding the effect of fuel type (ULSD and biodiesel blends) and the effect of CPF PM loading level on oxidation kinetics are primary goals. A test plan and protocol were developed that allowed passive oxidation rates to be determined from engine test cell data.

Task 5 of this project was designed to characterize DPF loading and passive oxidation, while Task 6 was designed to yield the same for active regeneration of the DPF loaded to a pre-specified PM loading level (≈ 2.2 g/l) by means of in-cylinder and/or post-turbo injection of diesel fuel. Both tasks have been completed and an initial model calibration has been performed to selected cases from both sets of experimental data. The following sections of this report explain each of these tasks in detail.

The objective of this task was to experimentally quantify, calibrate and validate the MTU 1-D CPF model and provide details for controls and OBD development. Results from experiments conducted involving loading and passive oxidation over a wide range of NO_2 /PM ratios, temperatures and exhaust flow rates using ULSD and Biodiesel/ULSD blends (B10 and B20) were used to determine global PM oxidation rates and PM filter characterization appropriate for the MTU 1-D CPF model and control (reduced order) model under passive oxidation operating conditions. The 1-D CPF model was used to determine the PM distribution in the wall and cake and the split of pressure drop components (channel, wall and cake).

Experimental efforts in this task were recorded and reported through two (2) Michigan Tech deliverables – DOE/EE0000204-2 [18] and DOE/EE0000204-4 [19]. These efforts were also published in two technical papers published and presented at the 2012 SAE World Congress at Detroit, MI [20,21], based on MS theses [13, 22]. The effort described in DOE/EE0000204-2 [18] primarily established a procedure for conducting experiments designed to study loading of a CPF and subsequent oxidation of

this PM via passive means. This procedure entails conducting each experiment in various stages. In stage 1 (called “S1”), the CPF is loaded at a pre-determined engine operating condition from a clean state for approximately ½ hour. At this point, the CPF is dismantled from the exhaust pipe and weighed to get a total substrate weight measurement. In stage 2 (called “S2”), the CPF is re-connected to the exhaust and loaded to a pre-specified PM loading level (≈ 2.2 g/l), followed by another substrate weight measurement. Then in the passive oxidation (called “PO”) stage, the engine is operated for a pre-determined duration of time at the passive oxidation engine operating condition at the end of which a certain percentage of the PM already loaded in the CPF is targeted. After this, in stage 3 (called “S3”), the engine is operated at the same operating condition as stage 1 and stage 2 for a pre-determined duration (in this case, 30 minutes). The substrate weight is again recorded. Figure 11 shows a graphical depiction of the CPF pressure drop and PM mass retained at the end of the different stages that have been explained here, along with the duration of the different stages shown by double-headed arrows.

Figure 11: Overview of the four main stages of the passive oxidation test procedure [18]

Also, DOE/EE0000204-2 [18] outlines the development of two test matrices for experiments conducted on two engines, a 2002 Cummins ISM 256 kW (330 hp) engine and a 2007 Cummins ISL 272 kW (365 hp) engine. A total of fifteen experiments were carried out, five on the ISM engine and ten on the ISL engine, details of which can be found in Table 5 of reference [18]. Stage-wise results from loading stages and passive oxidation stage were presented. A summary of the various experiments performed was also given, followed by conclusions drawn thereof and a list of recommendations for future experiments. Figure 12 shows the overall PM oxidation reaction rates obtained from experiments as reported in reference [18], where the reaction rates are calculated from the measured and/or calculated masses of PM before and after the passive oxidation (PO) stage.

Figure 12: Overall average PM reaction rates during passive oxidation tests [18]

Based on the recommendations from the work done using ULSD fuel [18,20], the work described in DOE/EE0000204-4 [19] was conducted on one engine, a 2007 Cummins ISL 272 kW (365 hp) engine using Soy Methyl Ester (SME)-based biodiesel blended with ULSD to 10% by volume (B10) and 20% by volume (B20). The procedure followed was based on that described in the previous work [18], but with some improvements to repeatability of measured variables during passive oxidation. These improvements included the addition of a 15 minute loading condition (called stage 3 or “S3”) between the end of stage 2 and the beginning of passive oxidation stage and continuing the passive oxidation stage with a return to loading engine operating conditions for 30 minutes (called stage 4 or “S4”), weighing the substrate and loading the CPF for another 60 minutes in what is called a post-loading stage (called stage 5 or “S5”). Figure 13 shows a graphical depiction of the various stages and the general nature of variation of the pressure drop across the CPF and PM retained in the CPF.

Figure 13: Overview of the different stages of the modified passive oxidation test procedure used during ISL tests 11-18 [19]

A total of eight tests were conducted, four (called “Test 14”, “Test 15”, “Test 16” and “Test 17”) with B10 and four (called “Test 11”, “Test 12”, “Test 13” and “Test 18”) with B20, the details of which are tabulated in Table 8c and Table 8d respectively in reference [19]. As with the previous work, this work also focused on presenting experimental results stage-wise and arriving at the global reaction rates during passive oxidation. Figure 14 shows a plot of experimentally obtained reaction rates during passive oxidation tests plotted against $1000/T$ where T is the average absolute temperature at which passive oxidation occurs. This plot also includes the data presented in Figure 12 for ease of comparison. The procedure followed to obtain these rates is also the same as that in reference [13].

Figure 14: Average overall PM reaction rates during passive oxidation tests plotted versus $1000/T$ where T is the average CPF temperature during passive oxidation expressed in Kelvin [19]

Through a detailed analysis of experimental data that was available from all passive oxidation experiments, six passive oxidation experiments were determined to contain reliable data for calibration of the high-fidelity CPF model [6]. These tests are listed in Table 3 below. Corrections to the inlet PM and NO_2 concentrations as obtained from analysis of experimental PM retained data along with calibrated outputs of the PM mass balance from multiple runs were applied to get better fits of PM retained along with a single set of kinetic parameters that fit all passive oxidation experiments as described in reference [12].

Table 3: List of passive oxidation experiments used for calibration of high-fidelity CPF model [15, 19, 21]

No.	Expt. Name [13]	Fuel Type	New Name [12]	PO Temp. [°C]	PO Time [min.]	CPF inlet NO_2/NO_x [ppm/ppm]	CPF inlet O_2 [% Vol.]
1	TEST 14	B10	PO-B10-14	253	101	112/257	12.55
2	TEST 15	B10	PO-B10-15	355	81	101/194	8.91
3	TEST 16	B10	PO-B10-16	408	43	61/209	7.13
4	TEST 17	B10	PO-B10-17	356	80	90/178	8.74
5	TEST 12	B20	PO-B20-12	350	81	109/206	9.40
6	TEST 13	B20	PO-B20-13	403	42	64/204	7.31

The high-fidelity CPF model developed as part of this effort was described and calibrated to one passive oxidation experiment from references [19, 13] (called “ISL B20 Test 12” in reference [13] or PO-B20-12 as given in Table 3) in order to demonstrate model capabilities in a technical paper presented in reference [6]. The CPF model was calibrated using data from all six experiments listed in Table 3. Specifics about the model calibration approach and procedure can be found in reference [12]. Calibration of the CPF model resulted in PM reaction rate constants being determined and used for optimization which resulted in the determination of a minimal set of PM kinetics parameters that can be

used to predict the PM retained in the CPF and the pressure drop across the CPF, details of which are given in reference [12].

All rate constants obtained from calibration of the CPF model were plotted in an Arrhenius plot since PM oxidation rate equations follow the following form:

$$\frac{dm_{ox,i}}{dt} = m_{ret,i} \sum_{m=NO_2}^{th} (-1)R_{m,i}$$

where $R_{m,i} = \rho_p A_p A_{m,i} e^{\left(\frac{Ea_{m,i}}{RT}\right)} [Y_m]$ are the rates of thermal/ NO_2 -assisted PM oxidation reactions (expressed in [1/s]), ρ_p is the packing density of PM in PM cake layer (expressed in kg/m^3), A_p is the specific surface area of PM (expressed in m^2/kg), $A_{m,i}$ are the pre-exponential factors (expressed in [m/s]), $Ea_{m,i}$ are the activation energies (expressed in [kJ/gmol]), Y_m are the mole fractions of oxidants

(O_2/NO_2 – unit-less), $i = \begin{cases} cake \\ wall \end{cases}$, and $m = \begin{cases} th (thermal - O_2) \\ NO_2 (NO_2 - assisted) \end{cases}$

Since the reaction rate constants follow the simple Arrhenius form, a linear fit of natural logarithms of the reaction rate constants obtained from calibration versus the inverse of the average absolute temperatures during NO_2 -assisted oxidation of PM can be used to iterate towards a single set of PM oxidation kinetics. Such a plot of reaction rate constants of the NO_2 -assisted PM oxidation reaction from the loading phase ($1000/T \cong 1.9$) and passive oxidation phases of all passive oxidation experiments is shown by location (PM cake layer and substrate wall) in Figure 15. Thermal PM oxidation kinetic parameters used for the calibration of these experiments have been obtained from optimized values of kinetics for thermal PM oxidation reaction using the active regeneration data collected in Task 6. The development of the thermal PM oxidation kinetic parameters will be discussed in the next section (3.6) covering Task 6 of this research work.

Figure 15: Natural logarithms of reaction rate constants for NO_2 -assisted PM oxidation reactions in the CPF during all passive oxidation experiments showing: a) NO_2 -assisted PM oxidation in PM cake layer, and b) NO_2 -assisted PM oxidation in substrate wall

As a result of model calibration, the pressure drops across the CPF and PM retained in the CPF were simulated and compared to experimental data for all 6 passive oxidation experiments. Figure 16 shows the result from the calibrated model compared to the experimental data for pressure drop and PM retained (PM cake and wall) for PO-B20-13. This figure shows the accumulation of PM in the wall initially (from time = 0 to ~0.3 hrs) and subsequently in the PM cake layer till the end of loading when the total PM mass retained in the CPF reaches ~40 g (time = 4.8 hrs). This is then followed by a passive oxidation event (at 403°C CPF inlet temperature and 64/204 CPF inlet NO_2/NO_x ratio – time = 5.1 hrs to 5.6 hrs) where the PM mass retained in the PM cake layer as well as substrate wall decrease due to oxidation to reach a final value of 24 g of total PM mass retained. After the passive oxidation event, the PM mass retained in the filter increases due to another loading event (called post-loading as explained in Figure 13 from reference [19]) from time = 5.7 hrs to 7.2 hrs. The model is able to simulate both total pressure drop across the CPF as well as total PM retained in the CPF throughout the experiment within acceptable limits.

Figure 16: Model-predicted values of CPF pressure drop (blue line) and total PM retained in the CPF (green line) compared with experimental total pressure drop across CPF (red line) and experimental PM retained at the end of stage 1, stage 2, stage 3 and stage 4 (black stars) and simulated PM retained in the wall (magenta dashed line) for test PO-B20-13 (as shown in Table 3).

The overall goal of detailed characterization of the CPF during passive oxidation has been accomplished by the experimental efforts described in references [18] and [19] and the modeling effort as described in reference [12]. Optimized values of kinetic parameters for passive PM oxidation reaction are as shown in Table 4. The range of values for filtration parameters and gaseous species reaction kinetic parameters used for the calibration of the passive oxidation as well as active regeneration (as explained in Task 6 – section 3.6) experiments are as shown in Table 5.

Table 4: Optimized passive PM kinetics developed in reference [12]

Fuel Type → Parameter ↓	ULSD	B10	B20	Units
$A_{NO_2, cake}$	0.21	0.06	0.015	[m/s]
$Ea_{NO_2, cake}$	74.1	68.3	59.4	[kJ/gmol]
$A_{NO_2, wall}$	0.21	0.06	0.015	[m/s]
$Ea_{NO_2, wall}$	74.1	68.3	59.4	[kJ/gmol]

Table 5: Filtration and gaseous species reaction kinetics from calibration of high-fidelity CPF model

Parameter	Units	Value (range)
FILTRATION		
$k_{s,0}$	[m ²]	1.15×10^{-13} - 1.19×10^{-13}
k_{trans}	[m ²]	0.74×10^{-13} - 1.19×10^{-13}
$C_{1,ppw}$	[1/m ³]	2.11 - 2.35
$C_{2,ppw}$	[kg/m ³]	1.48 - 1.61
$\alpha_{p,0}$	[.]	0.05
$k_{p,0}$	[m ²]	6.47×10^{-15} - 7.58×10^{-15}
$\rho_{p,0}$	[kg/m ³]	104
A_η	[.]	0.937
GASEOUS KINETICS		
A_{HC}	[m ³ /kmol.s]	6.00×10^8
Ea_{HC}	[J/kmol]	4.35×10^7
A_{CO}	[m ³ /kmol.s]	3.00×10^8
Ea_{CO}	[J/kmol]	3.90×10^7
A_{NO_2}	[m ^{3/2} /kmol ^{1/2} .s]	1.50×10^7
$Ea_{NO_2}^1$	[J/kmol]	3.00×10^7

3.6 Task 6. CPF Active Regeneration

Goal 1: Develop test protocol, instrumentation, and data templates for Michigan Tech and OEM CPF active regeneration engine testing. This includes a test plan for both ULSD and bio-diesel fuels, identification of independent variables, and collaboration with OEM's on similar test plans.

The focus of this activity is the detailed characterization of active regeneration including determination of global reaction rates and the dependence of these rates on dosing method, temperature, and PM loading for ULSD and biodiesel fuel blends as described in reference [12, 23].

As a result of the data collection and analysis methods used throughout the CPF active regeneration study, a test plan was developed for use on the 2007 Cummins ISL engine which allows for the use of

¹ Kinetic parameters (pre-exponential factor (A_{NO_2}) and activation energy (Ea_{NO_2})) of NO-NO₂ oxidation were optimized from this set of values as shown in reference [12].

ULSD and B10 (10% Vol.) and B20 (20% Vol.) blends of biodiesel fuel, in-cylinder and post-turbo dosing injection methods, as well as 2.2 and 4.1 ± 0.2 g/L CPF PM loading test cases.

Through the data analysis methods utilized, a method to determine the PM reaction rate at each time step through active regeneration, global activation energy for all three test fuels, and pre-exponential factors for each test fuel have been determined. As part of the data analysis, the effects of CPF temperature, fuel type, and dosing method on CPF active regeneration have been determined. A summary of the findings is shown below [14, 15]

- A method to calculate the PM reaction rate at each time step through the entire active regeneration phase of the experiments has been developed.
- The PM reaction rate was shown to increase with increasing test fuel percent biodiesel and CPF inlet temperature.
- An active regeneration model was developed and used to predict the active regeneration time given a set of experimental test conditions.
- Optimization methods were used to determine a global activation energy of 139 kJ/gmol for all test fuels.
- Optimization methods were used to determine the pre-exponential factor for each test fuel. The pre-exponential factor for B20 was the highest, followed by B10 and ULSD. The pre-exponential factors for B20 and ULSD were shown to be statistically different while they were statistically similar for B10 and ULSD.
- DOC HC conversion efficiency is increased by 3% or more with in-cylinder compared to post-turbo dosing methods.
- Efficiency of PM oxidation is increased as exhaust flow rate is decreased. This results because the amount of dosing fuel that is required to achieve a given CPF inlet temperature increases with proportionally increasing flow rate.
- Efficiency of PM oxidation at a constant CPF temperature increased with B20, as compared to ULSD, leading to shorter regeneration times and decreased fuel consumption during active regeneration.
- A lower temperature is required to achieve the same efficiency of PM oxidation with B20 when compared to B10, and a lower temperature is required with B10 compared to ULSD. A lower CPF temperature requires less dosing fuel to be consumed during dosing, decreasing fuel consumption during active regeneration.

Figure 17 illustrates the PM reaction rate for each test case as well as the model trends obtained by using the global activation energy and pre-exponential factors according to the test fuel determined using the optimization methods as discussed in reference [15]. The use of optimization methods allowed for determination of the global activation energy of 139 kJ/gmol and the pre-exponential factors for ULSD (9.8×10^6 1/sec), B10 (12.2×10^6 1/sec), and B20 (20.1×10^6 1/sec) [14, 15].

Figure 17: Optimized Results with All Tests Included in the Optimization

It can be seen that the PM reaction rate increases with increasing biodiesel content in the test fuel as well as with increasing CPF temperature. These trends were expected based on previous work related to CPF active regeneration.

Figure 18 illustrates the efficiency of PM oxidation (grams of PM oxidized per gallon of dosing fuel injected) data from this study as well as the data from previous active regeneration studies. The data from previous studies was normalized by the ratio of exhaust flow rates in order to analyze the effects of exhaust flow rate on the efficiency of PM oxidation. The flow rate used during active regeneration in this study was approximately ½ of that which was used in the data shown from the active regeneration studies by previous research, which means that the efficiency of PM oxidation increases with a proportional decrease in exhaust flow rate [14, 15].

As a result of this normalization process, it can be seen in Figure 18 that the regeneration efficiency of fuel dosing for any given temperature is increased with increasing test fuel biodiesel content. It is also shown that a lower CPF temperature is required to achieve a given efficiency of PM oxidation as the test fuel biodiesel content increased. Higher efficiency of PM oxidation at a constant temperature leads to shorter regeneration times, thereby decreasing the overall fuel consumption during active regeneration. Similarly, a lower temperature required to achieve a given efficiency of PM oxidation requires less dosing fuel to be consumed, which also decreases the overall fuel consumption during active regeneration.

Figure 18 Grams of PM oxidized per equivalent gallon of fuel injected during dosing as a function of average CPF temperature including data from reference [1] in reference [15] normalized by exhaust volumetric flow rate ratio [15]

In order to compare the effect of method of fuel dosing on CPF temperatures during active regeneration, data from 6 tests (as listed in Table 6) were analyzed. Tests ULSD-3, ULSD-4, ULSD-5, and ULSD-6 were test cases with experimental CPF inlet temperatures of $525 \pm 1^\circ\text{C}$ using ULSD. B20-5 and B20-6 were test cases with experimental CPF inlet temperatures of $527 \pm 1^\circ\text{C}$ using B20. Out of these 6 tests, ULSD-6 and B20-6 were the only test cases which used the post-turbo dosing method (all others used in-cylinder dosing method).

Table 6: Active Regeneration Test Data

Variable	Dosing Method	Estimated Doser Flow Rate	Estimated Engine Out HC Conc.	CPF Inlet HC Conc.
Test/Units	-	g/sec	ppmC	ppmC
B20 1	in-cyl.	0.517	7600	226
B20 2	in-cyl.	0.608	8900	374
B20 5	in-cyl.	0.695	10300	355
ULSD 3	in-cyl.	N/A	N/A	N/A
ULSD 4	in-cyl.	0.648	10100	289
ULSD 5	in-cyl.	0.636	9800	346
ULSD 6	exhaust	0.667	10300	571
B20 6	exhaust	0.749	10900	644
B20 4	in-cyl.	0.594	8800	300
B10 1	in-cyl.	0.654	10100	430
B10 2	in-cyl.	0.646	9900	342
B10 3	in-cyl.	0.648	9900	371
ULSD 1	exhaust	0.759	11700	585
ULSD 8	in-cyl.	0.635	10100	698
ULSD 9	in-cyl.	0.727	11400	894
B10 4	in-cyl.	0.738	11400	600
ULSD 7R	in-cyl.	0.709	11300	560
ULSD 2R	in-cyl.	0.893	14300	513
ULSD 10	in-cyl.	0.663	9900	365

From Table 6, it can be seen that the DOC inlet (Engine-out) HC concentration was nearly the same for all 6 test cases, while the CPF inlet HC concentration was 200-300 ppmC higher for the post-turbo dosing cases. This means that the DOC HC conversion efficiency with in-cylinder dosing is increased when compared to post-turbo dosing. Therefore, in order to achieve the same CPF inlet temperature, post-turbo dosing requires more fuel than in-cylinder dosing, regardless of fuel type [15].

The tests which were run with the post turbo dosing injector had elevated CPF temperatures when compared to tests run with in-cylinder dosing at the same test conditions. It can be seen in Table 7 that the ULSD and B20 cases had CPF inlet temperatures within 1°C and average CPF temperatures increased by 11 and 6°C, respectively, for the exhaust dosing cases. This could have been caused by the increase in doser flow rate required for post-turbo regeneration to reach the same CPF inlet temperature, allowing more HC to reach the CPF, thereby increasing the exotherm generated during active regeneration. Table 7 shows the average CPF temperature for ULSD and B20 in-cylinder dosing compared to post-turbo dosing test conditions [15].

Table 7: Average CPF Temperature as a Function of Dosing Method for ULSD and B20

Variable	CPF Inlet Temp.	Average CPF Temp.
Test/Units	°C	°C
ULSD in-cyl	525	529
ULSD post-turbo	524	540
B20 in-cyl	527	534
B20 post-turbo	528	540

Through the data analysis methods utilized, a method to determine the PM reaction rate at each time step through active regeneration including global activation energy and pre-exponential factors for each test fuel have been determined. As part of the data analysis, the effects of CPF temperature, fuel type, and dosing method on CPF active regeneration have been determined. A summary of the findings is shown below [14, 15]:

- A method to calculate the PM reaction rate at each time step through the entire active regeneration phase of the experiments has been developed.
- The PM reaction rate was shown to increase with increasing test fuel percent biodiesel and CPF inlet temperature.
- An active regeneration model was developed and used to predict the active regeneration time given a set of experimental test conditions.
- Optimization methods were used to determine a global activation energy of 139 kJ/gmol for all test fuels.
- Optimization methods were used to determine the pre-exponential factor for each test fuel. The pre-exponential factor for B20 was the highest, followed by B10 and ULSD. The pre-exponential factors for B20 and ULSD were shown to be statistically different while they were statistically similar for B10 and ULSD.
- DOC HC conversion efficiency is increased by 3% or more with in-cylinder compared to post-turbo dosing methods.

- Efficiency of PM oxidation is increased as exhaust flow rate is decreased. This results because the amount of dosing fuel that is required to achieve a given CPF inlet temperature increases with proportionally increasing flow rate.
- Efficiency of PM oxidation at a constant CPF temperature increased with B20, as compared to ULSD, leading to shorter regeneration times and decreased fuel consumption during active regeneration.
- A lower temperature is required to achieve the same efficiency of PM oxidation with B20 when compared to B10, and a lower temperature is required with B10 compared to ULSD. A lower CPF temperature requires less dosing fuel to be consumed during dosing, decreasing fuel consumption during active regeneration.

From an analysis of the experimental data [12], twelve experiments were determined to be used for calibration of the high-fidelity CPF model as given in Table 8

Table 8: List of active regeneration experiments used for calibration of high-fidelity CPF model

No.	Expt. Name [15]	Fuel Type	New Name [12]	AR Temp. [°C]	AR Time [min.]	CPF inlet NO ₂ /NO _x [ppm/ppm]	CPF inlet O ₂ [% Vol.]
1	ULSD-1	ULSD	AR-ULSD-1	554	15	4/106	7.2
2	ULSD-2	ULSD	AR-ULSD-2	581	6	7/141	6.9
3	ULSD-4	ULSD	AR-ULSD-4	526	21	8/122	7.6
4	ULSD-5	ULSD	AR-ULSD-5	524	22	6/131	7.7
5	ULSD-6	ULSD	AR-ULSD-6	532	21	4/130	7.7
6	B10-1	B10	AR-B10-1	530	26	4/119	7.8
7	B10-2	B10	AR-B10-2	528	19	7/110	7.8
8	B10-4	B10	AR-B10-4	554	15	3/124	7.5
9	B20-1	B20	AR-B20-1	476	35	10/152	8.8
10	B20-2	B20	AR-B20-2	503	39	4/138	8.0
11	B20-5	B20	AR-B20-5	528	19	7/140	8.2
12	B20-6	B20	AR-B20-6	531	16	10/124	8.2

Corrections to the active regeneration experimental data were required to ensure accuracy of data. These corrections are described in section titled “Data Integrity Analysis for Modeling” and Appendix H in reference [14].

The high-fidelity CPF model was calibrated to an active regeneration test as part of the SAE modeling technical paper [6]. Comparisons of model-predicted results to experimental quantities measured and comparison of different cases to determine the effect of temperature and fuel type on thermal PM oxidation rates are given in reference [12].

For the calibration of thermal PM oxidation kinetics, the NO₂-assisted PM oxidation kinetics were those derived from the optimized values obtained from calibration of the high-fidelity CPF model to passive oxidation data (as shown in Table 4 by test fuel type). The parameters adjusted for optimization of thermal PM kinetics were: $A_{th, cake}$ such that the model-predicted PM retained simulated the experimental PM retained at the end of stage-2, stage-3 and stage-4, and $A_{th, wall}$ such that the slopes of model-predicted pressure drop during loading and active regeneration simulated the slopes of the experimental pressure drop during the phases. Results obtained for individual active regeneration experiments and reaction rate constants obtained from the optimized values of thermal PM oxidation kinetic parameters for PM cake and substrate wall are as shown in Figure 19 (a) and (b) respectively.

Figure 19 Natural logarithms of reaction rate constants for thermal (O_2)PM oxidation reactions in the CPF during all active regeneration experiments showing: a) Thermal (O_2) PM oxidation in PM cake layer, and b) Thermal (O_2) PM oxidation in substrate wall

The corresponding model-predicted pressure drop and total PM mass retained to experimental data is shown in Figure 20 for active regeneration experiment AR-B10-1. This shows an accumulation of PM in the substrate wall from time = 0 hrs to ~0.2 hrs followed by PM cake formation and growth till time = 5.3 hrs when the maximum PM mass retained in the CPF reaches ~47 g. This is then followed by a different exhaust mass flow rate condition (time = 5.3 hrs to 5.5 hrs, corresponding to the engine being switched to active regeneration speed-load point). This is followed by active regeneration by fuel dosing (from time = 5.5 hrs to 5.8 hrs) in-cylinder in this case where the PM mass retained in the PM cake layer and substrate wall decrease to a final total PM retained of about 13 g. This is followed by a post-loading phase till time = 7.3 hrs where the PM mass accumulates mainly in the PM cake layer to about 28 g. The CPF high-fidelity model is able to simulate both total pressure drop across the CPF and total PM mass retained in the CPF to within reasonable tolerances.

Figure 20: Model-predicted values of CPF pressure drop (blue line) and PM retained in the CPF (green line) compared with experimental total pressure drop across CPF (red line) and experimental PM retained at the end of stage 1, stage 2, stage 3 and stage 4 (black stars) and PM mass retained in the substrate wall (magenta dashed line) for test AR-B10-1 (as shown in Table 8).

The stated goal of Task 6 has been achieved through collection, analysis, correction and interpretation of experimental data along with use of these as inputs to the high-fidelity CPF model to calibrate the model using the corrected input data. The thermal PM kinetic parameters developed as a result of optimization [12] of reaction rate constants from the active regeneration data is shown in Table 9.

Table 9: Optimized Thermal PM kinetic parameters [12]

Fuel Type →	ULSD	B10	B20	Units
Parameter ↓				
$A_{th,cake}$	0.96	0.96	1.04	[m/s]
$Ea_{th,cake}$	139			[kJ/gmol]
$A_{th,wall}$	0.96	0.96	1.04	[m/s]
$Ea_{th,wall}$	139			[kJ/gmol]

From the results obtained from the calibrated high-fidelity CPF model, the following conclusions can be drawn:

1. Oxidation rate of PM during passive oxidation in the PM cake layer and substrate wall increased with increasing biodiesel blend level in the fuel. This is reflected in the optimized NO₂-assisted PM kinetics obtained as shown in Table 4.
2. Oxidation rate of PM by thermal means did not show significant difference between ULSD and B10 fuel types. However, B20 showed an increase in PM oxidation rate as compared to B10 and/or ULSD. This is also reflected in the optimized values of PM kinetics obtained as shown in Table 9.

The details of the CPF calibration and the optimized PM kinetics obtained are the focus of a planned SAE technical paper in 2014.

Optimized PM kinetics as shown in Table 4 and Table 9 as well as filtration and gaseous species kinetic parameters from the high-fidelity CPF model calibration (as shown in Table 5) were used as inputs to the CPF reduced order model as initial values in order to simulate the same set of experimental data (such as pressure drop, total PM retained, PM in wall and overall filtration efficiency). The calibration of reduced order model and further use of this model with a Kalman filter-based estimator for estimating the PM mass retained based on the measurement of experimental pressure drop is discussed in reference [16] and in section titled “CPF Estimator Development” of this report in 3.3.

3.7 Task 7: CPF PM Loading Maldistribution

The focus of this activity is to experimentally characterize maldistribution behavior, and the dependency on regeneration parameters.

Goal 1: Develop testing protocol for testing at MTU with ULSD examining repeated controlled loading and partial regenerations following the works of Chilumukuru 2008. Non- destructive testing with the support of our OEM partners will be applied to determine quantitative distribution measures. Additionally alternative destructive methods of determination of PM distribution will be investigated.

Goal 2: The MTU 1D multilayer model run in a multi-channel configuration to estimate maldistribution effects.

Goal 3: OEM partner testing for transient cycles including HD FTP with normally scheduled active regenerations and additional partial regenerations.

The objective of Task 7 was to develop an understanding of PM maldistribution. There originally were three objectives associated with Task 7: 1) MTU Engine Tests, 2) MTU Model Correlation, and 3) OEM Engine Tests. The PM maldistribution was to be experimentally studied using both destructive and non-destructive techniques, with data collected from loaded and partially regenerated substrates. The results of the experiments were to be compared with the maldistribution effects that were determined by the MTU 1D multilayer model, run in a multichannel configuration. The OEM partners were to run additional tests that would focus on transient cycles, biofuels, and high PM out regimes of engine operation. The OEM partners were to also perform destructive testing on the substrates. The original hypothesis for the maldistribution study had two parts:

1. The extent to which passive oxidation may be performed is limited by maldistribution.
2. A partial regeneration may provide a uniform distribution and therefore, complete regenerations of the filter should be limited to lower the fuel penalty associated with the aftertreatment device.

The original objectives were modified slightly during the duration of the Task 7 work. The first major modification was that no destructive tests were conducted. The partnership with Cummins and Advantest, and the use of the TAS7000 3D Imaging Analysis system, shifted the priority from destructive to non-destructive testing. The TAS7000 provided enough high quality data to satisfy the data acquisition requirements for this study. More information on the TAS7000 is available in reference [24]. Since the capability to do repeated tests on a substrate and measure the maldistribution each time is fairly new, the focus of this study shifted to understanding the system and developing a method to analyze the data produced by the TAS7000, rather than gathering large amounts of data and attempting to model it all. The MTU 1D model was not developed in a multichannel model, so no maldistribution was ever estimated with it. Instead, the model development was focused on the inclusion of NO₂ back diffusion during passive oxidation. The OEM maldistribution engine tests were not carried out because OEM's were not able to have dyno time available. Instead, the OEM's focused on validating that the models that were developed. The OEMs validated the MTU models using engine, reactor, and their own model data. At this time, there has been no impact on the project results due to the modifications made to the objectives. The removed pieces of the study are considered as future work.

The research that was conducted consisted of 4 tests and 7 filter scans. The filter scans were completed on clean and PM loaded substrates. The PM loaded substrate scans were completed after the substrate was exposed to loading, passive oxidation, and active regeneration engine conditions. The original statement for the MTU Engine Test objective (Task 7.1) states that repeated loading and partial regenerations will be examined. This was satisfied in this test matrix as a total of three active regeneration tests, one passive oxidation test, and one loading test were completed. The full test matrix is given in Figure 21 [24]. The test matrix did not provide enough information to either confirm or refute the original hypothesis. However, additional work is being performed that will provide more information on passive oxidation and active regeneration trends.

Figure 21: Task 7 Test Plan [24]

An analysis method was developed that would quantify the amount of maldistribution in the PM, using the data from the Advantest system. The analysis method was based on an equation for flow uniformity, known as a uniformity index. The uniformity index gives a measure of the variation in the PM distribution. To assist in understanding variations, the substrate was divided into axial sections, axial segments, radial sections, quadrants, and angular increments. The result was that the PM distribution trends in a particular region of the substrate could be studied and compared against other regions. The full analysis method is described in further detail in reference [24].

There were many conclusions that were drawn from this work. The TAS7000 system was found to be capable of producing high resolution data that was capable of being analyzed using the developed method. Maldistribution of the PM was found for all engine conditions, particularly in the axial direction. The loading engine condition resulted in a PM density that was 12% higher than the substrate average near the outlet of the filter. The active regeneration engine condition resulted in a PM density that was 55% lower than the substrate average near the outlet of the substrate. The passive oxidation engine condition resulted in a PM density near the middle of the substrate that was 18% higher than the substrate average. It was also found that the PM distribution is more uniform near the centerline of the substrate. The data also showed that there may be an amount of PM oxidation that would result in a uniform radial PM distribution. The radial distribution was uniform when the amount of PM oxidized was around 40% or 90%, and was not uniform between 40 and 90%. The full results of this work, and a detailed analysis of each test conducted, are found in reference [24].

3.8 Task 8: Fuel-Optimal CPF Regeneration

Goal 1: Identify the fundamental relationships and limitations of the trade-off between reduction of pressure and increase engine efficiency with partial regeneration and PM Loading maldistribution in the CPF.

Goal 2: Develop practices for reducing wall mass in a near-optimal way while enabling accurate PM estimation and limit the impacts of maldistribution of PM in the CPF.

The combustion strategy in a diesel engine has an impact on the emissions along with the brake specific fuel consumption and the exhaust temperatures. While the CPF loading is a function of NO, NO₂ and PM concentrations in addition to the exhaust temperatures and the flow rates. Thus indirectly, the engine combustion strategy affects engine efficiency which has an impact on the CPF loading. The original goals specified in Task 8 of this project were modified during the duration of work, with the new goals focused on developing a process to understand this relationship between engine fuel consumption, in-cylinder combustion and its impact on CPF operation to find the most fuel optimal scenario for the system. To develop this process for finding the most fuel optimal scenario, a transfer function was developed which estimates the engine out emissions (PM, NO_x), exhaust temperatures and fuel consumption based on +/- percent deviations in the injection pressure and injection timing over the calibrated injection pressure and timings.

Transfer Function Development:

Work carried out by Ye, Boehman [25] was concerned with the impact of injection pressure and start of injection timings on the NO_x, PM emissions along with the fuel conversion efficiency at three engine operating points. This data were used along with experimentally collected data for the transient surrogate FTP cycle on the 2010 Cummins ISB engine at MTU, to generate the transfer function. The transfer function was developed for this engine and fuel considered was ULSD. The transfer function estimates the engine out NO_x, PM, BSFC and exhaust temperature for a transient surrogate FTP cycle as a function of steady state data for the same parameters as published by Ye, Boehman [25]. Thus transient PM concentrations were required for this analysis, hence a PM model was developed which estimates PM concentrations as a function of speed and load. In this model, a 2D lookup table was created using interpolation of scattered PM concentration data. To validate the PM model, the model predicted concentrations were compared with the experimentally measured PM concentrations from tests conducted at MTU. So as to factor in the difference in between the experimentally measured and model predicted PM concentrations, a correction factor was calculated and the PM concentrations predicted by the model for the surrogate FTP cycle were multiplied by this correction factor.

The steps followed in developing the transfer function model are as follows:

1. 3D surfaces (X-Injection pressure, Y-Injection Timing, Z-NO_x/PM/BSFC) were generated using interpolation at three operating point from the data published by Ye, Boehman [25].
2. To generate surfaces at all the operating points occurring in the surrogate FTP cycle, 'Reference Points' were selected on surfaces created in step 1).
3. A multiplication factor was calculated using the experimental data from the surrogate FTP cycle and the reference point values.
4. Reference surfaces were chosen from amongst the three surfaces created in Step 1). These surfaces were then scaled using the multiplication factor to generate surfaces for PM/NO_x/BSFC at all operating points occurring in the surrogate FTP cycle.
5. On these scaled surfaces, knowing the X (Injection Pressure) and Y (Injection Timing) co-ordinate values of the original calibrated point, and the +/- % deviation from this point, the new X and Y co-ordinates were located and used to predict the Z co-ordinate (PM/NO_x/BSFC) values for the various test cases.

To estimate the engine out exhaust temperatures, an equation was derived based on an energy balance which correlated the percent deviations in fuel consumptions with the percent deviations in the engine out exhaust temperatures.

Test Cases Considered:

The transfer function takes in the +/- percent deviations from the calibrated values of injection pressure/timing as input. The test cases defined and their results from the transfer function model for a run for the surrogate FTP transient cycle are shown in Table 10

Table 10: Transfer Function model results for various test cases over 20 mins of surrogate FTP cycle

	Test Case Name	% deviation from Calibrated Value	Cumulative engine out PM at the end of 20 mins (grams)	Fuel Consumed (Gallons)	Average engine out NO _x (g/kW-hr)
Injection Pressure	TC 1	Calibrated Value + 10 %	1.31	1.61	5.07
	TC 2	Calibrated Value - 10 %	1.70	1.62	4.25
	TC 3	Calibrated Value + 20 %	1.14	1.61	5.48
	TC 4	Calibrated Value - 20 %	1.93	1.62	3.85
Injection Timing	TC 5	Calibrated Value + 20%	1.41	1.61	5.16
	TC 6	Calibrated Value - 20 %	1.52	1.62	4.27
	TC 7	Calibrated Value + 40%	1.33	1.61	5.70
	TC 8	Calibrated Value - 40%	1.55	1.63	3.92
-	Base	Base Calibrated Values	1.48	1.61	4.63

The test cases considers an increase/decrease in injection pressure or an advanced/retarded SOI timing over the calibrated injection pressure/timing at all the operating points occurring in the 20 min surrogate FTP cycle. For example, TC 1 implies that the injection pressure at each operating point was increased by 10% over the calibrated value of injection pressure at the corresponding point.

The following observations were drawn from the transfer function model results:

1. An increase in injection pressure over the calibrated value (TC 1 and TC 3) results in a reduction in PM concentrations and fuel consumption and an increase in average NO_x concentrations, as compared to 'Base' results. Reduction in fuel consumption can be attributed to the fact that the engine was operating at higher fuel conversion (thermal) efficiencies. While the increase in NO_x is due to higher thermal efficiencies corresponding to higher in-cylinder combustion temperatures.
2. An advanced injection timing (TC 5 and TC 7) leads to a decrease in PM concentrations and fuel consumptions and vice versa.

Note: In this study, advanced injection timing was considered as start of injection taking place earlier with reference to the ATDC (After top dead center). For example if the calibrated SOI was -5° ATDC, then 20% advancement in injection timing causes the timing to become -6° ATDC. Similarly, 40% advancement in the injection timing causes the timing to become -7° ATDC.

To find the most fuel optimal scenario with respect to the penalties associated with active regeneration and backpressure, the transfer function model outputs are inputted into the 1D DOC and the 0D CPF models. The 1D DOC model [1] has been calibrated and validated for the surrogate FTP transient cycle and the results are published by Song et al. [3]. The reduced order CPF model [16] has not recently been calibrated for ULSD. Once the reduced order CPF model validation is complete, the various test cases can be simulated to find the most optimal scenario.

3.9 Task 9. Spatial Distribution of Ammonia Study

Goal 1: Measure spatial variation of ammonia storage and understand the cause; experimental test execution at ORNL.

Goal 2: Analysis of experimental data and model development, and impact on SCR state estimator

Summary

The objective of Task 9 was to investigate the SCR spatial storage characteristics. The approach was executed as proposed and consisted of a combination of modeling and experimental studies using both an engine test cell and a bench reactor. The modeling exercise explored differences between a computationally expensive, two-dimensional approach and a one-dimensional, computationally efficient approach. It was found that the computationally efficient approach matched well with experimental data, and thus the higher fidelity, two-dimensional model was not necessary for state estimation objectives. Supporting studies were performed using experimental data from both the engine test cell and the bench reactor. A new measurement technique (spaci-IR) was developed during the bench reactor studies that permitted the comparison of spatially resolved gas concentration measurements to simulation results within an SCR. Ammonia storage levels were computed based on the spatially resolved gas concentration data. The global kinetics, one-dimensional model predicted similar trends in spatial NH_3 distribution as compared to the measurements on the bench reactor. Thus, the objective of understanding NH_3 storage characteristics was achieved. A radial maldistribution study was also performed on the engine test cell using different exhaust / urea mixing stages. By measuring the gas concentrations at the outlet of the 1st SCR brick at multiple radial locations, the effect of the mixing stage on NH_3 distribution was investigated. It was found that a practical mixing stage can create a mixture of exhaust and urea at the SCR inlet such that the outlet concentration is well-mixed. Thus, modeling radial storage of ammonia is not necessary if the mixing stage is adequate.

Two approaches were used to investigate the performance of the model postulated for the SCR estimator – one was based on model simulation and the other was experimental studies. The simulation approach relied on a commercially available multiphysics modeling code (COMSOL). It was used to model the adsorption and desorption features of an SCR. COMSOL Multiphysics solves general partial differential equations based on finite element methods allowing for both stationary and time-dependent analyses. The COMSOL SCR model was used to validate the 1D high fidelity SCR model by comparing the simulation results of the NH_3 adsorption and desorption process. The experimental approach used a new bench reactor technique developed by Oak Ridge National Laboratory for measuring gas concentrations at known axial locations inside an SCR core sample. The spatially resolved gas concentrations were compared to the 1D SCR model predictions along with the computed axially resolved NH_3 storage levels. Both the COMSOL simulation and bench reactor experiments showed that the 1D, global kinetics SCR model was valid.

Comparison of COMSOL Model to the High Fidelity SCR Model

The steps for developing the COMSOL model were described in detail in reference [9]. The steps involved in the development and the solution of a typical COMSOL model are: (1) defining the geometry, (2) specifying the physics through a set of model equations, (3) applying spatial boundary conditions, (4) applying temporal initial conditions and system parameters, (5) solution generation and (6) post-processing the results. The development of the SCR model was based on the COMSOL 3.5a example on Transport and Adsorption described in reference [26]. Once the model is defined and its boundary conditions are described, initial conditions and other parameters for the solution of the problem were determined and the average flow velocity and storage capacity of the catalyst were calculated and used as the input to the model.

After setting the parameters of the COMSOL and the 1D high fidelity SCR model to the same values, both simulations were run and their spatial results compared as shown in Figure 22. Four spatial

locations of NH_3 gas concentration are shown at .25L, 0.5L, 0.75L and L where the length of the channel is $L = 2.46$ cm. It should be noted that ammonia gas concentration is an equivalent indicator of ammonia storage since this study only considers the adsorption and desorption mechanism of the SCR. Figure 22 shows a coarse solution to the NH_3 for the COMSOL model when the NH_3 concentration is below 50 ppm. Above 150 ppm, both models agree well.

Figure 22: COMSOL model results compared to the 1D model at 250°C and SV 60K hr⁻¹

The computational expense of the COMSOL model was significant compared to the faster-than-real-time execution of the 1D SCR model. The comparison indicated that the 1D SCR model form was sufficient to capture adsorption and desorption without the additional computational complexity introduced by the COMSOL model. Therefore, the 1D, global kinetics model was deemed sufficient for the continued evaluation for use within the SCR state estimator and the COMSOL study was not pursued further. The next section describes the successful calibration of the 1D global kinetics SCR model to experimental bench reactor data.

Comparison of the High Fidelity SCR Model to Spatially Resolved Reactor Data

The Cu-zeolite SCR core samples taken from the Cummins ISB engine were tested in a flow bench-reactor using the Spaci-IR technique. The 1-D high fidelity SCR model with mass transfer and SCR reactions between stored NH_3 and other species was optimally calibrated to the Spaci-FTIR experimental results by identifying the key parameters of the model including NH_3 storage capacity, activation energy and the pre-exponential constants for the major SCR reactions [8].

The Spaci-FTIR approach allowed measurements of gas concentrations axially within the core sample and computation of axial distributions of ammonia storage. The tests were run at three different temperatures (250, 300, and 350 °C) with a space velocity of 60,000 hr⁻¹. The spatially resolved (0.05, 0.1, 0.2, 0.3, 0.4, 0.6, and 0.8 of the catalyst length) gaseous concentrations of NH_3 , NO, NO_2 , and N_2O were measured during a test protocol with NH_3 saturation, NO_x SCR reaction, and NO SCR reaction conditions. The NH_3 storage distributions at different axial locations of the catalyst were quantified for the three temperature conditions. The SCR model has two storage sites. NH_3 adsorption and desorption take place on both sites. However, the first site also supports all SCR reactions. The storage capacities of

both sites were quantified to fit best the experimental data by comparing the simulation results of a one-site model, two-site model, and the experimental results. Activation energies and pre-exponential constants of key SCR reactions were calculated using axial gradients of gaseous concentrations and were further tuned using an optimization process. The calibration procedure was introduced in reference [8] the calibrated SCR model was able to correctly predict both spatially resolved concentrations and NH_3 storage distributions under NH_3 saturation and NO_x SCR reaction conditions as shown in Figure 23.

Figure 23: Comparison of axial NO_x , NH_3 concentration and NH_3 storage profiles between model simulation and experimental results

NH_3 Maldistribution Study

The high fidelity SCR model calibration developed from the Spaci-IR data served as a basis to develop a calibration that works for the SCR reactor data under different space velocity and temperature conditions [4]. Then a new calibration was developed using SCR engine test data [5]. The purpose of this approach was to determine if reactor-based calibration alone is sufficient for calibrating the model for later use within an SCR estimator. This exercise illuminated key differences between the reactor bench and engine test cell calibrations as shown in reference [5]. Additional NH_3 maldistribution testing indicated a maldistribution of NH_3 entering and within the SCR as the probable cause.

The NH_3 maldistribution engine tests were designed to determine the SCR inlet NH_3 and NH_3/NO_x ratio (ANR) distribution profile with different mixer setups. The tests were carried out on a 6.7 L Cummins 2010 ISB engine. The SCR inlet NH_3 concentration cannot be directly measured using emission analyzers because the urea injected in the exhaust flow may crystallize in the sample and damage the analyzer. As a result, the SCR inlet NH_3 maldistribution was determined by comparing the NO_x distribution at the outlet face of the 1st SCR brick with and without the SCR upstream urea injection. The distribution of the NO_x reduced across the SCR with urea injections was considered to be related to the NH_3 distribution of the SCR inlet face. In order to determine the distribution profiles, gas sampling was taken

from different radial positions downstream of the 1st SCR brick using ¼ inch stainless steel sampling probes. A total of 25 different sampling positions were measured.

The gaseous measurements of NO and NO₂ at each position were measured with and without the urea injection. For each maldistribution test, the NO and NO₂ concentrations at each measurement location were measured after the engine and aftertreatment system conditions reached steady state. Next, urea injection was initiated upstream of the SCR to give an average ammonia to NO_x ratio (ANR) of 0.3. The NO and NO₂ concentrations at each measurement location were measured again after the SCR reached equilibrium. The NO_x reduced by the NH₃ formed from decomposition of the injected urea is assumed to be equal to the NH₃ consumed. Based on this assumption, the SCR inlet ANR distribution profile was calculated as shown in Figure 24. The uniformity index (UI) of the SCR inlet ANR at this condition was 0.79. The test results of other test conditions showed that the test condition had little effect (≤ 0.02) on the UI of SCR inlet NH₃. The engine operating condition for this test was 1450 rpm and 203 N·m with the exhaust mass flow rate of 4.23 kg/min and a SCR inlet temperature of 350 °C.

Figure 24: Determined NH₃ distribution profile with SCR upstream urea injection

A swirl mixer was installed into the SCR inlet cone and the maldistribution of the NH₃ and ANR were measured again with the mixer installed. The results showed that better mixing performance was achieved. The UI of SCR inlet ANR was improved from below 0.8 to about 0.9.

In order to determine the NH₃ maldistribution effects on the SCR performance under different operating conditions and on the SCR model parameters, a simulation study was performed by considering the maldistribution effects using a multi-channel SCR model. The model contained 24 separate channels with different inlet ANR levels to simulate the measured maldistribution. The average ANR was multiplied by a maldistribution factor for each individual channel. The maldistribution factors representing different UI were generated from normal distributions based on a mean value of 1.0 and different standard deviations.

The simulation was conducted under different temperature, NO₂/NO_x ratio and NH₃ maldistribution levels. The simulated NO_x reduction efficiencies and NH₃ slip as a function of the average ANR for different UI under the SCR temperature of 300 °C and NO₂/NO_x ratio of 0.0 is shown in Figure 25 and Figure 26. It can be observed that the UI has negative effects on NO_x reduction and NH₃ slip when the average inlet ANR is above 0.6. When changing the UI from 0.7 to 1.0 with an average of 1.0, the NO_x reduction efficiency was increase by 10% and the NH₃ slip was reduced by 15 ppm. However, the SCR

performance with UI of 0.9 and 1.0 is close. The UI effects were similar for the average ANR of 1.0 and 1.2 and were less obvious with lower average ANRs. Similar effects were observed in the other simulation runs. The NO_x reduction was reduced by 5-10% with 10 to 20 ppm increase in NH_3 slip for the different conditions.

Figure 25: NO_x reduction efficiency and NH_3 slip as a function of average ANR for different UI

Figure 26: NH_3 storage as a function of average ANR for different UI

In order to determine if the NH_3 maldistribution is a factor causing the differences in the model parameters developed from the reactor and engine data, a simulation study of the engine test data was carried out by running the SCR model calibrated to the reactor data with multi-channel setup and nonuniform inlet NH_3 . The multi-channel model gave simulation results which are closer to the engine test data by taking maldistribution effects into consideration. It was determined that the maldistribution effect is a factor causing the different model parameters between the SCR model calibrated to reactor and engine test data. The SCR model calibrated to the engine test data takes the complex engine exhaust conditions into account and is able to simulate the SCR system with those effects.

Conclusions

Showing its ability to be calibrated to the experimental data and to predict both species concentration and stored NH_3 , the postulated 1D, global kinetics SCR model was a suitable form for estimator development. Both simulation and experimental techniques were used and it was shown that it could be successfully calibrated to data. It was concerning that the calibration was different between engine and reactor data sets. Further experimentation and simulation showed that the likely cause was maldistribution of ammonia entering the SCR. A possible solution, that could affect estimator model design, was to use a multi-channel SCR model. This was investigated and shown to alleviate some of the mismatch between engine versus reactor calibrations. Since the calibration difference resulted in less than a 10% error in outlet species and ammonia storage predictions and since using a multi-channel model would add significant complication to the state estimation task, it was concluded that a single channel, 1D, global kinetics SCR model with calibration to engine data was the best choice for continued SCR estimator development.

3.10 Task 10: Aged SCR Studies

Goal 1: The focus of this task is to quantify the effect of SCR performance as a function aging.

Goal 2: Model this effect and incorporate it into an SCR model structure suitable for OBD and control system design.

This task was changed mid-project from an HC masking focus to aging. The approach used bench reactor data from SCR core samples of both a degreened (unaged) catalyst and a hydrothermally aged catalyst. The spaci-IR technique, developed during this project, was used to quantify the aging effects of not only exit concentrations and total storage, but also the internal change in spatial distribution of ammonia as the catalyst ages. A corresponding modeling study was executed to relate the experimentally observed aging effects to the model's calibratable parameters.

The objective of this project is to create state estimation strategies for diesel engine aftertreatment components using differential equation models of each aftertreatment device. The performance of a state estimator is limited by (1) the ability of the model used within the estimator to predict the states of the system for known inputs and (2) the quality of the sensor signals used as inputs to the estimator. A 1D, axially discretized, global kinetics model has been postulated as the basis for the SCR estimator. Its states are the concentrations of the NO, NO₂ and NH₃ in both the bulk exhaust stream and a thin layer in the vicinity of the catalyst for each element and the amount of stored NH₃. Its inputs are the NO, NO₂ and NH₃ concentrations, flow rate and temperature of the inlet gas. The outlet concentration of the NO, NO₂, and NH₃ is highly dependent on the amount of stored NH₃. Therefore, the estimator's performance will be limited by the ability of its SCR model to predict amounts of stored NH₃. Reference [8] focused on quantifying the impacts of spatial nonuniformities in NH₃ storage on device operation, and on verifying the ability of the 1-D model to handle spatial variations where necessary. This report focuses on another aspect of catalyst operation that must be considered in the context of model, control strategy, and system design: aging of the catalyst over the life of the vehicle. In particular, the focus was on measuring the potential impacts of catalyst aging on NH₃ storage distributions within the catalyst.

Experimental

Catalyst Samples

This investigation focused on a commercial Cu-exchanged zeolite urea SCR catalyst. Researchers at MTU removed the catalyst from the exhaust system of a 2010 Cummins ISB engine and shipped pieces of it to ORNL. ORNL cut two core samples from a face of the catalyst (it was not determined whether the face was the front or back of the catalyst brick, but the catalyst supplier informed us that this should not matter). Each core sample was 8 cm long and roughly 2 cm in diameter, and contained exactly 162 channels. Both core samples were hydrothermally aged in a laboratory furnace under a flow of 20% O₂, 10% H₂O, and balance N₂. One core sample was aged for 4 h at 700 °C, the supplier-recommended degreening conditions. The other core sample was aged for 16 h at 800 °C. These conditions were chosen based on the work of Schmieg [27] and coworkers, who found that a commercial Cu-exchanged zeolite urea SCR catalyst core sample hydrothermally aged in the laboratory at 800 °C for 16 h showed similar performance to one that was aged on a vehicle for 220000 km (approximately the end of full useful life for a light duty application). While this project used a different commercial catalyst material and was focused on heavy duty applications (which have a much longer catalyst life requirement), these conditions provided a starting point for aging the catalyst to a relevant state where catalyst function was impacted without completely destroying all catalyst activity. The goal was to understand how aging

might impact NH_3 storage, and in particular axial distributions of NH_3 storage, over the full useful life of the catalyst.

Flow reactor

Experimental evaluation of the aged core samples was conducted in an automated flow reactor at ORNL. The reactor uses mass flow controllers to create synthetic exhaust gas mixtures from compressed gas bottles. Water is delivered by an HPLC pump through a custom vaporization/injection system. Reactive gases are introduced through pneumatically actuated heated four-way valves to create reasonably fast (<0.5 s) transients in gas composition. Gases are routed through 6.4 mm diameter stainless steel tubing heated to approximately 200 °C. High temperature electrically actuated solenoid valves direct the gas flows to either the catalyst sample or a bypass line. The catalyst cores are wrapped in fiberglass strands and loaded into a 25 mm diameter quartz tube. The upstream portion of the quartz tube is filled with 3 mm quartz chips to enhance gas heating and improve temperature uniformity. The quartz tube is fitted with graphite ferrules and custom stainless steel end caps that connect to the reactor gas lines and provide inlet ports for thermocouples and other instrumentation. Three 0.5 mm diameter type K thermocouples are used to measure gas temperatures around the catalyst core sample: 5 mm upstream from the front face of the catalyst, 5 mm downstream from the rear face of the catalyst, and near the axial midpoint of the center channel inside the core sample. The quartz tube is loaded in a tube furnace for temperature control of the catalyst sample. Reactor pressures are monitored with silicon-diaphragm absolute pressure transducers. Data acquisition and automated system control are accomplished through National Instruments hardware components and a custom LabVIEW interface.

Spaci-IR

To measure spatially resolved gas concentrations and surface NH_3 inventories, we modified the spatially resolved capillary inlet infrared spectroscopy (Spaci-IR) approach developed by Epling and coworkers [28]. Their approach uses a capillary inserted inside a catalyst core sample channel to sample the gas from a particular axial location. The capillary can be translated to develop axially resolved maps of gas composition. A dilution flow is added to the sample gas stream at the outlet of the reactor to reduce gas transient times, and the diluted flow is sent to an FTIR spectrometer (MKS Instruments Multigas 2030HS) for analysis. The transient experiments were designed to measure surface NH_3 inventories which required better temporal and concentration resolution than the Epling group reported. To improve both the transient response characteristics and the accuracy of the concentration measurements, the sample flow rate was increased by deploying four larger diameter (0.68 mm outer diameter) sampling capillaries (arranged as shown in Figure 27(a)). An effort was also made to minimize the impact of the sampling capillaries on the overall flow distribution within the catalyst core sampling by sampling a fraction of the channel flow equal to the fractional area of the channel blocked by the capillary. A dilution ratio of 10:1 was found as the optimal balance between temporal response and gas concentration resolution. Dilution ratio was measured with CO_2 (which was included in the feed gas at a fixed concentration) and used to correct the sample gas concentrations back to their undiluted values. A schematic of the sampling system is included in Figure 27(b).

Figure 27: Schematics of (a) the catalyst core sample cross section showing positions of the sampling capillaries (orange circles) and mid-catalyst thermocouple (gray circle) and (b) the Spaci-IR sampling system.

Experimental protocol

The experimental protocol (summarized in Table 11) was designed to measure surface NH_3 inventory under three steady state operating conditions: complete NH_3 saturation (in the presence of O_2), NO SCR, and $\text{NO}+\text{NO}_2$ (fast) SCR. For each step, operating conditions were held constant until the measured gas concentrations reached a steady state. For cases with NH_3 in the feed (steps 2, 4, and 7), after steady state was achieved, NH_3 was turned off while NO_x was left on (or turned on). Total NH_3 inventory was calculated by adding the desorbed NH_3 and the NO_x converted by the stored NH_3 .

Table 11: Protocol steps

Step	Description	NO (ppm)	NO ₂ (ppm)	NH ₃ (ppm)	O ₂ (%)	H ₂ O (%)	CO ₂ (%)
1	stabilize	0	0	0	10	5	5
2	NH ₃ adsorption	0	0	500	10	5	5
3	NH ₃ inventory: NO ₂ / NO _x = 0.0	500	0	0	10	5	5
4	SCR: NH ₃ /NO _x = 1.0; NO ₂ / NO _x = 0.0	500	0	500	10	5	5
5	NH ₃ inventory: NO ₂ / NO _x = 0.0	500	0	0	10	5	5
6	stabilize NO ₂ / NO _x = 0.5	250	250	0	10	5	5
7	SCR: NH ₃ / NO _x = 1.0; NO ₂ / NO _x = 0.5	250	250	500	10	5	5
8	NH ₃ inventory: NO ₂ / NO _x = 0.5	250	250	0	10	5	5
9	clean	500	0	0	10	5	5

Figure 28: An example of the concentrations of NH_3 (purple), N_2O (blue), NO (green), and NO_2 (orange) measured during a Spaci-IR experiment. Vertical black lines separate the protocol sections.

Figure 28 shows an example of the concentrations measured during a Spaci-IR experiment run according to the protocol in Table 11. After the protocol was completed at one position within the catalyst, the capillaries were moved to a different position, and the protocol was run again. This process was repeated until the concentrations were mapped across the length of the catalyst core (a total of 8 axial positions including one upstream of the catalyst to measure inlet composition). The entire protocol was run at three different temperatures (250, 300, 350 °C) for each core sample. All experiments were run at a space velocity of 40000 hr^{-1} .

Results and discussion

We began our investigation into the impacts of hydrothermal aging on NH_3 storage by comparing cumulative NH_3 stored across the length of the catalyst for the two different hydrothermal pretreatments. Figure 29 shows the total NH_3 on the catalyst surface under steady state conditions at three different temperatures (250, 300, and 350 °C) under:

- (a) NH_3 saturation (500 ppm NH_3);
- (b) NO SCR (500 ppm NH_3 , 500 ppm NO); and
- (c) NO+ NO_2 SCR (500 ppm NH_3 , 250 ppm NO, 250 ppm NO_2).

As expected, NH_3 storage is a strong function of catalyst operating temperature. Higher temperatures destabilize the NH_3 on the catalyst surface, resulting in lower surface inventories. An increase of catalyst temperature by 100 °C decreases the storage capacity by roughly half. Increased hydrothermal aging also clearly impacts the catalyst NH_3 surface inventories. Aging at 800 °C decreases the total NH_3 storage capacity under saturation conditions by about one fourth. This decrease implies a loss in the total number of stable sites available to store NH_3 on the catalyst surface. This loss of sites is also apparent under NO SCR conditions (step 4 of Table 11), where the surface NH_3 inventory also drops with hydrothermal aging, though not quite to the same extent as under NH_3 saturation conditions. Interestingly, the NH_3 inventory under NO+ NO_2 SCR operating conditions (step 7 of Table 11) is essentially unchanged by hydrothermal aging. Understanding this apparent inconsistency requires a closer look inside the catalyst at the spatially resolved NH_3 storage profiles.

Figure 29: Total NH₃ stored on surface of catalyst (measured near the catalyst outlet) as a function of temperature and aging state under (a) 500 ppm NH₃; (b) 500 ppm NH₃, 500 ppm NO; (c) 500 ppm NH₃, 250 ppm NO, 250 ppm NO₂. All experiments run at GHSV of 40000 hr⁻¹ and included 10% O₂, 5% H₂O, and 5% CO₂ in feed gas.

Figure 30 shows the local NH₃ inventory as a function of axial position under NH₃ saturation conditions for both aging states. The symbols represent the calculated difference in NH₃ uptake between adjacent sampling points inside the catalyst divided by the catalyst volume between the sampling points. Since both the NH₃ uptake and catalyst volume slices are relatively small, there is scatter apparent in the data points. To help reveal the trends in the NH₃ inventory data, a second method for calculating local NH₃ inventory was employed: a polynomial curve was fit to the cumulative NH₃ storage data, and the curve was analytically differentiated to generate the lines plotted in Figure 30. Under ideal NH₃ saturation conditions, the NH₃ storage density should be the same across the entire catalyst length, generating horizontal lines for plots of inventory as a function of position. For the 800 °C aged sample, the lines are nearly horizontal, as expected. The NH₃ inventory decreases somewhat toward the back of the catalyst for the 700 °C aged sample, resulting in a downward slope in the inventory lines. This could be due to scatter in the data, or it could result from a nonuniform washcoat distribution inside the catalyst sample. Regardless, we see that the NH₃ storage profiles are consistent with the integral NH₃ storage capacities reported in Figure 29: the higher aging temperature (open symbols and dashed lines) results in a loss of stable NH₃ storage sites at all three temperatures.

Figure 30: NH₃ inventory on catalyst surface as a function of axial position and temperature at steady state under a feed of 500 ppm NH₃, 10% O₂, 5% H₂O, 5% CO₂, balance N₂ (40000 h⁻¹ GHSV) after two different hydrothermal aging pretreatments: 700 °C for 4 h (filled symbols and solid lines) and 800 °C for 16 h (open symbols and dashed lines).

Adding NO_x to the feed gas mixture significantly alters the NH_3 storage profiles. Figure 31 shows the spatially resolved NH_3 inventories under 500 ppm NH_3 and 500 ppm NO . The catalyst is quite active in the NO SCR reaction at these temperatures, resulting in a steady decrease in both NH_3 and NO concentrations along the catalyst length. Since the NH_3 adsorption equilibrium is controlled in part by the gaseous NH_3 concentration, a steadily decreasing NH_3 concentration results in a steadily decreasing surface NH_3 inventory. Thus, the NH_3 inventory approaches saturation near the front of the catalyst sample, but drops toward zero at the back. In addition to reducing the saturation capacity (and thus the NH_3 inventory near the front of the catalyst), hydrothermal aging also decreases the catalyst activity in the NO SCR reaction. Since the nature and function of the active site(s) in these copper zeolite SCR catalysts has not been definitively established, it is hard to say whether this drop in activity is a direct effect of the reduced NH_3 inventory, or due to a loss of some other site that plays a role in the NO SCR mechanism. Either way, the reduced SCR activity consumes NH_3 more slowly, yielding less steep NH_3 inventory profiles in Figure 31.

Figure 31: NH_3 inventory on catalyst surface as a function of axial position and temperature at steady state under a feed of 500 ppm NH_3 , 500 ppm NO , 10% O_2 , 5% H_2O , 5% CO_2 , balance N_2 (40000 h^{-1} GHSV) after two different hydrothermal aging pretreatments: 700 °C for 4 h (filled symbols and solid lines) and 800 °C for 16 h (open symbols and dashed lines).

The complex interplay between SCR activity and NH_3 inventory is even more apparent under the $\text{NO}+\text{NO}_2$ SCR conditions depicted in Figure 32. Due to the higher reaction rates of the “fast” SCR mechanism which occurs when both NO and NO_2 are present in the feed mixture, all of the NH_3 is consumed about half way through the catalyst, resulting in zero NH_3 inventory in the back half of the catalyst. As above, hydrothermal aging reduces the nearly saturated storage capacity at the front of the catalyst, and it results in storage profiles that decrease more gradually across the catalyst.

Figure 32: NH₃ inventory on catalyst surface as a function of axial position and temperature at steady state under a feed of 500 ppm NH₃, 250 ppm NO, 250 ppm NO₂, 10% O₂, 5% H₂O, 5% CO₂, balance N₂ (40000 h⁻¹ GHSV) after two different hydrothermal aging pretreatments: 700 °C for 4 h (filled symbols and solid lines) and 800 °C for 16 h (open symbols and dashed lines).

The reason for the change in the NH₃ inventory distribution becomes more obvious after analyzing the gaseous NH₃ concentration profiles plotted in Figure 33. The NH₃ concentration drops rapidly over the front portion of the catalyst due to consumption by the “fast” (NO + NO₂) SCR reaction. For the catalyst aged at 700 °C, all of the NH₃ is consumed within the front 40% of the catalyst length. Consistent with this observation, the NH₃ inventory in Figure 33 also drops to zero at about 40% of the catalyst length. For the 800 °C aged catalyst, the gaseous NH₃ concentration persists deeper into the catalyst due to a lower fast SCR reaction rate. So, while the NH₃ inventory starts out lower near the front of the catalyst due to the loss of stable storage sites, the deeper penetration of the gaseous NH₃ into the catalyst spreads the surface inventory along more of the catalyst length. The combination of a lower site density with NH₃ spread across more of the catalyst results in practically no change in total NH₃ inventory Figure 29) under NO+NO₂ SCR operating conditions.

Figure 33: Gaseous NH₃ concentration as a function of axial position and temperature at steady state under a feed of 500 ppm NH₃, 250 ppm NO, 250 ppm NO₂, 10% O₂, 5% H₂O, 5% CO₂, balance N₂ (40000 h⁻¹ GHSV) after two different hydrothermal aging pretreatments: 700 °C for 4 h (filled symbols and solid lines) and 800 °C for 16 h (open symbols and dashed lines).

Conclusions

In our prior work, we determined that the spatial distribution of NH_3 on the catalyst surface depends on two primary factors: (1) the NH_3 adsorption properties of the catalyst (number of sites and stability of NH_3 on those sites), and (2) the gaseous NH_3 concentration profile imposed by the consumption of NH_3 through SCR and NH_3 oxidation reactions. These two aspects are not completely independent since reaction rates depend on the NH_3 inventory on the catalyst surface at any point in space and time, but an accurate accounting of both elements should enable accurate predictions of NH_3 inventory and catalyst performance.

Here, we observed that hydrothermal aging impacts both factors controlling NH_3 storage. It reduces the number and/or stability of NH_3 storage sites. And it impacts NH_3 concentration profiles by reducing the rates of certain reactions. Once again, it's not clear if these two impacts are independent or directly related since it's possible that the reduced reaction rates are a direct result of the lower surface NH_3 inventories. Regardless, the result is that hydrothermal aging can have a significant impact on spatial distributions of NH_3 storage. The changes in NH_3 storage distributions could propagate through to impact overall device performance, particularly during transient operating conditions where accurate NH_3 storage predictions are critical to maintaining high NO_x conversion with low NH_3 slip. Thus, control models and strategies may need to account for aging impacts on NH_3 storage.

3.11 Task 11: SCR Optimal Ammonia Storage

Goal 1: The focus of this task is to control the amount of stored ammonia where the set-point ammonia storage level is a function of engine conditions.

Goal 2: Conduct simulation studies to develop guidance of optimal ammonia storage levels, and compute sensitivity functions.

The proposed objective was to develop quantitative relationships between engine operating conditions and optimal ammonia storage. This was motivated by a postulated method of SCR control using the ammonia storage level as the control set point. The outcomes of the study were different where the optimal storage was integrated into a control strategy specific to a priori drive cycle definitions. This approach computes the optimal ammonia injection, and thus storage, for a given drive cycle. This creates an upper bound on SCR closed loop performance in terms of both NO_x reduction and ammonia slip. Its primary use is for comparing the performance of any SCR control strategy to the upper bound of performance.

System Description

A depiction of the SCR system of interest is shown in Figure 34. The inputs to the model based controller are the sensed NO_x concentrations upstream and downstream of the SCR. The control law computes the dosing command for the next update to minimize the expected downstream, production NO_x sensor reading. Since production NO_x sensors are known to have cross-sensitivity to NH_3 , this approach favors high NO_x conversion and low NH_3 slip. A calibrated Cu-zeolite SCR model [5] is used to simulate SCR dynamics to evaluate the performance of the control law. Details on the model, parameter settings, and calibration can be found in reference [5].

Figure 34: SCR exhaust & data flow. 'S' is a NO_x sensor.

System Identification

The SCR model accurately represents the nonlinear physics but cannot be readily used to solve for an optimal urea dosing schedule. Thus, a data-driven model that can be used to obtain an optimal dosing strategy was developed. We assume that the input-output relationships of the SCR system can be represented by a linear time-invariant state-space-innovations model [29] given by:

$$\begin{aligned} x_{t+1} &= Ax_t + Bu_t + Ke_t, \\ y_t &= Cx_t + e_t, \end{aligned} \quad (1)$$

where x_t is the system state, y_t is the output, e_t is assumed to be Gaussian noise, and K is the Kalman gain matrix. More details on the model and parameter identification process can be found in reference [30]. To identify the model parameters, a surrogate heavy-duty diesel (HD)-FTP data set was used. Details about the experimental setup and data collection process can be found in reference [5].

Validation

The ability of the identified model to predict SCR performance outside of the calibration data was explored. The approach was to compare its prediction of SCR outlet NO_x sensor values to experimental values where the inlet NO_x was the same, but the inlet urea dosing was scaled by: 30, 50, 80, and 120% from the injection levels used in the calibration data set. It was found that the model was not sensitive to initial conditions (i.e. the model will converge after a few time steps). Thus, choosing $x_0 = 0$ did not have an appreciable effect on the model fit and helps generalize the model.

The goodness-of-fit of the identified model was evaluated using a prediction-error metric. Prediction-error is the difference between the model output prediction (downstream NO_x) for the next time step and the actual value for the next time step. The root mean squared error (RMSE) over all predictions for the 120% case was 5 ppm, so the average error at each time point was within ± 7.5 ppm and for most samples it was much lower. The RMSEs for the 80%, 50%, and 30% data were 5, 7, and 9 ppm, respectively. Detailed results and discussion can be found in reference [30].

Optimal Control

Using the linear quadratic estimator form of the model, the predicted downstream NO_x sensor reading at the next time step can be computed from the NO_x sensor reading at the current time step. In this way, it is possible to determine the optimal NH₃ input. A model-based controller was developed that minimizes the cost function (2) a combination of the predicted outputs and the controllable inputs. Here we derive the analytic solution to (2). The objective function to be minimized is:

$$F(u_{1:k}) = \|\hat{y}_{t+1|t}\|^2 + \|\Lambda u_{1:k}\|^2 = \|Qx + Ru + Sy\|^2 + \|\Lambda u_{1:k}\|^2 \quad (2)$$

$$= x^T Q^T Q x + u^T R^T R u + y^T S^T S y + x^T Q^T R u + u^T R^T Q x + x^T Q^T S y + y^T S^T Q x + u^T R^T S y + y^T S^T R u + u_{1:k}^T \Lambda^T \Lambda u_{1:k},$$

where, $u_{1:k} = [u_1, \dots, u_k]^T$, and $\Lambda \in \mathbb{R}^{k \times k}$ is the weighting matrix of tuning parameters for the k controllable inputs. The controller was implemented in MATLAB® and resulted in a computationally efficient calculation cycle.

Simulation

Although the optimal control law was calibrated to experimental data, it was not possible to test it on the same experimental setup used to acquire the calibration data. Instead a simulated comparison was performed. This yielded simulated outlet NO_x concentrations that could be compared to simulated NO_x outlet conditions in which the urea dosing was computed using the method described in the previous section.

The controller for computing optimal urea dosing was inserted into a calibrated Cu-zeolite SCR model described by Song, et al. [5]. The doser was assumed to be capable of applying any nonnegative control signal. Also, we did not simulate NO_x sensor cross sensitivity, so the controller received the actual, simulated, NO_x value. It should be noted that the urea dosing controller used for obtaining the experimental data was started 30 seconds after the engine was started and so this same constraint was applied to the simulation study.

Table 12 gives a synopsis of the relevant performance metrics for the comparison between the nominal production controller and proposed optimal controller. The optimal controller performs better than the production controller for every metric in Table 12. The optimal controller converts a larger mass of NO_x while using and expelling a smaller mass of NH₃/Urea.

Table 12: Synopsis of controller comparison

	Nominal	Optimal
Upstream NO_x Mass	63.09 g	63.09 g
Downstream NO_x Mass	4.78 g	4.60 g
NO_x Conversion Efficiency	92.43%	92.71%
Upstream NH₃ Mass	18.67 g	16.33 g
Downstream NH₃ Mass	2.15 g	0.22 g
NH₃ Conversion Efficiency	88.49%	98.67%
Urea Mass	32.92 g	28.79 g

Using the default settings for the SCR simulator and the optimal controller the NH₃ storage profile shown in Figure 35 was obtained. The upper plot is the storage site that reacts with NO_x while the second site, at bottom, only participates in adsorption and desorption. The ten lines on each plot represent the ten axial elements used in the SCR model. An interesting feature is present at 700 seconds, where the temperature at the inlet increases substantially, for storage the NO_x-reactive storage site (top plot). The NH₃ in the first three elements desorbs while the last four elements accumulate NH₃.

Figure 35: Optimal NH₃ storage fractions using a transient test cycle and a 10 element axially discretized SCR global kinetics model.

Conclusion

A data-driven modeling and optimal control strategy that allows the optimal performance of the SCR to be computed for a particular drive cycle of interest was developed. The NH₃ storage capability and sensitivity of the control strategy was analyzed. A data-driven state-space SCR estimator was validated against several surrogate HD-FTP data sets and found to fit with low error. The controller, in simulation, showed specific areas in which a production controller could improve and gave a possible upper bound for these improvements. The strategy developed can be used as an SCR profiling tool, so that engineers can fine-tune their controllers. Analysis of the storage profile admitted by the SCR controller showed that the storage profiles were insensitive to changes in simulated model parameters.

4. Schedule Status

A summary of the reports required on this contract, due dates, and actual delivery dates are shown in Table 13. Delivery dates were modified as a result of the no-cost time extension which extends the completion of this project to April 30, 2013.

Table 13: Milestone Report and Test Plan / Studies Due Dates

Budget Period	Milestone Name	Proposal Due Date	Modified Due Date	Actual Delivery Date
Budget Year 1	Data Inventory System Report	Month 3	Month 6	3/31/2010
	PM Loading Report	Month 9	Month 16	1/31/2011
	Axial Storage Study Report Combined below****	Month 12		Combined below
Budget Year 2	SCR, CPF, Sensor Estimator Models Report	Month 15	Month 21	06/30/2011
	Estimator Strategy Report	Month 15	Month 29	01/27/2012
	PM Loading Test Report (Engine Test Report)	Month 18	Month 21	07/28/2011
	Model Correlation (Active Regeneration) Report	Month 21	Month 22	10/12/2011
	PM Loading Test Plan Completion	Month 24		11/07/2011
Budget Year 3	Estimator Engine Test Report	Month 27	Month 46	
	Model Adaptation Report	Month 36	Month 44	06/07/2013
	CPF Active Regeneration Report	Month 36	Month 46	
	Maldistribution Report	Month 36	Month 41	03/28/2013
	Fuel Optimal Regeneration Report Combined below*	Month 27		Combined below
	Fuel Optimal Regeneration & Test Report*	Month 36	Month 46	
	Ammonia Storage Impact Report****	Month 27	Month 44	06/03/2013
	Flow Reactor & Engine Test Results Combined below**	Month 27		Combined below
	Aged SCR Report **	Month 36	Month 44	06/03/2013
	Optimal Ammonia Storage Report Combined below***	Month 27		Combined below
	Optimal Ammonia Storage & Sensitivity***	Month 36	Month 41	04/23/2013

* This report is a combination of Fuel Optimal Regeneration Process Development report and DPF Fuel Optimal Regeneration Test report.

** This report is a combination of Flow Reactor and Engine Test Results and Aged SCR report.

*** This report is a combination of Optimal Storage report and Optimal Storage Model Sensitivity Study report.

**** This report is a combination of Axial Storage Study Report and Ammonia Storage Impact Report.

5. Ancillary Results

This section summarizes publications, web site development, additional collaborations fostered by the project, and inventions.

Publications

- "Model Adaptation Study Report," Surenahalli, H., and Parker, G., *Technical Report to DOE*, DOE Report Number DOE/EE0000204-12, 2013, dated June 7, 2013.
- "Axial Storage Study and Ammonia Storage Impact Report," Song, X., Khajuee, S.M.H.S.H., Parker, G., Phil, J., *Technical Report to DOE*, DOE Report Number DOE/EE0000204-11, dated June 3, 2013.
- "Aging Impact on Ammonia Storage," Song, X., Parker, G., Pihl, J., *Technical Report to DOE*, DOE Report Number DOE/EE0000204-10, dated June 3, 2013.
- "Optimal NH₃ Storage in SCR," Stevens, A., Sun, Y., Lian, J., Devarakonda, M., Parker, G., *Technical Report to DOE*, DOE Report Number DOE/EE0000204-9, dated April 23, 2013.
- "Analysis Report for Particulate Matter Maldistribution in a Catalyzed Particulate Measured with a Terahertz Wave Scanner," Ryan Foley, Jeffrey Naber, John Johnson, *Technical Report to DOE*, DOE Report Number DOE/EE0000204-8, dated March, 28, 2013.
- "An Experimental and Modeling Study of SCR Reaction Kinetics for a Cu-Zeolite SCR Based on SCR Engine Experiments," Xiaobo Song, Jeffrey D. Naber, Gordon G. Parker, John H. Johnson, SAE Technical Paper No. 2013-01-1054, 2013 SAE World Congress.
- "A Modeling Study of SCR Reaction Kinetics from Reactor Experiments," Xiaobo Song, Gordon G. Parker, John H. Johnson, Jeffrey D. Naber, Josh A. Pihl, SAE Technical Paper No. 2013-01-1576, 2013 SAE World Congress.
- "Extended Kalman Filter Estimator for NH₃ Storage, NO, NO₂, and NH₃ Estimation in a SCR," Harsha S Surenahalli, Gordon G Parker and John H Johnson, SAE Technical Paper No. 2013-01-1581, 2013 SAE World Congress.
- "An Experimental Investigation into the Effects of Biodiesel Blends on Particulate Matter Oxidation in a Catalyzed Particulate Filter during Active Regeneration," MS Thesis, James Pidgeon, 2012.
- "An Engine Experimental Investigation into the Effects of Biodiesel Blends on Particulate Matter Oxidation in a Catalyzed Particulate Filter on an Engine during Active Regeneration," James Pidgeon, Jeffrey D. Naber, and John H. Johnson, SAE Technical Paper No. 2013-01-0521. 2013 SAE World Congress.
- "Development of a 1-D Catalyzed Diesel Particulate Filter Model for Simulation of the Oxidation of Particulate Matter and Gaseous Species during Passive Oxidation and Active Regeneration," Kiran Premchand, John Johnson, and Song-Lin Yang, SAE Technical Paper No. 2013-01-1574, 2013 SAE World Congress.
- "Experimental and Modeling Study of a Diesel Oxidation Catalyst (DOC) under Transient and CPF Active Regeneration Conditions," Xiaobo Song, Harsha Surenahalli, John Johnson, and Gordon Parker, SAE Technical Paper No. 2013-01-1046, 2013 SAE World Congress.
- "Optimal Feedback SCR Control with a Data-Driven State-Space Model," Andrew Stevens, Maruthi Devarakonda, Gordon Parker, SAE Technical Paper No. 2013-01-1573, SAE 2013 Congress.
- "Measuring PM Distribution in a Catalyzed Particulate Filter Using a Terahertz Wave Scanner," Ryan Foley, Jeffrey D. Naber, John H. Johnson- Michigan Technological University, Leigh Rogoski-Cummins Inc., Makoto Shinohara- Advantest Corporation, 2012 DEER Conference.
- "A Kalman Filter Estimator for a Diesel Oxidation Catalyst During Active Regeneration of a CPF", Surenahalli, H., Parker, G., Johnson, J., and Devarakonda, M., *American Control Conference* 2012.
- "A Study of the Effect of Biodiesel Fuel on Passive Oxidation in a Catalyzed Particulate Filter" Ken L. Shiel, Master Thesis, Michigan Technological University, 2012.

- "Catalyzed Particulate Filter Passive Oxidation Study with Ultra Low Sulfur and Biodiesel Blended Fuel," Kenneth Lee Shiel, Jeffrey Naber, John Johnson, Chris Hutton, Michigan Technological University, SAE Paper No. 2012-01-0837, SAE International Congress April 25, 2012.
- "Procedure Development and Experimental Study of Passive Particulate Matter Oxidation in a Diesel Catalyzed Particulate Filter," Chris Hutton, John Johnson, Jeffrey Naber, Jason Keith, Michigan Technological University, SAE Paper No. 2012-01-0851, SAE International Congress April 25, 2012.
- "Estimator Strategy Report," Surenahalli, H., Parker, G., Johnson, J., and Devarakonda, M., *Technical Report to DOE*, DOE Report Number DOE/EE0000204-7, 2013, dated Jan 27, 2012.
- "Investigation of NO₂ Oxidation Kinetics and Burning Mode for Medium Duty Diesel Particulate: Contrasting O₂ and NO₂ Oxidation", Strzelec, A., *DEER Conference*, 2011.
- "NO₂ Oxidation Kinetics and Burning Mode in Medium Duty Diesel Particulate," *DEER Abstract - Paper Presentation – 2011 Annual Meeting*.
- "Engine Test and Analysis Report for Catalyzed Particulate Filter Particulate Matter Loading and Passive Oxidation with Ultra Low Sulfur Diesel and Biodiesel Fuels," Christopher Hutton, Professor John H Johnson, Professor Jeffrey Naber, *Technical Report to DOE*, DOE Report Number DOE/EE0000204-6, dated Nov 7, 2011.
- "A Parameterized Iron-Zeolite SCR Model Calibrated to Reactor Data" Seth DeLand, Jason Keith, Gordon Parker, John Johnson, AICHE No. 222827-2011, *AIChE Annual Meeting* October 2011.
- "Engine Test and Analysis Report for the Effects of Biodiesel Blends on Particulate Matter Oxidation in a Catalyzed Particulate Filter during Active Regeneration," James Pidgeon, Professor John H Johnson, Professor Jeffrey Naber, *Technical Report to DOE*, DOE Report Number DOE/EE0000204-5, dated Oct 12, 2011.
- "Engine Test and Analysis Report for Catalyzed Particulate Filter Particulate Matter Loading and Passive Oxidation with Ultra Low Sulfur Diesel and Biodiesel Fuels," Kenneth Shiel, Harsha Surenahalli, Christopher Hutton, Professor John H Johnson, Professor Jeffrey Naber, *Technical Report to DOE*, DOE Report Number DOE/EE0000204-4, dated July 28, 2011
- "Baseline Estimator Study Form", Surenahalli, H., Parker, G., and Devarakonda, M., *Technical Report to DOE*, DOE Report Number DOE/EE0000204-3, dated June 30, 2011.
- "Modeling Study of Active Regeneration of a Catalyzed Particulate Filter Using One-Dimensional DOC and CPF Models," Surenahalli, Harsha S., et al. 2011, 2011 SAE World Congress, SAE Technical Paper No. 2011-01-1242, April 12-14, 2011.
- "Engine Test and Analysis Report for Catalyzed Particulate Filter Particulate Matter Loading and Passive Oxidation with Ultra Low Sulfur Diesel," Christopher Hutton, Harsha Surenahalli, Kenneth Shiel, Professor John H Johnson, Professor Jeffrey Naber, *Technical Report to DOE*, DOE Report Number DOE/EE0000204-2, dated Jan 31, 2011.
- "Data Inventory System" " Professor John Johnson, Professor Jason Keith, Professor Jeffrey Naber, Professor Gordon Parker, Professor Song-Lin Yang, *Technical Report to DOE*, DOE Report Number DOE/EE0000204-1, dated March, 31, 2010.
- "An Experimental Investigation into the Passive Oxidation of Particulate Matter in a Catalyzed Particulate Filter," Hutton, Christopher, Master Thesis, Michigan Technological University, 2010.
- "Development and Parameter Identification of an Iron-Zeolite SCR Catalyst Model Using Reactor Data," DeLand, Seth, Master Thesis, Michigan Technological University, 2010
- "A Modeling Study of a Diesel Oxidation Catalyst and Catalyzed Particulate Filter During Loading and Active Regeneration." Surenahalli, Harsha S, Master Thesis, Michigan Technological University, 2010.
- "A SCR Model based on Reactor and Engine Experimental Studies for a Cu-zeolite Catalyst," Song, Xiaobo, PhD Thesis, Michigan Technological University, 2013.
- "Dynamic Model Based State Estimation in a Heavy Duty Diesel Aftertreatment System for Onboard Diagnostics and Controls," H. Surenahalli, PhD thesis, Michigan Technological University, 2013.

Publications currently in progress:

- "Modeling and Parameter Identification for an Iron-Zeolite SCR Catalyst," Seth DeLand, Gordon Parker, Jason Keith, and John Johnson, *in preparation*

Presentations

- "A Parameterized Iron-Zeolite SCR Model Calibrated to Reactor Data," AICHE Abstract Submission #222827-2011 Annual Meeting.
- "Trends in Particulate Nanostructure: Impact of Engine Size and Biofueling," DEER Abstract - Poster Presentation – 2011 Annual Meeting.
- "DOC Efficacy on the Soluble Organic Fraction with Biofuel Blending on a HD-Engine," DEER Abstract - Poster Presentation – 2011 Annual Meeting.
- "Advances in Exhaust Temperature Sensing and their Applicability for Diesel Emission Diagnostics" - 2011 SAE OBD Symposium
- "Catalyzed Particulate Filter Passive Oxidation Study with Ultra Low Sulfur and Biodiesel Blended Fuel," Kenneth Lee Shiel, Jeffrey Naber, John Johnson, Chris Hutton, Michigan Technological University, SAE Paper No. 2012-01-0837, SAE International Congress April 25, 2012.
- "Procedure Development and Experimental Study of Passive Particulate Matter Oxidation in a Diesel Catalyzed Particulate Filter," Chris Hutton, John Johnson, Jeffrey Naber, Jason Keith, Michigan Technological University, SAE Paper No. 2012-01-0851, SAE International Congress April 25, 2012.
- "Spatial Variations in NH₃ Storage on Copper Zeolite SCR Catalysts," J.A. Pihl, C.S. Daw, Presentation to the CTI 4th International Conference on NO_x Reduction, Detroit, MI, June 20, 2012
- "Local Ammonia Storage in a Monolithic SCR Catalyst: Comparing Model & Commercial Catalyst Performance," W.P. Partridge, J.A. Pihl, X. Auvray, L. Olsson, T.J. Toops, J.-S. Choi, C.S. Daw, K. Kamasamudram, A. Yezerets, N.W. Currier, presentation to the 9th International Congress on Catalysis and Automotive Pollution Control, Brussels, Belgium, August 29, 2012.
- "Local Ammonia Storage in a Monolithic SCR Catalyst: Comparing Model & Commercial Catalyst Performance," W.P. Partridge, J.A. Pihl, X. Auvray, L. Olsson, T.J. Toops, J.-S. Choi, C.S. Daw, K. Kamasamudram, A. Yezerets, N.W. Currier, presentation to the 7th International Conference on Environmental Catalysis, Lyon, France, September 5, 2012.
- "A Study and Comparison of SCR Reaction Kinetics from Reactor and Engine Experimental Data," Xiaobo Song, Gordon G. Parker, Jeffrey D. Naber, John H. Johnson, Josh A. Pihl, Poster 2012 DEER Conference.
- "Measuring PM Distribution in a Catalyzed Particulate Filter Using a Terahertz Wave Scanner," Ryan Foley, Jeffrey Naber, John Johnson, and Leigh Rogoski, Presentation 2012 DOE DEER Conference.
- "An Experimental and Modeling Study of SCR Reaction Kinetics for a Cu-Zeolite SCR Based on SCR Engine Experiments," Xiaobo Song, Jeffrey D. Naber, Gordon G. Parker, John H. Johnson, SAE Technical Paper No. 2013-01-1054, 2013 SAE World Congress.
- "A Modeling Study of SCR Reaction Kinetics from Reactor Experiments," Xiaobo Song, Gordon G. Parker, John H. Johnson, Jeffrey D. Naber, Josh A. Pihl, SAE Technical Paper No. 2013-01-1576, 2013 SAE World Congress.
- "Extended Kalman Filter Estimator for NH₃ Storage, NO, NO₂, and NH₃ Estimation in a SCR," Harsha S Surenahalli, Gordon G Parker and John H Johnson, SAE Technical Paper No. 2013-01-1581, 2013 SAE World Congress.
- "An Engine Experimental Investigation into the Effects of Biodiesel Blends on Particulate Matter Oxidation in a Catalyzed Particulate Filter on an Engine during Active Regeneration," James Pidgeon, Jeffrey D. Naber, and John H. Johnson, SAE Technical Paper No. 2013-01-0521. 2013 SAE World Congress.

- “Development of a 1-D Catalyzed Diesel Particulate Filter Model for Simulation of the Oxidation of Particulate Matter and Gaseous Species during Passive Oxidation and Active Regeneration,” Kiran Premchand, John Johnson, and Song-Lin Yang, SAE Technical Paper No. 2013-01-1574, 2013 SAE World Congress.
- “Experimental and Modeling Study of a Diesel Oxidation Catalyst (DOC) under Transient and CPF Active Regeneration Conditions,” Xiaobo Song, Harsha Surenahalli, John Johnson, and Gordon Parker, SAE Technical Paper No. 2013-01-1046, 2013 SAE World Congress.
- “Optimal Feedback SCR Control with a Data-Driven State-Space Model,” Andrew Stevens, Maruthi Devarakonda, Gordon Parker, SAE Technical Paper No. 2013-01-1573, SAE 2013 Congress.

Web Site Development:

Web site developed and deployed during quarter 2, (<http://www.diesel.mtu.edu>.) It is used for both a data archive system and a place to share project-related documents and results. It is a password protected site to protect data generated by OEMs

Collaborations Fostered:

There were significant collaborations between the industrial and National Lab partners which will be extended into a Diesel Aftertreatment Consortium which is being organized by Michigan Tech with a start date of August 1, 2013.

Technologies/Techniques: DOC, CPF, and SCR Reduced Order Estimator Models

Inventions/Patent Applications: None

Licensing Agreements: None

MODELS DEVELOPED:

DIESEL OXIDATION CATALYST (DOC) MODELS

DOC High-Fidelity Model

Model Description

The MTU DOC model used in this study is a 1-D single channel representation of the DOC. The DOC model simulates the gas and surface phase concentrations and temperatures. The heat and mass transfer is limited by the heat and mass transfer coefficients. The DOC model was developed using Matlab/Simulink® c-sfunction. A variable time step solver is used to solve the species and energy conservation equations.

The goal of the model was to simulate the DOC during steady state and active regeneration conditions. The intended use of model was to provide a basis for development of a reduced order DOC model and state estimator. This requires the model to be able to simulate the DOC outlet concentrations of CO, NO, NO₂ and HC under different space velocities and temperatures.

Assumptions in the DOC Model

The important assumptions made in the High Fidelity 1D DOC model are as follows:

1. The channels in the DOC are square (channel shape can be changed with some modifications to the code).
2. The species concentration and exhaust gas velocity are cross sectional mass averaged quantities and the bulk flow is modeled.
3. Reaction rate constants and adsorption equilibrium factors used in the model are of the Arrhenius form.
4. Particulate matter oxidation is neglected.
5. C₃H₆ is considered to be representative of the hydrocarbon oxidation in the DOC.
6. NO-NO₂ oxidation is reversible and CO and HC oxidation is forward only.
7. A single channel is considered to be representative of the entire DOC and hence radial variation of the gaseous concentrations, velocity and temperature is neglected.
8. Exhaust gas is assumed to be an ideal gas.
9. The pressure along the axial length of the DOC is assumed to be constant.
10. Axial heat conduction in the channels is neglected.
11. Heat transfer to the ambient is considered to be through free convection.

The DOC consists of a circular outer cross-section, filled internally with square channels. The square channels in the DOC catalyst, have a hydraulic diameter of 'a' and a wall thickness, 'wt'. Characteristic physical properties such as length (L), diameter (D), wall thickness (wt) and cell density are used to calculate the open frontal area (ϵ) and geometric surface area (A_g) to model the chemical kinetics in a channel. The exhaust gas pressure used as input to the model is the averaged pressure calculated from the test data upstream and downstream of the catalyst.

Reactions Considered in the Model

CO, NO and HC oxidation reactions are simulated in the DOC model. C₃H₆ is considered to be representative of the hydrocarbon oxidized in the DOC. NO oxidation is modeled as a reversible reaction. CO and HC oxidation reactions are considered to be forward only reactions. All the oxidation

reactions are assumed to take place on the surface of the catalyst. The chemical reactions considered are shown in Equations (1) to (3).

CO Oxidation:

NO $\leftrightarrow$ NO₂ Oxidation:

C₃H₆ Oxidation:

Species Conservation

As the exhaust gas moves through the DOC catalyst, molecules of CO, HC, NO and NO₂ are transported to the stagnant boundary layer at the surface of the monolith wall and then take part in the catalytic reactions. Reaction products are desorbed back into the boundary layer and then are transported into the bulk flow and to the monolith exit. Thus, concentrations of both gas and surface phase of the participating species are modeled in the simulation. The partial differential equations for CO, NO, NO₂, HC and O₂ surface and gaseous species conservation are as shown in Equations (4) to (5) [1].

$$\epsilon \frac{\partial C_{g,j,i}}{\partial t} = -\epsilon u \frac{\partial C_{g,j}}{\partial x} - \beta_j A_g (C_{s,j,i} - C_{g,j,i}) \quad (4)$$

$$(1 - \epsilon) \frac{\partial C_{s,j,i}}{\partial t} = -\beta_j A_g (C_{s,j,i} - C_{g,j,i}) - R_{j,i} \quad (5)$$

Where, u is the bulk velocity of the exhaust (m/s), ϵ is the open frontal area or void fraction, A_g is the geometric surface area (m²), $C_{g,j,i}$ are the gaseous concentrations of the species (j^{th} = CO, NO, NO₂, HC and O₂) in mol/m³ and $C_{s,j,i}$ are the surface concentrations of the species (j^{th} = CO, NO, NO₂, HC and O₂) in mol/m³. β_j is the mass transfer coefficient and is defined as

$$\beta_j = Sh_j \frac{D_m}{L}$$

Where, Sh_j is the limiting Sherwood number, L is the characteristic length (m) and D_m is the hydraulic diameter of the square channel.

$$Sh_j = 0.766 \times \left(\frac{d}{L} \times Re \times Sc \right)^{0.483}$$

Where Re and Sc are the Reynolds and Schmidt numbers.

Reaction Rate Calculations

The reaction rates for the CO, NO and C₃H₆ oxidation reactions are as shown in Equations (6) to (8) [1].

$$R_{CO} = \frac{K_{CO}[C_{S,CO}C_{S,O_2}]}{G_1} \quad (6)$$

$$R_{NO} = \frac{K_{NO}\left[C_{S,NO}C_{S,O_2} - \frac{C_{S,NO_2}}{K_p}\right]}{G_2} \quad (7)$$

$$R_{C_3H_6} = \frac{K_{C_3H_6}[C_{S,C_3H_6}C_{S,O_2}]}{G_3G_4} \quad (8)$$

K_p in the NO oxidation reaction rate equation is the equilibrium constant which determines the relative magnitude of the reverse reaction and is given by:

$$K_p = e^{\frac{-\Delta G_T}{RT}}$$

Where, ΔG_T is the Gibb's free energy for NO, NO₂ and O₂ mixtures at temperature T (Kelvin) and R is the universal gas constant. The reaction rate constants K_{CO} , K_{NO} and $K_{C_3H_6}$ are of the Arrhenius form and represented as:

$$K_i = A_i e^{-\frac{E_{a,i}}{RT}} \quad i = CO, NO, C_3H_6$$

G_1 , G_2 , G_3 and G_4 are the inhibition terms to account for the inhibition of the oxidation reactions due to the availability of catalyst sites.

G_1 , G_2 and G_3 are of the form (1):

$$G_i \left[(1 + K_{a,j}C_{S,CO} + K_{a,j+1}C_{S,C_3H_6})^2 (1 + K_{a,j+2}C_{S,CO}^2 C_{S,C_3H_6}^2) (+K_{a,j+3}C_{S,NO}^{0.7}) \right]$$

$$j = 1, 2, 3$$

And G_4 is of the form

$$G_4 = (1 + K_{a,j}C_{S,O_2})^{1.5}$$

Where $K_{a,j}$ are of the Arrhenius form and are called inhibition factors

$$K_{a,j} = A_{a,j} e^{-\frac{\Delta H_{a,j}}{RT}}$$

Where, $A_{a,j}$ are the adsorption constants and $\Delta H_{a,j}$ are the adsorption heats. 3.1.5. Conservation of Energy

Species Conservation

Applying conservation of energy for the surface and gas phase results in two partial differential equations for the gas and the surface temperature respectively. The heat source by oxidation of the species is included in the surface temperature equation. The resulting differential equations are [1]:

$$\rho C_v \frac{dT_g}{dt} = -\rho u C_p \frac{dT_g}{dx} - h_g \frac{4}{a_w} (T_g - T_w) \quad (9)$$

$$\rho_w C_w \frac{dT_w}{dt} = h_g \frac{4a_w}{a_p^2 - a_w^2} (T_g - T_w) - h_a \frac{4a_p}{a_p^2 - a_w^2} (T_w - T_a) + \frac{A_g}{1-\epsilon} \sum_i \frac{-\Delta h_i R_i}{MW_i} \quad 10$$

Equation (9) is the gas phase energy balance and Equation 10 is the surface phase energy balance equation.

Files needed to run the model

The DOC simulink model requires 15 files to be present in the current folder to run successfully. The files required along with a brief description are as below:

1. setup5.m: This file sets up the user input constants and inputs to the model. The geometric properties of the DOC, the reaction rate constants for the reactions, the inhibition constants for the reaction inhibition and also the total simulation time and time step for integration is specified in this file.
2. DOCLobalsandConstants5.m: Contains constants used in the “setup5.m” and “loadparams5.m”
3. Load_Inputs5.m: This file creates transient inputs based on the inlet conditions specified in the “SampleInputs.mat”.
4. SampleInputs.mat: Is a Matlab® file which contains a sample set of inputs for simulating the model. This file contains the DOC inlet and outlet concentrations, temperatures along with mass flow rates and pressures.
5. doc_hom5.c: This is the main C-sfunction file that calls several function to simulate the model
6. doc_constants5.h: This file contains definitions of the constants used in the C Sfunction.
7. support5.c : This file contains the supporting functions that are used in the “doc_hom5.c”.
8. support5.h: Contains definitions of the functions in “support5.c”
9. nelem5.h: Is a C header file the number of elements in the model. Changing the number of elements in the header file requires the recompilation of the code.
10. loadparams5.m: Processes all the inputs from setup5.m and copies it to Sfunction parameters.
11. vectors5.h : Contains Vectors used in “support5.c”
12. hom_doc5.mdl: This is the simulink model file to simulate the DOC model. Figure 1 shows a screen capture of the simulink estimator model. The figure highlights the Inputs, model and output blocks of the simulink model. The simulation results are stored in two separate arrays for temperatures and concentrations. The temperatures are stored in an array with name “Temperatures” and species concentrations are stored in an array with the name “Concentrations”. For a 2 axial element model the values in the “Temperatures” array represents as follows:
 - 1) Column 1- Simulation time
 - 2) Column 2&4- Gas temperature for element 1 and 2
 - 3) Column 3 &5- Surface temperature for element 1 and 2

Similarly for a 2 axial element model the values in the “Concentrations” array represents as follows:

- 1) Column 1- Simulation time
- 2) Columns 2 & 12 – Gas phase CO concentration for element 1 and 2.
- 3) Columns 3 & 13 – Gas phase NO concentration for element 1 and 2.
- 4) Columns 4 & 14 – Gas phase NO₂ concentration for element 1 and 2.
- 5) Columns 5 & 15 – Gas phase HC concentration for element 1 and 2.
- 6) Columns 6 & 16 – Gas phase O₂ concentration for element 1 and 2.
- 7) Columns 7 & 17 – Surface phase CO concentration for element 1 and 2.
- 8) Columns 8 & 18 – Surface phase NO concentration for element 1 and 2.
- 9) Columns 9 & 19 – Surface phase NO₂ concentration for element 1 and 2.
- 10) Columns 10 & 20 – Surface phase HC concentration for element 1 and 2.
- 11) Columns 11 & 21 – Surface phase O₂ concentration for element 1 and 2.

Figure 1: Screen capture of the model with the inputs and outputs to the DOC model.

13. Plot_Results.m: Is a Matlab plotting script which plots the simulated and experimental DOC outlet concentrations and temperatures.
14. Define_Plot_Colors.m: Defines the colors to be used in the Plot_Results.m
15. DispStatus.m: This is a Matlab® function that prints the status of the simulation in the Matlab® command prompt.

Running a Simulation

1. Specify inputs in “setup5.m” and run the Matlab script to setup the inputs.
2. Line 147 of the “setup5.m” calls the “Load_Inputs5.m” which contains commands to load the sample inputs to the Matlab® work space. Hence executing “setup5.m” also sets up the transient inputs.
3. Open the “hom_doc5.mdl” and from the simulation drop down menu select the start.

Figure 2: Screen capture of the model highlighting the menu to start the simulation.

4. After the completion of the simulation open the file "Plot_Results.m" and run the script to generate the plots. Each subplot show comparison of the estimated DOC outlet Temperature, NO₂/NO_x ratio, HC and CO concentration.

Model Performance

The DOC model was simulated on steady state, active regeneration and transient data. The data to simulate the model was acquired on a 2010 Cummins ISB engine with a production. The aftertreatment system consists of DOC, CPF, SCR and AMOX devices. The details of the model and the results from the simulation is reported in an SAE paper at 2013 SAE World Congress [3]. The paper presents an experimental and modeling study of a production DOC catalyst under different engine operating conditions including steady state, active regeneration during in-cylinder fuel injection, and surrogate heavy-duty federal test procedure (HD-FTP) transient cycle tests. The kinetic parameters associated with the HC, CO, and NO were identified in the process.

Hardware Requirements

Operating Systems: Windows XP Service Pack 3, Windows XP x64 Edition Service Pack 2, Windows Server 2003 R2 Service Pack 2, Windows Vista Service Pack 2, Windows Server 2008 Service Pack 2 or R2, Windows 7.

Processors: Any Intel or AMD x86 processor supporting SSE2 instruction set

Disk Space: 1 GB for MATLAB only, 3–4 GB for a typical installation

RAM: 1024 MB (At least 2048 MB recommended)

DOC Reduced Order Estimator

Model Description

An Extended Kalman Filter (EKF) based state estimation strategy for the Diesel Oxidation Catalyst (DOC) was developed using reduced order DOC model. The reduced order model is derived from the high fidelity model. The DOC estimator uses the exhaust mass flow rate, CO, C₃H₆ and O₂ concentrations from the engine maps along with the NO_x sensor and temperature measurement upstream of the DOC and a temperature measurement downstream of the DOC to estimate the states of the DOC.

The goal of the reduced order DOC estimator was to simulate the DOC outlet concentrations of CO, NO, NO₂, HC concentrations and temperatures. The reduced order model was simulated using steady state and active regeneration tests. The DOC reduced order estimator was simulated using the surrogate FTP test data.

Assumptions in the DOC Model

The important assumptions made in the development of the reduced order model are:

1. The reactions are instantaneous $\frac{\partial C_g}{\partial t} = \frac{\partial C_s}{\partial t} = 0$
2. The surface phase and gas phase concentrations are identical and can be assumed to be equal, C = C_g = C_s.
3. The surface phase and gas phase temperatures are identical and can be assumed to be equal, T = T_g = T_s.

Reactions Considered in the Model

CO, NO and HC oxidation reactions are represented in the DOC reduced order estimator. C₃H₆ is considered to be representative of the hydrocarbon oxidized in the DOC. NO oxidation is modeled as a reversible reaction. The chemical reactions considered are shown in Equations (1) to (3).

CO Oxidation:

NO ↔ NO₂ Oxidation:

C₃H₆ Oxidation:

DOC Mass and Energy Balance

The mass and the energy balance equations describing the model are given in Equations (4) and (5).

$$\epsilon u \frac{\partial C_i}{\partial x} = -R_i \quad (4)$$

$$i = CO, NO, NO_2, C_3H_6 \& O_2$$

$$(\rho_s C_s + \rho C_v) \frac{dT}{dt} = -\rho u C_p \frac{dT}{dx} - \frac{1}{1-\epsilon} \sum_{i=CO, NO, C_3H_6} \frac{-\Delta h_i R_i}{MW_i} \quad (5)$$

where, ρ_s and $c_{p,s}$ are the density and specific heats of the substrate, ρ is the density of the exhaust gas, c_p and c_v are specific heats of the exhaust gas, Δh_i is the enthalpy of the CO, NO and C_3H_6 oxidation reactions and MW_i is the molecular weight of i^{th} species .

Reaction Rate Calculations

The reaction rates for the CO, NO and C_3H_6 oxidation reactions are as shown in Equations (6) to (8) [1].

$$R_{CO} = \frac{K_{CO} [C_{CO} C_{O_2}]}{G_1} \quad (6)$$

$$R_{NO} = \frac{K_{NO} \left[C_{NO} C_{O_2} - \frac{C_{NO_2}}{K_p} \right]}{G_2} \quad (7)$$

$$R_{C_3H_6} = \frac{K_{C_3H_6} [C_{C_3H_6} C_{O_2}]}{G_3 G_4} \quad (8)$$

K_p in the NO oxidation reaction rate equation is the equilibrium constant which determines the relative magnitude of the reverse reaction and is given by:

$$K_p = e^{\frac{-\Delta G_T}{RT}}$$

Where, ΔG_T is the Gibb's free energy for NO, NO_2 and O_2 mixtures at temperature T (Kelvin) and R is the universal gas constant. The reaction rate constants K_{CO} , K_{NO} and $K_{C_3H_6}$ are of the Arrhenius form and represented as:

$$K_i = A_i e^{\frac{E_{a,i}}{RT}} \quad i = CO, NO, C_3H_6$$

G_1 , G_2 , G_3 and G_4 are the inhibition terms to account for the inhibition of the oxidation reactions due to the availability of catalyst sites.

Files needed to run the model

The DOC estimator simulink model requires 6 files to be present in the current folder to run successfully. The files required along with a brief description are as below:

16. Simsetup.m: This file sets up the user input constants and inputs to the model. The geometric properties of the DOC, the reaction rate constants for the reactions, the inhibition constants for the reaction inhibition and also the total simulation time and time step for integration is specified in this file.
17. DOC_est_const.m: This file contains all the constants used in the simulation of the DOC EKF estimator. The constants include the number of axial elements.
18. DOC_estimator_discrete.m: This file contains the sfunction which simulates the EKF estimator.

19. estimator_doc_discrete.mdl: This is the simulink model file to simulate the EKF estimator. Figure 1 shows a screen capture of the simulink estimator model. The figure highlights the Inputs, estimator and output blocks of the simulink model. The simulation results are stored in an array with name "Estimated_States". For a 13 axial element model the values in the array represent as follows:

- 1) Column 1- Simulation time
- 2) Column 2-14 – Temperature along the axial length from inlet to outlet.
- 3) Column 15-27 – NO concentration along the axial length from inlet to outlet.
- 4) Column 28-40 – NO₂ concentration along the axial length from inlet to outlet.
- 5) Column 41-53 – CO concentration along the axial length from inlet to outlet.
- 6) Column 53-66 – HC concentration along the axial length from inlet to outlet
- 7) Column 67 – Pressure drop across the DOC.

Figure 1: Screen capture of the model with the inputs and outputs to the estimator.

20. Estimator_Inputs.mat: This file contains sample inputs to run the estimator. This file executed from the setup file.
21. Plot_Results.m: This file is used to generate plots to compare the simulation results with the estimated results.
22. DispStatus.m: This is a Matlab® function that prints the status of the simulation in the Matlab® command prompt

Running a Simulation

1. Specify inputs in “Simsetup.m” and run the Matlab script to setup the inputs.
2. Line 9 of the Simsetup.m contains command to load the sample inputs to the Matlab® work space. Hence executing “Simsetup.m” also sets up the transient inputs.
3. Open the “estimator_doc_discrete.mdl” and from the simulation drop down menu select the start.

Figure 2: Screen capture of the model highlighting the menu to start the simulation.

4. After the completion of the simulation open the file “Plot_Results.m” and run the script to generate the plots. Each subplot show comparison of the estimated DOC outlet Temperature, NO2/NOX ratio, HC and CO concentration along with the DOC inlet values..

Model Performance

The DOC reduced order model was simulated on steady state and active regeneration data. The reduced order DOC estimator was simulated on the transient FTP data. The data to simulate the model was acquired on a 2010 Cummins ISB engine with a production Cummins aftertreatment system consisting of DOC, CPF, SCR and AMOX devices. The details on the reduced order model and the reduced order estimator and the simulation results are published in a conference paper submitted American Controls Conference [2] and in a report submitted to DOE [16]. The paper presents the development and simulation of the DOC reduced order estimator to steady state, active regeneration during in-cylinder fuel injection, and also shows the development and simulation of the DOC reduced order estimator on surrogate heavy-duty federal test procedure (HD-FTP) transient cycle tests.

Hardware Requirements

Operating Systems: Windows XP Service Pack 3, Windows XP x64 Edition Service Pack 2, Windows Server 2003 R2 Service Pack 2, Windows Vista Service Pack 2, Windows Server 2008 Service Pack 2 or R2, Windows 7.

Processors: Any Intel or AMD x86 processor supporting SSE2 instruction set

Disk Space: 1 GB for MATLAB only, 3–4 GB for a typical installation

RAM: 1024 MB (At least 2048 MB recommended)

CATALYZED PARTICULATE FILTER (CPF) MODELS

CPF High-Fidelity Model

The catalyzed diesel particulate filter (CPF) is applied to reduce carbonaceous particulate matter emissions from diesel engines. As the exhaust gas mixture passes through the particulate filter, it is forced to flow through the porous walls of the substrate which causes a physical filtration of PM by the substrate. The collection of PM in the substrate wall causes the wall pores to get filled with PM, causing the deposition of PM on the inlet channel surfaces of the substrate wall as a PM cake layer. Subsequently, this PM cake layer forms an efficient (filtration efficiency > 90%) filter of subsequent incoming PM. This filtered PM is oxidized either by O_2 to form CO and CO_2 or by NO_2 to form CO, CO_2 and NO. Both O_2 and NO_2 are already present in the exhaust gas mixture. In addition, NO_2 is produced (by means of oxidation of NO) in the DOC as a function of temperature and space velocities inside the DOC which is placed upstream of the CPF in a typical aftertreatment system. The oxidation of PM via O_2 and NO_2 can be enhanced by elevating the temperature of the exhaust gas mixture passing through the CPF, thereby increasing the temperature at which the thermal and passive PM oxidation reactions occur. This can be achieved by oxidation of fuel either in-cylinder (by means of a post-injection) or in the exhaust stream (using a doser pump). Numerical modeling of the CPF provides a method for identifying the kinetics of all reactions occurring in the CPF including gas phase reactions and PM oxidation reactions as well as being able to predict the pressure drop across the CPF during different engine conditions where PM is being accumulated or regenerated at different rates.

Model Description

The CPF high-fidelity model version 4.0 [6] is a numerical model developed at MTU that constitutes a 1-dimensional single channel representation of a CPF. The model simulates one inlet channel, one substrate wall and one outlet channel of the CPF. It contains sub-models to predict the flow, filtration and oxidation of solid particulate matter and variation of concentrations of gaseous species constituting exhaust gas mixture due to chemical reactions occurring in the catalyst. These sub-models solve the mass, axial momentum, energy and species mass balance governing equations along with filtration efficiency calculations in order to calculate the velocity, pressure, temperature and molar composition of the exhaust gas mixture as it passes through the inlet channel, PM cake layer, catalyst washcoat, substrate wall and outlet channel as well as rate of deposition of particulate matter in the substrate wall and PM cake layer of the particulate filter. The current version of CPF high-fidelity model source code is v4.0 dated May 31st, 2013. The entire source code is written in FORTRAN programming language.

Assumptions

- Single channel is representative of the entire geometry of the particulate filter. No radial variation in any calculated variables is considered.
- Exhaust gas mixture is an ideal gas of molecular weight determined by the mole fractions of all gaseous species that constitute the gas mixture.
- $C_{12}H_{24}$, O_2 , N_2 , CO_2 , H_2O , CO , NO and NO_2 are the gaseous chemical species constituting the exhaust gas mixture.
- Quasi-steady state of all governing equations is assumed, except for substrate wall energy balance which is considered transient.
- Flow of exhaust gas mixture into, out of and through the CPF inlet channel, substrate wall and outlet channel is of the steady-state, compressible, fully-developed and laminar kind.
- Particulate matter (PM) is to be solid elemental carbon and flows into the CPF by the exhaust gas mixture at a rate proportional to the cross-sectional average volumetric flow rate of the exhaust gas mixture at the inlet of the CPF.
- There are 3 chemical reactions involving gaseous species that can occur in the CPF: $C_{12}H_{24}$ oxidation, CO oxidation and NO oxidation/ NO_2 dissociation. All these chemical reactions take place in the catalyst washcoat layer.
- There are 2 mechanisms for PM oxidation reaction; thermal (O_2) and passive (NO_2). These reactions occur at two locations in the model; PM cake layer and substrate wall.

The intended use of the CPF high-fidelity model is to support the development of a reduced order CPF model which in turn would be used for a Kalman filter-based estimator to be used towards controls and on-board diagnostics applications of the CPF in an aftertreatment system. In order for the high-fidelity model to be validated, it needs to be able to predict the pressure drop, PM retained, exhaust gas temperatures at CPF outlet and NO/NO_2 concentrations at CPF outlet for the experiment data which included both passive oxidation and active regeneration cases.

Features

A detailed description of all sub-models used in the CPF high-fidelity model as well as sample calibration results have been published in a peer-reviewed SAE technical paper in April 2013 [6]. Calibration results from passive oxidation and active regeneration experiments conducted at MTU were also published in reference [12].

The following sub-sections briefly describe the processes that are simulated in the model.

Filtration of PM occurs via 2 mechanisms in the substrate wall and PM cake layer: Brownian diffusion and direct interception. Filtration is modeled based on the concept of unit collectors in the substrate wall and PM cake layer. The equivalent filtration efficiency of the PM cake layer or the substrate wall is the resultant of the filtration efficiencies of the 2 mechanisms of filtration. The filtration efficiency of a unit collector in the substrate wall or PM cake layer is expressed mathematically as:

$\eta_{DR,i} = \eta_{D,i} + \eta_{R,i} - \eta_{D,i}\eta_{R,i}$ where $i = \text{cake/wall}$, η_D is the filtration efficiency due to Brownian diffusion and η_R is the filtration efficiency due to direct interception.

At clean state, substrate wall is the only filter present. The permeability of the substrate wall at this point is defined as a pre-determined constant known as initial substrate wall permeability ($k_{0,wall}$). The filtration efficiency of the CPF at this point is equal to the filtration efficiency of the substrate wall. As and when the substrate wall gets filled with PM, the permeability of the substrate wall decreases and leads to the formation of a PM cake layer. This is determined in the CPF high-fidelity model by the use of a parameter called the 'transition permeability of the substrate wall' (k_{trans}). When the instantaneous

permeability of the substrate wall at any axial location has reached below the value of transition permeability of wall that has been specified, a PM cake layer starts to form at that particular axial location. The filtration efficiency of the PM cake layer is dependent on the thickness and porosity of the PM cake layer itself and diameter and filtration efficiency of a single unit collector in the PM cake layer [6].

Oxidation of PM occurs in the PM cake layer and substrate wall through thermal (O_2) and passive (NO_2) mechanisms, the rate of which influences the rate of PM mass retained and hence the total PM mass retained over a period of time. The overall rate of oxidation of PM is dependent on the instantaneous amount of PM available in the particulate filter for oxidation, kinetics of thermal and passive reactions, absolute local temperature of the substrate wall and local oxidant (O_2 , NO_2) concentrations. The rate of oxidation of PM is expressed as [6]:

$$\frac{d(m_{ox,i})}{dt} = m_{ret,i} [-RR_{th,i} - RR_{NO_2,i}], i = cake/wall$$

where $m_{ret,i}$ is the mass of PM retained in the cake or wall, $RR_{th,i}$ is the rate of thermal PM oxidation reaction (with O_2) and $RR_{NO_2,i}$ is the rate of passive PM oxidation reaction (with NO_2).

Catalyst washcoat is modeled as a separate layer on the inlet channel side of the substrate wall or in the pores of the substrate wall. This is the domain of all 3 gaseous chemical reactions considered. Stoichiometric reactions are assumed for all gaseous species reactions. Solution of gaseous species concentrations considers the rate of mass transfer of a particular chemical species across the boundary layer between the inlet channel and the substrate wall as the exhaust gas mixture passes through the inlet channel. Also, the rate of diffusion, convection and reaction of each chemical species in the transverse direction is included in the species concentrations solution in the PM cake layer, catalyst washcoat and substrate wall.

An **Iterative solution procedure** is followed since quasi-steady state of all governing equations except substrate wall temperature is assumed and all chemical reactions depend on the substrate wall temperature solution. Solution at any time point is iterated till convergence is reached for all major variables; namely absolute pressure, velocity, temperature and species concentrations (mole fractions).

Inputs Required

The following CPF inlet conditions need to be supplied to the CPF high-fidelity model at all points in time that are simulated:

- Mass flow rate of exhaust gas mixture,
- Exhaust gas temperature,
- Concentrations of gaseous species ($C_{12}H_{24}$, O_2 , CO_2 , CO , NO and NO_2) and particulate matter (C).

These inputs are specified in an ASCII text file named 'input_exhaust_flow_v4_b04.dat'.

Also, the constant input parameters that specify the substrate geometry, physical and thermal properties of PM, filtration and kinetics (of both PM and gaseous species oxidation reactions) and simulation convergence criteria need to be specified. These inputs are specified in the following ASCII text files:

1. gas_prop_coeff_v4_b04.dat.dat
2. input_adsorption_parameters_v4_b04.dat
3. input_dia_distup_v4_b04.dat
4. input_gas_kinetics_v4_b04.dat

5. input_optim_parameters_v4_b04.dat²
6. input_parameters_v4_b04.dat
7. input_pm_cake_density_vs_time_v4_b04.dat³
8. input_pm_cake_efficiency_vs_time_v4_b04.dat²
9. input_pm_cake_permeability_vs_time_v4_b04.dat²
10. input_pm_kinetics_v4_b04.dat
11. timepoints_v4_b04.dat

Outputs

The CPF high-fidelity model code writes the following outputs to ASCII text files:

- Total pressure drop across the CPF and its components (across channels, PM cake and substrate wall) versus simulation time,
- PM mass balance (cumulative inlet, oxidized, retained and outlet and distribution of retained in the PM cake layer and substrate wall) versus simulation time,
- Total filtration efficiency and its components (PM cake and substrate wall) versus simulation time,
- Total oxidation rate of PM and its components by location (PM cake layer, substrate wall) and mechanism (thermal, passive) versus simulation time,
- PM cake layer thickness versus simulation time and its axial variation at different points in simulation time,
- CPF outlet, axial and transverse gas phase concentrations (expressed in ppm/%Vol. as appropriate) of C₁₂H₂₄, O₂, CO₂, H₂O, CO, NO and NO₂ versus simulation time, and
- Inlet channel, substrate wall and outlet channel temperatures at different axial locations versus simulation time as well as axial variation of the same at different points in time.

In addition, the model source code can output several intermediate variables mainly for testing/debugging purposes which can be switched on/off by changing specific input parameter values.

Code Structure and How to Run a Simulation

The model source code is written in FORTRAN programming language which consists of a main body followed by individual sub-models and functions called from within the main body as well as the sub-models which form several subroutines. All commands are included in a text-based "Fortran" file (file extension .f) and all variable declarations are included in a separate text-based "include" file (file extension .i). The current version of compiler used is Intel® Fortran Compiler 10.1.011 on the Windows 7 platform. For compilation of the model source code, the user is required to issue the following command at the command prompt:

```
\> ifort /real_size:64 /O3 codefilename.f /obj:outputfilename
```

where codefilename.f is the Fortran source code file, the option "/real_size:64" specifies all real numbers to be treated as double-precision floats and the option "/O3" is the third level Fortran code optimization specification option and the option "/obj" specifies the name of the output file(s). Accordingly, upon completion of this compilation command, there will be two files created named "outputfilename.exe" and "outputfilename.obj". Both files are needed in order

² Required if performing an optimization of input parameters using the CPF high-fidelity model source code.

³ Required if explicitly specifying PM cake layer properties

to run a simulation. In order to run the executable, the user is required to issue the following command at the command prompt:

```
\> outputfilename.exe
```

or simply:

```
\> outputfilename
```

The command window will show the progress of the simulation in percentage completed. When the simulation is complete, the output text files can be used for post-processing using a spreadsheet utility like Microsoft Excel or a graphical programming environment like Matlab.

Hardware Requirements

A Windows XP/7 PC with Intel® FORTRAN compiler 10.1.011 installed is required to compile the source code. 1GB RAM is required. 4GB RAM is preferred, although not required. Approximately 1GB of free space is required to store the output ASCII text files. A local installation of plotting software such as Microsoft Excel 2007-onwards or Matlab 2012a-onwards is recommended to post-process the data.

CPF Reduced Order Model

Model Description

The reduced-order model and state estimator are MATLAB Level 1 S-Functions. These S-Functions are used in Simulink models. The reduced-order model requires a vector of 12 signals, while the state estimator requires 13 with the same first 12 signals. The signals, in order from top to bottom, are: inlet temperature, inlet PM concentrations, inlet PM concentrations, inlet CO concentrations, inlet NO concentrations, inlet NO₂ concentrations, inlet HC concentrations, measured pressure drop, inlet O₂ concentrations, exhaust mass flow rate, the ambient temperature, and the barometric pressure. The estimator's 13th signal is used as a filtered pressure drop input.

The outputs of the model can be adjusted. By default, there are 8 outputs of the S-Function. In order from top to bottom: the substrate temperature, mass retained in the cake layer, mass retained in the wall, CO, NO, NO₂, HC, and the pressure drop. For the estimator, the outputs are: estimated substrate temperature, estimated mass retained in the cake layer, estimated mass retained in the wall, CO, NO, NO₂, HC, and estimated pressure drop.

The model is organized into 6 folders: data, documents, libraries, models, utilities, and work. The data folder is used to store all of the input data files, both loaded directly by the startup script and other auxiliary data files such as optimized parameters. The documents folder contains reference materials on the model, presentations, and figures used. The libraries folder contains all of the subfunctions used by other scripts and the models that aren't necessarily meant for the end user. The models folder contains the Simulink models, S-functions, and the reduced-order model function. The utilities folder contains scripts that can be used to ease the workflow of the end user. The work folder is a MATLAB specific folder used as a cache for JIT compilation during Simulink model acceleration.

To setup the model, the inputs need to be arranged in a specific manner. See the MAT files in '\data\', such as PO-B20-13.mat, for examples. A sample script called kiranConvert.m in utilities converts tab delimited data to the required format for the model. The MAT file needs to have separate variables, named case sensitively and filled as follows: tin, inlet temperature in Celsius; c_in, inlet PM

concentration in mg/m³; co_in, inlet concentration of CO in ppm; no_in, inlet concentration of NO; no2_in, inlet concentration of NO₂; c3h6_in, inlet concentration of HC (C₃H₆) in ppm; o2_in, O₂ in exhaust gas in mole percentage; mdota, exhaust mass flow rate in kg/s; pbaro, barometric pressure in kPa; time, simulation time in hours; pdrop, a column vector where the first column is time and the second is measured pressure drop in kPa. pm_cmp, no_cmp, no2_cmp are optional inputs used in plotting features. They are column vectors like pdrop. If these are unavailable, please uncomment the lines defining them in getInputParams, found in 'libraries\scripts'.

Once the input MAT file is created, line 10 in basicSetup (found in '.\utilities\') needs to be changed to reflect which data set should be loaded. By default, it loads the passive oxidation test 13, which uses B20 fuel type. Once this is done, running startup should load all of the data into the workspace which can be used to run the Simulink models found in '.\models\'

Key Assumptions

The key assumptions can be found in the Estimator Engine Test Report submitted to the DOE [16] and are summarized here:

- Exhaust gas is ideal
- Outlet temperature of gas is equal to the temperature within the CPF
- Total PM retained in the filter is divided into the mass in the cake layer and the mass in the wall
- Thermal and passive oxidation of the PM takes place in both the substrate wall and the cake layer
- Reaction rate constants are in Arrhenius form
- PM uniformly deposits into a single "slab" within the substrate wall and as a layer on top of the substrate wall for all cells in the filter

Intended Use

The purpose for this model and estimator is a practical proof of concept that a state estimator can improve the PM retained estimate using a pressure drop sensor signal. It has not been tested with transient FTP cycle data.

Performance Criteria

The major criteria of the reduced-order model is the capability of predicting the PM retained accurately. The estimator needs to improve the PM retained model prediction by improving the pressure drop estimate. Minor criteria include run-time to ensure the estimator could be used in real-time.

Test Results

The results are discussed in detail in reference [16]. To summarize, the model predicts the pressure drop well (<0.32 kPa RMS error) and the estimator improves the PM retained estimate by about 1 g RMS error by improving the pressure drop estimate.

Theory

The theory of the model can be found in detail in reference [16]. The model includes multiple submodels: reaction model, temperature model, PM filtration model, gaseous species model, and pressure drop model.

Formulas and Calculation methods

The formulas used can be found in [16]. The state differential equations solved using Simulink are:

$$\begin{aligned}\dot{T} &= \frac{\dot{Q}_r - \dot{m}_{exh}c_{p,exh}(T - T_{in}) - \dot{Q}_{amb}}{(m_{cake} + m_{wall})c_{p,PM} + \rho_{filter}c_{filter}V_w + \rho_{exh}c_{p,exh}V_{exh}} \\ \dot{m}_{cake} &= -(\beta RR_{cat,cake} + (1 - \beta)RR_{th,cake} + RR_{pas,cake}) + \dot{m}_d\eta_{cake} \\ \dot{m}_{wall} &= -(\beta RR_{cat,wall} + (1 - \beta)RR_{th,wall} + RR_{pas,wall}) + \dot{m}_d(1 - \eta_{cake})\eta_{wall} \\ \dot{c}_{CO} &= -U \left(\frac{c_{CO} - c_{CO,in}}{L} \right) - RR_{CO} + \frac{\Sigma(f_{CO}(\beta RR_{cat,i} + (1 - \beta)RR_{th,i}) + g_{CO}RR_{pas,i})}{\frac{\rho_{pw}}{m_i}MW_C} \\ \dot{c}_{NO} &= -U \left(\frac{c_{NO} - c_{NO,in}}{L} \right) - RR_{NO} + \frac{\Sigma(2 - g_{CO})RR_{pas,i}}{\frac{\rho_{pw}}{m_i}MW_C} \\ \dot{c}_{NO_2} &= -U \left(\frac{c_{NO_2} - c_{NO_2,in}}{L} \right) + RR_{NO} - \frac{\Sigma(2 - g_{CO})RR_{pas,i}}{\frac{\rho_{pw}}{m_i}MW_C} \\ \dot{c}_{HC} &= -U \left(\frac{c_{HC} - c_{HC,in}}{L} \right) - RR_{HC} \\ i &= cake, wall\end{aligned}$$

Hardware Requirements

The model and estimator require MATLAB and Simulink. Therefore, it has the same system requirements as MATLAB, which can be found on the MathWorks website. The genetic algorithm developed requires the global optimization toolbox. Simulink could generate code to run the simulation in real time on embedded hardware.

SELECTIVE CATALYTIC REDUCTION (SCR) MODELS

SCR High-Fidelity Model

Model Descriptions and Assumptions

The high fidelity SCR model was developed for Cu-zeolite catalyst [4, 5] based on an existing Fe-zeolite SCR model [7]. The input for the model includes space velocity (or exhaust mass flow rate), temperature, pressure and concentrations of NO, NO₂, NH₃, H₂O, CO₂ and O₂. The model simulates the temperature, concentrations of NO, NO₂, NH₃ and N₂O as well as the NH₃ storage at different axial positions of a catalyst channel. The model consists of a series of equations describing the mass transfer, heat transfer and SCR reactions. The key assumptions for the model include:

1. A single square channel of the SCR is representative of the catalyst. The channel is axially divided into finite axial element in the model
2. The exhaust gas is ideal gas and the molecular weight of air is used as an approximation of the exhaust gas
3. There are three states of gas associated with each channel element. They are gas phase, surface phase and storage phase. Mass transfer takes place between species in gas phase and surface phase. The chemical reactions take place between the species in surface phase and storage phase.

4. The NH_3 is the only species in storage phase
5. The model consists of two types of the NH_3 storage sites. Both storage sites adsorb and desorb NH_3 but only the 1st site supports other SCR reactions
6. The SCR reactions are 1st order in the reactants.
7. Heat transfer takes place between the gas flow and the substrate and between the substrate and the ambient

The intended use of model was to provide a basis for development of a reduced order SCR model and state estimator. This requires the model to be able to simulate the SCR outlet concentrations of NO , NO_2 , N_2O and NH_3 under different space velocities and temperatures.

SCR Reaction Mechanism

The reactions considered in the model are given in Table 14. There were two NH_3 storage sites with both sites supporting NH_3 adsorption and desorption reactions but only the 1st site supporting all the other SCR reactions. The 2nd site performed as a storage site which only adsorbs and desorbs NH_3 . Other reactions taking place on the 1st site included two NH_3 oxidation reactions with different selectivity to N_2 and NO respectively, two standard SCR reactions with different equivalence ratio between NH_3 and NO in the reactants, the fast SCR reaction, the slow SCR reaction, NO oxidation (the reverse of which is NO_2 decomposition), and an N_2O formation reaction.

R1 and 2 are the NH_3 adsorption and desorption reactions on the 1st storage site. R3 and 4 are the NH_3 adsorption and desorption reactions on the 2nd storage site. R5 to 12 are the SCR reactions that take place in the 1st storage site. There are two NH_3 oxidation reactions (R5 and 6) showing NH_3 oxidation selectivity to both N_2 and NO . R7 and 8 are two standard SCR reactions which have different stoichiometry NH_3/NO_x ratio. The 2nd standard SCR reaction (R8) had a higher stoichiometric NH_3 to NO_x ratio and was used to explain the NH_3 overconsumption observed from the reactor test results. R9 and 10 are the fast and slow SCR reactions respectively. R11 is the NO oxidation reaction which is considered as a reversible reaction of the NO_2 decomposition reaction. R12 is the N_2O formation from NO_2 and the stored NH_3 . The reaction rate calculation for each reaction is also given in the table. The reaction rate constant was assumed to be in Arrhenius form as shown in Equation 1.

$$k = Ae^{-\frac{E}{RT}} \quad (1)$$

Where, A and E are the pre - exponential factor and activation energy. R is the universal gas constant and T is the temperature in degree Kelvin.

Table 14 Reactions included in the model and reaction rate calculation for each reaction

No.	Description	Reaction Equation	Reaction Rate Equations	Unit of k
R1	Adsorption (Site 1)	$\text{NH}_3 + \text{S}_1 \rightarrow \text{NH}_{3,1}^*$	$R_{\text{Ads},1} = k_{\text{Ads},1} C_{\text{NH}_3,S} (1 - \theta_1) \Omega_1$	$\text{m}^3/\text{gmol}\cdot\text{s}$
R2	Desorption (site 1)	$\text{NH}_{3,1}^* \rightarrow \text{NH}_3 + \text{S}_1$	$R_{\text{Des},1} = k_{\text{Des},1} \theta_1 \Omega_1$	1/s
R3	Adsorption (Site 2)	$\text{NH}_3 + \text{S}_2 \rightarrow \text{NH}_{3,2}^*$	$R_{\text{Ads},2} = k_{\text{Ads},2} C_{\text{NH}_3,S} (1 - \theta_2) \Omega_2$	$\text{m}^3/\text{gmol}\cdot\text{s}$
R4	Desorption (Site 2)	$\text{NH}_{3,2}^* \rightarrow \text{NH}_3 + \text{S}_2$	$R_{\text{Des},2} = k_{\text{Des},2} \theta_2 \Omega_2$	1/s
R5	NH ₃ Oxidation1 (Site 1)	$4\text{NH}_{3,1}^* + 3\text{O}_2 \rightarrow 2\text{N}_2 + 6\text{H}_2\text{O}$	$R_{\text{Oxi1,NH}_3} = k_{\text{Oxi1,NH}_3} \eta_{\text{O}_2} \theta_1 \Omega_1$	1/s
R6	NH ₃ Oxidation2 (Site 1)	$4\text{NH}_{3,1}^* + 5\text{O}_2 \rightarrow 4\text{NO} + 6\text{H}_2\text{O}$	$R_{\text{Oxi2,NH}_3} = k_{\text{Oxi2,NH}_3} \eta_{\text{O}_2} \theta_1 \Omega_1$	1/s
R7	Standard SCR 1 (Site 1)	$4\text{NH}_{3,1}^* + 4\text{NO} + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$	$R_{\text{Std},1} = k_{\text{Std},1} C_{\text{NO},S} \eta_{\text{O}_2} \theta_1 \Omega_1$	$\text{m}^3/\text{gmol}\cdot\text{s}$
R8	Standard SCR 2 (Site 1)	$5\text{NH}_{3,1}^* + 3\text{NO} + 9/4\text{O}_2 \rightarrow 4\text{N}_2 + 15/2\text{H}_2\text{O}$	$R_{\text{Std},2} = k_{\text{Std},2} C_{\text{NO},S} \eta_{\text{O}_2} \theta_1 \Omega_1$	$\text{m}^3/\text{gmol}\cdot\text{s}$
R9	Fast SCR (Site 1)	$4\text{NH}_{3,1}^* + 2\text{NO} + 2\text{NO}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$	$R_{\text{Fst}} = k_{\text{Fst}} C_{\text{NO},S} C_{\text{NO}_2,S} \theta_1 \Omega_1$	$\text{m}^6/\text{gmol}^2\cdot\text{s}$
R10	Slow SCR (Site 1)	$4\text{NH}_{3,1}^* + 3\text{NO}_2 \rightarrow 7/2\text{N}_2 + 6\text{H}_2\text{O}$	$R_{\text{Slo}} = k_{\text{Slo}} C_{\text{NO}_2,S} \theta_1 \Omega_1$	$\text{m}^3/\text{gmol}\cdot\text{s}$
R11	NO Oxidation and NO ₂ decomposition (Site 1)	$2\text{NO} + \text{O}_2 \leftrightarrow 2\text{NO}_2$	$R_{\text{Oxi,NO}} = k_{\text{Oxi,NO}} (C_{\text{NO},S} \eta_{\text{O}_2}^{0.5} - C_{\text{NO}_2,S} / K_p)$	1/s
R12	N ₂ O Formation (Site 1)	$6\text{NH}_{3,1}^* + 8\text{NO}_2 \rightarrow 7\text{N}_2\text{O} + 9\text{H}_2\text{O}$	$R_{\text{N}_2\text{O}} = k_{\text{N}_2\text{O}} C_{\text{NO}_2,S} \theta_1 \Omega_1$	$\text{m}^3/\text{gmol}\cdot\text{s}$

Mass Transfer Equations

Mass transfer between the gas phase and surface phase is included in the model. The mass balance equations for the gas phase and surface phase is given in Equations ((2) and ((3). Equation ((2) describes the mass balance for the gas phase, and Equation (3 describes the mass balance for the surface phase.

$$\varepsilon \frac{\partial C_{g,i}^n}{\partial t} = -u \frac{\partial C_{g,i}^n}{\partial x} - \beta_i A_g (C_{g,i}^n - C_{s,i}^n) \quad (2)$$

$$(1 - \varepsilon) \frac{\partial C_{s,i}^n}{\partial t} = \beta_i A_g (C_{g,i}^n - C_{s,i}^n) - \sum_j N_{i,j} R_j \quad (3)$$

$i = \text{NO}, \text{NO}_2, \text{NH}_3,$

$j = \text{ads, des, fast SCR, standard SCR, slow SCR, etc.}$

Where, ε is the void fraction of the catalyst, u is the speed of the exhaust flow in m/s, A_g is the geometric surface area and β_i is the mass transfer coefficient shown in Equation ((4). C_g and C_s are the gas phase and surface phase gaseous concentrations in gmol/m^3 .

$$\beta_i = Sh_i D_{m,i} / d_h \quad (4)$$

Where, d_h is the hydraulic diameter of the channel and $D_{m,i}$ is the molecular diffusivity of the i th species. Sh_i is the Sherwood number of the i th species and is shown in Equation (5).

$$Sh_i = 0.766 \times (d/L \times Re \times Sc)^{0.483} \quad (5)$$

Where, d and L are the diameter and length of the channel. Re and Sc are the Reynolds number and Schmidt number. A multiplier factor of 4 was applied to the Sherwood number calculation when calibrating the model to better simulate the space velocity effects on the SCR performance.

Heat Transfer Equations

In order to predict the axial temperature gradients in the SCR as well as the outlet temperatures under transient conditions, the SCR model also includes heat transfer between the exhaust flow and the substrate as well as the heat transfer to the ambient. This is valuable for improving the model prediction performance under transient conditions by considering the axial temperature gradients in the model. The heat transfer equations for the SCR are given in Equations ((6) and ((7). Equation ((6) is the gas phase energy balance equation and Equation ((7) is the surface phase energy balance equation. The heat transfer to the ambient is through convection heat transfer from the outer surface of the channel with the heat transfer coefficient h_a and an ambient temperature T_a . The heat release due to the SCR reactions is negligible and was set to zero in this model.

$$\rho C_v \frac{dT_g}{dt} = -\rho u \frac{dT_g}{dx} - h_g \frac{4}{a_w} (T_g - T_w) \quad (6)$$

$$\rho_w C_w \frac{dT_w}{dt} = h_g \frac{4a_w}{a_p^2 - a_w^2} (T_g - T_w) - h_a \frac{4a_p}{a_p^2 - a_w^2} (T_w - T_a) + \sum_i \frac{-\Delta H_i R_i}{MW_i} \quad (7)$$

In Equations ((6) and ((7), ρ and ρ_w refer to the density of the exhaust gas and the substrate wall. T_w , T_g , and T_a refer to the temperatures of the wall, gas, and the ambient. h_g and h_a refer to the heat transfer coefficients. a_p and a_w are the width of the monolith element and the channel.

The model solves for the surface and gas phase concentrations of NO, NO₂, NH₃ and N₂O, as well as the NH₃ storage at different axial positions by integrating the model equations using the semi-implicit, variable time-step integrator ode15s in MATLAB [7].

Model Performance

The high fidelity SCR model was calibrated to both SCR reactor data collected from a reactor setup at ORNL and engine data collected from MTU engine test cell. The model as well as the detailed calibration procedures was introduced in references [4] and [5]. The NH₃ storage capacities for the two storage sites and the kinetic parameters for the SCR reactions were determined separately for the reactor and engine data. The performance of the calibrated model was validated by comparing the simulation results to the experimental data. The comparison results showed that the model is able to simulate the SCR outlet concentrations of NO, NO₂, N₂O and NH₃ under difference temperatures and space velocities. The ability of the model to predict the NH₃ storage was discussed in reference [8] as compared to the Spaci-IR reactor data.

The high fidelity SCR model calibrated to the engine data accounts for the more complex testing environments (complex urea decomposition process, NH₃ maldistribution at the SCR inlet, .etc) and served as a basis for developing the SCR reduced order model estimator [10].

Files needed to run the model

The SCR model requires 15 .m files and 2 .mat files to run successfully. The files required along with a brief description are as below:

1. SCROPT.m: this file is the main function of the model; it calls a series of functions to simulate the SCR chemical mechanism. User can change catalyst dimensions, overwrite kinetic parameters, change axial element number in the model, and choose to run with reactor model parameters or engine model parameters in this function.
2. Globalsandconstants.m: this file defines the constants and variables that are used throughout the model
3. InitDataStructure.m: this file initializes the big structure used to contain all the data
4. ErrorCheck.m: this file checks for some basic errors related to basic setup before simulating, print error messages if errors occur
5. SetDataStructureValues.m: this function is used to import experimental data of both SCR inlet and outlet from data files and Setup optimization parameters, etc. The heater transfer functions are called by this function to calculate the axial temperature gradients in the catalyst.
6. ThermalSimV3_withCv_ddt.m: this function simulates the heater transfer between bulk gas flow, substrate and the ambient. It calculates the temperature on each axial model element. This is meaningful for transient test data where exhaust gas temperature is changing. For steady state test, it is okay to neglect the temperature gradients from inlet to outlet.
7. run_nonlinear_scr2_ic.m: this file is used to prepare the initial conditions and parameters for the model
8. run_nonlinear_scr2.m: this file calls the model functions to run the model, convert the results from the model into the same form as the experimental data, and calculate the cost function (error between simulation and experiments)
9. nonlinear_scr3_inhib.m: this file calls the governing ODE equations to simulate the SCR reactions
10. calcrxnratecoeffs.m: this file contains the function for calculating the reaction rate constant for each SCR reaction included
11. calcbetas.m: this file contains the function for calculating the mass transfer coefficient for each major gas species
12. calculate_cij.m: this file contains the function for calculating the coefficients used to determine the mass transfer coefficients of all the species used in the chemical kinetics model
13. calcrxnrates.m: this file calculates the reaction rate for each SCR reaction included
14. superplot2_all.m: this function plots a time history of SCR outlet species including NO, NO₂, NH₃, N₂O compared to the experimentally measured SCR outlet concentrations
15. print_opt_params.m: this file prints the parameter optimization results in command window after finalizing the optimization
16. SV60kT300C_bpf.mat: this is the data file from experiments, it defines the SCR inlet conditions including temperature, pressure, space velocity, and gaseous concentrations of NO, NO₂, and NH₃. The parameter of each column of the file is listed as below,

Column 1	Time in second (the input data has to be 1Hz for the model to function)
Column 2 - 7	SCR inlet concentrations of NH ₃ , N ₂ O, NO, NO ₂ , H ₂ O, and CO ₂
Column 8 – 9	SCR inlet NO _x and O ₂ concentrations measured by NO _x sensor (not used in the model)
Column 10	SCR inlet temperature in °C
Column 11	SCR space velocity in 1/hr
Column 12	Pressure at SCR inlet in Pa
Column 13	SCR outlet temperature in °C

17. SV60kT300Cf.mat: this is the data file recording the SCR outlet conditions during a SCR test, the data is used to compared with the model simulation results. Major columns of the data file are listed as below,

Column 1	Time in second
Column 3 -6	SCR outlet concentrations of NH ₃ , N ₂ O, NO, and NO ₂

18. ModelParameters.mat: this file contains the model parameters for both SCR reactor and engine model. The model parameters include NH₃ storage capacity on each of the model sites as well as the pre-exponential and activation energy for the SCR reactions.

Preparation to Run the Model

In order to run the model with a different SCR catalyst and new test data sets, some parameters and data files need to be setup accordingly

1. Generate SCR inlet data files which contains SCR inlet gaseous concentrations and test conditions,
2. Prepare SCR outlet data file which contains measured SCR outlet gaseous concentrations, both data files are imported into the model by the functions in 'SetDataStructureValues.m'. The data files used for this model should be in a time interval of 1 second
3. Setup SCR catalyst dimensions, chose to run with reactor or engine model parameters, define model input name in 'SCROPT.m'
4. User can also chose to run the model with different axial element numbers.

Running a Simulation

Set Matlab 'current folder' to the folder which contains the scripts. Then open script named 'SCROPT.m' in Matlab, run this script to start the simulation. Simulation of outlet concentrations will be automatically plotted after simulation is complete. Other simulation results are accessible in Matlab Workspace.

Hardware Requirements

Operating Systems

Windows XP Service Pack 3
Windows XP x64 Edition Service Pack 2
Windows Server 2003 R2 Service Pack 2
Windows Vista Service Pack 2
Windows Server 2008 Service Pack 2 or R2
Windows 7

Processors

Any Intel or AMD x86 processor supporting SSE2 instruction set

Disk Space

1 GB for MATLAB only,

3–4 GB for a typical installation

RAM

1024 MB (At least 2048 MB recommended)

SCR Reduced Order Model Estimator

Model Description

An Extended Kalman Filter (EKF) based state estimation strategy for the Selective Catalytic Reduction (SCR) was developed using a reduced order SCR model. The reduced order SCR model was validated with engine experimental data. The SCR estimator uses the exhaust mass flow rate, NH_3 , NO, NO_2 and O_2 concentrations from the engine maps along with the temperature and the NO and NO_2 concentrations upstream (NO_x sensor upstream or NO and NO_2 out of the CPF from a model) of the SCR and NH_3 and/or NO_x sensor downstream of the SCR to estimate the states of the SCR.

The goal of the reduced order SCR estimator was to simulate the SCR outlet concentrations of NH_3 , NO, NO_2 concentrations and NH_3 storage. The SCR reduced order estimator was simulated using the surrogate FTP test data.

Assumptions in the SCR Model

The important assumptions made in the development of the reduced order model are:

1. The reactions are instantaneous $\frac{\partial c_g}{\partial t} = \frac{\partial c_s}{\partial t} = 0$
2. The surface phase and gas phase concentrations are identical and can be assumed to be equal, $C = C_g = C_s$.
3. The surface phase and gas phase temperatures are identical and can be assumed to be equal, $T = T_g = T_s$.

Reactions Considered in the Model

The reduced order model and estimator uses the same reactions as the SCR high fidelity model [5]. The NH_3 storage is modeled using two storage sites; site 1 participates in the NH_3 storage and NO_x reduction whereas site 2 participates only in the storage of NH_3 through adsorption and desorption. The reactions considered in the EKF's SCR reduced order model are shown in Equations (1) to (11). The reduction of NO_x takes place through three main reaction mechanisms: two standard reactions (Eq (6) and (7)), the fast reaction (Eq. (8)) and the slow reaction (Eq. (9)).

Adsorption:

Desorption:

NH₃ Oxidation reaction:

Standard SCR1 reaction:

Standard SCR2 reaction:

Fast SCR reaction:

Slow SCR reaction:

NO to NO₂ oxidation:

N₂O formation:

SCR Mass and Energy Balance

The mass and the energy balance equations describing the model are given in Equations (12) and (13).

$$\epsilon u \frac{\partial C_i}{\partial x} = -R_i \quad (12)$$

$$i = CO, NO, NO_2, C_3H_6 \& O_2$$

$$(\rho_s C_s + \rho C_v) \frac{dT}{dt} = -\rho u C_p \frac{dT}{dx} - \frac{1}{1-\epsilon} \sum_{i=CO, NO, C_3H_6} \frac{-\Delta h_i R_i}{MW_i} \quad (13)$$

where, ρ_s and $c_{p,s}$ are the density and specific heats of the substrate, ρ is the density of the exhaust gas, c_p and c_v are specific heats of the exhaust gas, Δh_i is the enthalpy of the CO, NO and C₃H₆ oxidation reactions and MW_i is the molecular weight of i^{th} species .

The NH₃ balance equations for the storage site 1 and site 2 are shown in Equations (14) and (15).

$$\Omega_1 \dot{\theta}_1 = R_{ads1} - R_{desp1} - 4R_{NH3oxi} - 4R_{std1} - 4R_{fst} - 4R_{slow} - 5R_{std2} - 6R_{N2O} \quad (14)$$

$$\Omega_2 \dot{\theta}_2 = R_{ads2} - R_{desp2} \quad (15)$$

where, θ_i are NH_3 storage fractions and Ω_i are storage capacities. The quantities $R_{\text{ads}1}$, $R_{\text{ads}2}$, $R_{\text{des}1}$ and $R_{\text{des}2}$ are the adsorption and desorption rates. $R_{\text{NH}_3\text{oxi}}$, R_{std} , R_{fst} and R_{slow} are the reaction rates for NH_3 oxidation, standard SCR, fast SCR and slow SCR reactions.

Reaction Rate Calculations

The rate equations for all the reactions in the SCR are shown in Equations (16) to (36).

Adsorption:

$$R_{\text{ads},1} = k_{\text{ads},1} c_{\text{NH}_3} (1 - \theta_1) \Omega_1 \quad (16)$$

$$R_{\text{ads},2} = k_{\text{ads},2} c_{\text{NH}_3} (1 - \theta_2) \Omega_2 \quad (17)$$

Desorption:

$$R_{\text{des},1} = k_{\text{des},1} \theta_1 \Omega_1 \quad (18)$$

$$R_{\text{des},2} = k_{\text{des},2} \theta_2 \Omega_2 \quad (19)$$

NH_3 Oxidation:

$$R_{\text{NH}_3 \text{ oxi}} = k_{\text{NH}_3 \text{ oxi}} Y_{\text{O}_2} \theta_1 \Omega_1 \quad (30)$$

Standard SCR 1 reaction:

$$R_{\text{Std}1} = k_{\text{Std}1} c_{\text{NO}} Y_{\text{O}_2} \theta_1 \Omega_1 \quad (31)$$

Standard SCR 2 reaction:

$$R_{\text{Std}2} = k_{\text{Std}2} c_{\text{NO}} Y_{\text{O}_2} \theta_1 \Omega_1 \quad (32)$$

Fast SCR reaction:

$$R_{\text{Fst}} = k_{\text{Fst}} c_{\text{NO}} c_{\text{NO}_2} \theta_1 \Omega_1 \quad (33)$$

Slow SCR reaction:

$$R_{\text{Slow}} = k_{\text{Slow}} c_{\text{NO}_2} \theta_1 \Omega_1 \quad (34)$$

NO Oxidation:

$$R_{\text{NO}} = k_{\text{NO}} \left(c_{\text{NO}} c_{\text{O}_2}^{0.5} - \frac{c_{\text{NO}_2}}{K_p} \right) \quad (35)$$

N_2O Formation

$$R_{\text{N}_2\text{O}} = k_{\text{N}_2\text{O}} c_{\text{NO}_2} \theta_1 \Omega_1 \quad (36)$$

The reaction rate constants, k_i , are of the Arrhenius form and are defined as:

$$K_i = A_i e^{-E_{a,i}/RT} \text{ where } i = \text{ads1, desp1, ... , Desorption, ... N}_2\text{O formation} \quad (37)$$

Files Needed to Run the Model

The SCR estimator simulink model requires 12 files to be present in the current folder to run successfully. The files required along with a brief description are as below:

23. Simsetup.m: This file sets up the user input constants and inputs to the model. The geometric properties of the DOC, the reaction rate constants for the reactions, the inhibition constants for the reaction inhibition and also the total simulation time and time step for integration is specified in this file.
24. SCR_est_const.m: This file contains all the constants used in the simulation of the DOC EKF estimator. The constants include the number of axial elements.
25. SCR_estimator_discrete.m: This file contains the sfunction which simulates the EKF estimator.
26. estimator_scr_discrete.mdl: This is the simulink model file to simulate the EKF estimator. Figure 1 shows a screen capture of the simulink estimator model. The figure highlights the Inputs, estimator and output blocks of the simulink model. The simulation results are stored in an array with name "Estimated_States". For a 13 axial element model the values in the array represent as follows:

- 4) Column 1- Simulation time
- 5) Column 2, 9... – NH_3 concentration at the first element.
- 6) Column 3, 10 ... – NO concentration at the first element.
- 7) Column 4, 11 ...– NO_2 concentration at the first element.
- 8) Column 5, 12 ... – N_2O concentration at the first element.
- 9) Column 6, 13 ... – NH_3 Storage for site 1.
- 10) Column 7, 14 ... – NH_3 Storage for site 2.
- 11) Column 8, 15 ...– Temperature at the first element.

Figure 1: Screen capture of the model with the inputs and outputs to the estimator.

27. Estimator_Inputs.mat: This file contains sample inputs to run the estimator. This file executed from the setup file.
28. Setup_Inputs_SCR.m: The file creates the structure 'scr' and copies the inlet concentrations, temperature, mass flow rate and pressure in the format that can be used for the estimator.
29. Plot_SCR_Results.m: This file is used to generate plots to compare the simulation results with the estimated results.
30. DispStatus.m: This is a Matlab® function that prints the status of the simulation in the Matlab® command prompt.
31. Define_Setup_Constants.m: This file contains all the constants used in setting up the inputs.
32. Clear_Setup_Constants.m: This is a Matlab® script that clears the variables that are not used.
33. Sample_SCR_Outputs.mat: This file contains sample results from the estimator.
34. SensorCoeffs.m: This file contains the coefficients for the NO_x and NH₃ sensor models.

Running a Simulation

1. Specify inputs in "Simsetup.m" and run the Matlab script to setup the inputs.
2. Line 26 of the Simsetup.m contains command to load the sample inputs to the Matlab® work space. Hence executing "Simsetup.m" also sets up the transient inputs.
3. Open the "estimator_scr_discrete.mdl" and from the simulation drop down menu select the start.

Figure 2: Screen capture of the model highlighting the menu to start the simulation.

4. After the completion of the simulation open the file “Plot_SCR_Results.m” and run the script to generate the plots. Each subplot show SCR inlet concentration and comparison of the estimated SCR outlet Temperature, NO, NO₂ and NH₃ concentrations.

Model Performance

The model used for EKF development was calibrated to transient engine data using a 2010 Cummins ISB engine with a production aftertreatment system consisting of a DOC, CPF and SCR. The EKF was then exercised for three different SCR outlet, sensor configurations: NO_x only, NH₃ only and both NO_x and NH₃. The EKF-estimated outlet NO, NO₂, and NH₃ concentrations were compared to measured experimental data using a mass spectrometer. The results from the simulation are described in reference [10].

Hardware Requirements

Operating Systems: Windows XP Service Pack 3, Windows XP x64 Edition Service Pack 2, Windows Server 2003 R2 Service Pack 2, Windows Vista Service Pack 2, Windows Server 2008 Service Pack 2 or R2, Windows 7.

Processors: Any Intel or AMD x86 processor supporting SSE2 instruction set

Disk Space: 1 GB for MATLAB only, 3–4 GB for a typical installation

RAM: 1024 MB (At least 2048 MB recommended)

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