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DYNAMIC MODEL BASED STATE ESTIMATION IN A HEAVY DUTY DIESEL AFTERTREATMENT SYSTEM FOR ONBOARD DIAGNOSTICS AND CONTROLS

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Michigan Technological University

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DYNAMIC MODEL BASED STATE ESTIMATION IN A HEAVY DUTY DIESEL AFTERTREATMENT SYSTEM FOR ONBOARD DIAGNOSTICS AND CONTROLS

By
Harsha S. Surenahalli

A DISSERTATION
Submitted in partial fulfillment of the requirements for the degree of

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LIST OF SYMBOLS

**Acronyms:**

DOC - Diesel Oxidation Catalyst
CPF - Catalyzed Particulate Filter
SCR - Selective Catalytic Reduction
OBD - Onboard Diagnostics
EKF - Extended Kalman Filter
SI - Spark Ignition
EPA - Environmental Protection Agency
PM - Particulate Matter
NMHC - Non Methane Hydrocarbons
ECU - Engine Control Unit

**Variables:**

ε - Void fraction of the catalyst

$C_g$ - Gaseous concentration of the species $\left( \frac{\text{mol}}{\text{m}^3} \right)$

$C_s$ - Surface concentration of the species $\left( \frac{\text{mol}}{\text{m}^2} \right)$

$C$ - Bulk concentration of the species $\left( \frac{\text{mol}}{\text{m}^3} \right)$
$A_g$ - Geometric surface area ($\frac{m^2}{m^3}$)

$\beta$ - Mass transfer co-efficient

$R_i$ - Reaction rates ($\frac{mol}{m^3.s}$)

$T_g$ - Gaseous temperature (K)

$T_s$ - Surface temperature (K)

$T$ - Bulk temperature (K)

$\rho$ - Density of exhaust gas ($\frac{kg}{m^3}$)

$C_v$ - Specific heat of exhaust at constant volume ($\frac{J}{kg.K}$)

$C_p$ - Specific heat of exhaust at constant pressure ($\frac{J}{kg.K}$)

$u$ - Velocity of exhaust gas ($\frac{m}{s}$)

$h_g$ - Heat transfer coefficient between gas and surface phase($\frac{J}{m^2.s.K}$)

$h_a$ - Heat transfer coefficient to ambient($\frac{J}{m^2.s.K}$)

$\Delta h$ - Enthalpy of reaction ($\frac{J}{mol}$)

$MW$ - Molecular weight ($\frac{mol}{g}$)

$\rho_s$ - Density of substrate ($\frac{kg}{m^3}$)

$C_{p,s}$ - Specific heat capacity of the substrate ($\frac{J}{kg.K}$)

$G$ - Inhibition factors

$K_P$ - Equilibrium constant

$k$ - Reaction rate constants

$A$ - Pre exponential factor

$E_a$ - Activation energy

$P$ - Exhaust gas pressure(kpa)

$\Delta G$ - Gibbs free energy

$R$ - Universal gas constant

$A_a$ - Adsorption constants
\( \Delta H_a \) - Adsorption heats
\( \theta \) - \( NH_3 \) Storage fraction
\( \Omega \) - Storage capacity \( \left( \frac{\text{mol}}{m^3} \right) \)

**Vectors:**

\( \vec{x}_k \) - State vector
\( \vec{u}_k \) - Input vector
\( \vec{y}_k \) - Output vector
\( \vec{v}_k \) - Observation noise vector
\( \vec{w}_k \) - Process noise vector
\( \vec{P}_k \) - Estimation error covariance
\( \vec{K}_k \) - Optimal Kalman Gain
Abstract

Estimating un-measurable states is an important component for onboard diagnostics (OBD) and control strategy development in diesel exhaust aftertreatment systems. This research focuses on the development of an Extended Kalman Filter (EKF) based state estimator for two of the main components in a diesel engine aftertreatment system: the Diesel Oxidation Catalyst (DOC) and the Selective Catalytic Reduction (SCR) catalyst. One of the key areas of interest is the performance of these estimators when the catalyzed particulate filter (CPF) is being actively regenerated.

In this study, model reduction techniques were developed and used to develop reduced order models from the 1D models used to simulate the DOC and SCR. As a result of order reduction, the number of states in the estimator is reduced from 12 to 1 per element for the DOC and 12 to 2 per element for the SCR. The reduced order models were simulated on the experimental data and compared to the high fidelity model and the experimental data. The results show that the effect of eliminating the heat transfer and mass transfer coefficients are not significant on the performance of the reduced order models. This is shown by an insignificant change in the kinetic parameters between the reduced order and 1D model for simulating the experimental data.

An EKF based estimator to estimate the internal states of the DOC and SCR was developed. The DOC and SCR estimators were simulated on the experimental data to show that the estimator provides improved estimation of states compared to a reduced order model. The results showed that using the temperature measurement at the DOC outlet improved the estimates of the $CO$, $NO$, $NO_2$ and $HC$ concentrations from the DOC. The SCR estimator was used to evaluate the effect of $NH_3$ and $NO_X$ sensors on state estimation.
quality. Three sensor combinations of $NO_X$ sensor only, $NH_3$ sensor only and both $NO_X$ and $NH_3$ sensors were evaluated. The $NO_X$ only configuration had the worst performance, the $NH_3$ sensor only configuration was in the middle and both the $NO_X$ and $NH_3$ sensor combination provided the best performance.
1. INTRODUCTION

Diesel engines are known for their high thermal efficiency and high torque characteristics compared to spark-ignition(SI) engines. The high torque characteristics of the diesel engine make them ideal for heavy load applications. Hence, diesel engines have been used to power most of the heavy duty trucks around the world. Diesel engines have also been used in light duty trucks and cars due to their low fuel consumption compared to SI engines. Similar to the SI engine, a diesel engine also produces undesirable green house gases and particle pollutants. Most of the countries around the world have some kind of regulations to regulate these emissions. In the Unites States, the emission regulations are set by the Environmental Protection Agency (EPA). The regulated emissions for heavy duty diesel engines are carbon monoxide ($CO$), nitrogen oxides ($NO_x$), unburnt hydrocarbons (HC) and particulate matter (PM). Table 1.1 shows the EPA emission standards from 1988 to 2010. It can be seen that the limits for all the regulated emissions have been progressively lowered from 1988 to 2010.
Table 1.1
EPA emission standards for heavy duty diesel engines [2]

<table>
<thead>
<tr>
<th>Year</th>
<th>HC</th>
<th>CO</th>
<th>NOx</th>
<th>PM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1988</td>
<td>1.30</td>
<td>15.50</td>
<td>10.70</td>
<td>0.60</td>
</tr>
<tr>
<td>1990</td>
<td>1.30</td>
<td>15.50</td>
<td>6.00</td>
<td>0.60</td>
</tr>
<tr>
<td>1991</td>
<td>1.30</td>
<td>15.50</td>
<td>5.00</td>
<td>0.25</td>
</tr>
<tr>
<td>1994</td>
<td>1.30</td>
<td>15.50</td>
<td>5.00</td>
<td>0.10</td>
</tr>
<tr>
<td>1998</td>
<td>1.30</td>
<td>15.50</td>
<td>4.00</td>
<td>0.10</td>
</tr>
<tr>
<td>2002</td>
<td>0.50</td>
<td>15.50</td>
<td>2.40</td>
<td>0.10</td>
</tr>
<tr>
<td>2007</td>
<td>0.14</td>
<td>15.50</td>
<td>0.20</td>
<td>0.01</td>
</tr>
</tbody>
</table>

To meet the 2010 EPA $NO_X$ and PM emission standards, a typical 2010 aftertreatment system for heavy duty diesel engines consists of a DOC, CPF and SCR as shown in Figure 1.1. The figure also shows a Ammonia Oxidation Catalyst (AMOX) downstream of the SCR. The AMOX is used to oxidize the ammonia slip from the SCR. The figure also shows a $NO_X$ sensor upstream of the DOC to measure inlet $NO_X$ to the aftertreatment system and a $NO_X$ sensor downstream of the AMOX to measure the $NO_X$ out of the SCR. The DP sensor is used to measure pressure drop across the CPF and temperature sensors are used to measure temperatures at different locations in the aftertreatment system. Likely, between 2013-2016, the aftertreatment system will still contain these three components with higher SCR $NO_X$ conversion efficiencies so that the fuel consumption of the engine can be reduced to meet the proposed 2014-2018 fuel consumption regulations [3]. The DOC oxidizes carbon monoxide ($CO$) and hydrocarbons in the exhaust to $CO_2$ and $H_2O$ and oxidizes $NO$ to $NO_2$. The CPF filters and oxidizes the PM in the exhaust and at the same time oxidizes the hydrocarbons to $CO_2$ and $H_2O$ and oxidizes $NO$ to $NO_2$ and consumes $NO_2$ in oxidizing the PM. During normal engine operation ($T < 400^0C$), the retained PM in the CPF is oxidized using $NO_2$ [5] and the exhaust temperature. Active regeneration is
performed periodically by injecting the diesel fuel into the exhaust to oxidize the PM using $O_2$ at higher temperatures ($T > 500^\circ C$) [6]. The SCR catalyst reduces $NO$ and $NO_2$ in the exhaust to $N_2$ and water. This is achieved by injecting urea upstream of the SCR catalyst, which thermally decomposes into $NH_3$ and reacts with $NO$ and $NO_2$ on the active sites of the catalyst. The DOC either directly or indirectly affects the performance of the CPF and SCR and the CPF affects the SCR performance by the $NO_2/NO_X$ ratio out of the filter.

The onboard diagnostic (OBD) systems that monitors the emission control system has

![Figure 1.1. Schematic of a typical 2010 heavy-duty diesel aftertreatment system](image)

been implemented on SI engines since 1991 and more stringent OBD standards were implemented in 1996. All light duty diesel engines have been required to meet OBD standards since 2004. From 2010 onwards, the OBD standards were implemented for heavy-duty diesel engines. By 2013 all the diesel engines manufactured are required to meet the OBD standards. Table 1.2 shows the OBD monitoring requirements for heavy duty diesel aftertreatment systems. The table shows specifications related to the performance and failure related monitoring systems for the DOC, CPF and SCR aftertreatment system components. Along with the performance related monitoring, the table also indicates the monitoring of catalyst aging. With regards to the sensors, the rule also specifies the monitoring of the
Table 1.2
Monitoring requirements of EPA and California OBD systems[3]

<table>
<thead>
<tr>
<th>System/Component</th>
<th>Parameter Requiring Monitoring</th>
</tr>
</thead>
</table>
| NMHC(Non Methane Hydrocarbons) catalyst | Conversion efficiency  
SCR NOx catalyst | SCR reductant: 
- delivery performance, 
- tank level, quality, and 
- injection feedback control  
Catalyst aging |
| NOx adsorber | NOx adsorber capability  
Desorption function fuel delivery  
Feedback control |
| DPF Filtering performance | Frequent regeneration  
NMHC conversion  
Incomplete regeneration  
Missing substrate  
Active regeneration fuel delivery  
Feedback control |
| Exhaust gas sensors | For air-fuel ratio and NOx sensors:  
- performance,  
- circuit faults,  
- feedback, and  
- monitoring capability  
Other exhaust gas sensors  
Sensor heater function  
Sensor heater circuit faults |

 failure of the sensors and circuits and any auxiliary devices associated with the sensors such as heaters.

Table 1.3 shows the thresholds for detecting the failure of these systems. The thresholds are specified either in terms of the multiples of the emission standards (indicated with a ’x’
Table 1.3
EPA thresholds for 2010 and later heavy-duty diesel engines[^4]

<table>
<thead>
<tr>
<th>Monitor</th>
<th>Model Year</th>
<th>Diesel Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>NMHC</td>
</tr>
<tr>
<td>$NO_X$ catalyst system</td>
<td>2010-2012</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2013 &amp; later</td>
<td>-</td>
</tr>
<tr>
<td>DPF system</td>
<td>2010-2012</td>
<td>2.5x</td>
</tr>
<tr>
<td></td>
<td>2013 &amp; later</td>
<td>2x</td>
</tr>
<tr>
<td>$NO_X$ sensors</td>
<td>2010-2012</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2013 &amp; later</td>
<td>-</td>
</tr>
<tr>
<td>Other monitors with emissions</td>
<td>2010-2012</td>
<td>2.5x</td>
</tr>
<tr>
<td>thresholds</td>
<td>2013 &amp; later</td>
<td>2x</td>
</tr>
</tbody>
</table>

after a number in the table) or in terms of absolute value of the species (indicated by ‘+’ in front of a number). The onboard diagnostic strategies are required to detect and inform the driver when any of the regulated emissions exceed the limits indicated in Table 1.3.

The DOC, CPF and SCR contain un-measurable states (such as PM retained in the CPF and $NH_3$ storage in the SCR) that need to be estimated for diesel fuel injection for active regeneration and urea injection control systems on-board the vehicle. To optimize the performance of the aftertreatment system, it is necessary to estimate the internal states in real time and use them for control system and onboard diagnostics (OBD) strategy implementation. In order to meet the 2014-18 fuel consumption standards, the use of fuel for active regeneration must be minimized and the fuel injection control strategy must be optimized. To achieve this, it is important to know the hydrocarbon and temperature states in the DOC and to optimize the urea injection so as to minimize the urea use and maximize the $NO_X$ reduction.

One of the important aspects of state estimation is to have a reduced order model of
the dynamic system. A reduced order DOC and SCR model and corresponding Extended Kalman Filter (EKF) state estimation strategy is discussed relative to the research that has been conducted for this thesis.

The literature review of section 3 shows that models and sensors are valuable tools to assist in estimating states that cannot be measured. The models provide additional information based on the inputs to the system. The limitations of using the models to estimate states is that the error between the estimated and true states is high if the model is not an accurate representation of the system. With an optimal state estimator, even if the system is not well known, the estimation error is minimized. Hence, the main objective of this research is to create state estimation strategies for the DOC and SCR heavy duty diesel aftertreatment components. The state estimation strategies include development of reduced order models, evaluation of state estimation strategies and evaluation of estimation quality based on several different sensor combinations. The general objectives can be divided into reduced order model development and state estimator development.

1. The objectives for the reduced order models: (a) Develop reduced order model for the DOC and SCR. (b) Validate the performance of the reduced order models with the experimental data and the high-fidelity models.

2. The objectives for the state estimation: (a) Develop Kalman Filter based state estimators to estimate states in the DOC and SCR. (b) Validate the performance of the estimators with the experimental data. (c) Evaluate the several different sensor combinations needed to estimate the states in both the DOC and SCR.
2. Background and Literature Review

This section provides a review of the significant relevant literature with respect to the reduced order model development and state estimation strategy development. There are four subsections:

1. Onboard Diagnostics and Controls.

2. State Estimations Strategies and Onboard Diagnostics - describes the state estimation strategies and the onboard diagnostics.

3. Reduced Order Models and Controls - describes the reduced order models and controls

2.1 Onboard Diagnostics (OBD) and Controls

Onboard Diagnostics or OBD are tools which provide the ability to monitor and detect the status of different subsystems in a vehicle. On-Board-Diagnostics concepts assist in trouble shooting the problems in the vehicle subsystem and help manufacturers monitor the state of the different components and also detect any failures. A failure in the aftertreatment
system would result in the vehicle exceeding the legal emission limits. OBD strategies can detect any critical failures and provide the user the limp home capability to prevent any serious damage and reduce the cost of repairs[7].

Any physical failure of aftertreatment devices can be detected with the sensors already present in the production system. To detect any performance related failures, models could be used to check the performance of the actual device with the simulated values. To do this, the models need to be very accurate and computationally efficient. For an SCR an efficient and robust control system would be useful in controlling the urea injection and the performance of the SCR. There are two kind of control systems that have been reported in the literature - open loop and closed loop control systems.

**Open Loop Control Systems:** The heavy duty diesel industry have used open loop control systems to control the urea injection into the SCR. The open loop control strategies provide good $NO_X$ conversion performance and are very stable and easy to implement. The open loop control strategies inject urea based on the $NO_X$ estimate at the SCR inlet. The control laws determine the $NO_2 / NO_X$ ratios from the engine maps for a particular engine speed and load and then estimate the amount of urea injection. This often results in the over injection of urea and results in higher $NH_3$ slip at the SCR outlet. To overcome this problem, manufacturers have used a Ammonia Oxidation Catalyst (AMOX), which oxidizes the $NH_3$ in the exhaust to $N_2$ and $H_2O$. This increases the total cost of the aftertreatment system.

**Closed Loop Control Systems:** Another solution is to use a closed loop control system. The closed loop control system would minimize the ammonia slip at the SCR outlet and it is also possible to retain the high $NO_X$ conversion efficiency. A closed loop control on an SCR is challenging due to the slow dynamics of the SCR and the response of the urea
injection system. Several researchers have proposed \( NO_X \) and \( NH_3 \) sensor based control strategies. These control strategies use the \( NH_3 \) or \( NO_X \) sensors located at the SCR outlet to determine the amount of urea injection. The objective of these strategies have been to maintain the \( NH_3 \) storage in the SCR at a optimum level. To achieve this, the control system use models to estimate the \( NH_3 \) storage along with a linearized first order model for the SCR to determine the urea injection quantity. The first order models are developed from the CFD models and are an approximation of the SCR. Since the SCR is a non linear system, all the controls oriented models use variable parameters in the transfer function of the system. The parameters in the first order transfer function vary as a function of SCR inlet temperature and mass flow rates. To estimate the \( NH_3 \) storage, \( NH_3 \) balance models are used. Several researchers have compared the performance of different control strategies. Some of the important literature are reviewed in this section.

The researchers in reference [8] compared the performance of a closed loop feedforward and an open loop control system for urea injection. The performance of the controllers were evaluated at steady state conditions and the results showed that closed loop control reduced the steady state error to 5% which was not possible with an open loop controller. The evaluation of the control strategies on transient conditions showed that closed loop controller improves the transient SCR \( NO_X \) reduction performance. The authors concluded that the closed loop control is a must to meet the EPA 2010 emission standards.

The goal of the study in reference [9] was to evaluate the modeling approaches and to develop models which can be used for control system development. The paper infers that simplistic models might lack physical representations and such models will have limited applications. The paper states that the kinetics parameters of the catalyst should be included in the models in some way to enable the control systems to account for the aging
related performance changes. The authors concluded that more complex models and observers would be useful to develop advanced control strategies and could help in increasing the conversion efficiencies of the aftertreatment system.

The goal of the research work in reference [10] was to develop a control oriented model for the SCR and develop a feedforward control system for urea injection. The model developed consisted of ODE’s for the gas and surface phase concentrations and PDE’s for temperature and $NH_3$ storage on a single storage site. The model was then used to develop model based feedforward controls for urea injection. The feedforward control system was developed with a goal to maintain constant $\frac{NO_X}{NH_3}$ ratio at the SCR outlet. The controller was implemented and validated on an engine dynamometer. The controller achieved up to 85% $NO_X$ conversion efficiency with reduced $NH_3$ slip compared to a open loop controller.

In reference [11] the researchers evaluated the possibility of using the $NO_X$ sensor to monitor the health of the SCR. The $NO_X$ sensor signals were compared to chemiluminescence detector (CLD) measurements. The $NO_X$ sensor’s cross sensitivity toward $NH_3$ and other components in the exhaust were evaluated. The authors concluded that $NO_X$ sensors are robust enough to implement in production systems and are very useful to implement control strategies.

The objective of the research in reference [12] was to develop an SCR control strategy for urea injection. A 1D single channel model to simulate the SCR was developed and calibrated to the experimental data. Using the 1D model a first order transfer function was derived to represent the SCR. The parameters for the transfer function model were estimated using Model Reference Adaptive Control with composite adaptation law. The first order model was used to develop a closed loop self tuning control strategy with online adaptation of the controller gains. The transfer function model parameters are estimated...
using time history of the SCR catalyst inlet concentrations, exhaust flow rates and temperatures. The controller was able to reduced the mean $NH_3$ slip to less than 7 ppm and maximum slip to less than 55 ppm. The authors concluded that knowledge of the $NH_3$ storage and temperature is very important for the performance of the controller.

The goal of reference [13] was to evaluate several OBD concepts for the SCR catalyst. The monitoring requirements and challenges associated with open and closed loop control strategies were discussed. The authors concluded that to meet the 2010 SCR OBD requirements, a closed loop control strategy is needed.

The objective of the research in reference [14] was to compare a $NO_X$ sensor based control strategy with an open loop control strategy for the SCR. The authors compared a $NO_X$ sensor based closed loop SCR surface coverage / $NH_3$ slip control strategy with cross sensitivity compensation with an open loop control strategy. The authors concluded that the SCR catalyst dynamics, time delay in urea injection system and maximum $NH_3$ slip targets limit the dynamic performance of the SCR closed loop control. The open loop control had high (>85%) $NO_X$ conversion efficiency but was unable to adapt to 30% higher SCR inlet $NO_X$.

The objective of the research in reference [15] was to evaluate $NO_X$ sensor based and $NH_3$ sensor based control strategies. The $NH_3$ sensor was used with a surface coverage / $NH_3$ slip control strategy. The $NH_3$ sensor signal was used as a feedback for $NH_3$ slip and also to estimate $NH_3$ coverage fraction. The $NH_3$ sensor based control strategy achieved similar $NO_X$ conversion efficiency but with lower $NH_3$ slip.

The goal of the research in reference [16] was to compare $NO_X$ based and $NO$ and $NO_2$ based control strategies. A linearized SCR model was used to develop and compare
Nitrogen Oxides (NOx) based and NO and NO2 based control strategies. The NO and NO2 based control strategy produced less SCR outlet NOx compared to the NOx based control strategy.

The objective of the research in reference [17] was to analyze the limitations and requirements for open loop and closed loop control systems for the SCR urea injection. The authors concluded that for feedforward open loop control strategies, the controller needs a good estimate of NO and NO2. Since most of the time the NO and NO2 is not known accurately, the controller ends up injecting excess urea, which results in excess NH3 slip. For optimal NOx conversion efficiency, the knowledge of accurate NH3 storage is important. This is especially important during transients and low temperature operation. The amount of NH3 stored in the SCR determines how long the high NOx conversion at low temperatures can be maintained. The closed loop control system is affected by the quality of the sensor signals, the maximum NH3 slip limits, slow SCR dynamics and urea injection system delays. The major conclusion was that the performance of the SCR control system is a strong function of the estimated NH3 storage.

The authors in reference [18] compared the performance of a closed loop control strategy with NH3 sensor at the mid brick of an SCR and an open loop control strategy with a NOx sensor. The performance of the closed loop control strategy was significantly improved by the inclusion of a NH3 sensor at mid brick location. The NH3 sensor located mid brick had faster response compared to the NH3 sensor at the SCR outlet. The faster NH3 sensor response improved the performance of the closed loop control system.

The objective of the research in reference [19] was to compare the performance of a proportional integral (PI) controller with NH3 storage estimate as feedback and an adaptive PI controller. The model for the controls was approximated by a first order transfer function. The parameters in the transfer function were estimated as a function of engine condition.
The results showed that both the controllers were able to achieve over 90% conversion efficiency and less that 2 ppm of peak $NH_3$ slip.

The focus of the research in reference [20] was to experimentally evaluate $NH_3$ storage as a function of aging. The storage capacity of the SCR was calculated with an hydrothermally aged SCR. The results showed that the SCR storage capacity changes with aging on exposure to high temperatures.

This objective of the reference [21] was to evaluate the cross sensitivities of the $NO_X$ sensor to $HCNO$, $HCN$, $NH_3$ and other components of the exhaust. The results show that the $NO_X$ sensor is only sensitive to the $NH_3$ in the exhaust.

Based on the literature review of the control systems for the SCR, it can be concluded that the both closed loop and open loop controls can achieve high $NO_X$ Conversion efficiency, but a closed loop control strategy can also reduce the $NH_3$ slip at the SCR outlet. The implementation of a closed loop control system on an SCR is limited by slow SCR dynamics, inaccurate estimate of the $NH_3$ storage and the time delay in the urea injection system. One of the critical parameters in the control strategy performance for both open and closed loop control system is the accurate $NH_3$ storage estimate.

### 2.2 State Estimation Strategies and Onboard Diagnostics

To meet the increasingly stringent emission control standards, better control strategies need to be developed. Control strategy performance is a direct function of the ability to measure, estimate and use internal states. This is usually done using sensors, however implementing sensors to measure all the states needed for a controller is usually not possible.
nor cost effective. Sometimes models and state estimators can be used as virtual sensors to estimate states that cannot be measured by a sensor. For the diesel engine application, these models and estimators must be implementable in the ECU. Thus, computational efficiency is of great importance in virtual sensor algorithm development. State estimators can also be used to detect degradation in the performance or failure of the system within an OBD strategy.

Either linear or nonlinear state estimation strategies should be implemented depending on the system’s input output model form. Linear state estimation techniques are simpler and easier to implement as compared to nonlinear estimators. Since the models of after treatment devices are nonlinear, there is a performance penalty associated with using a linear state estimation strategy for this application. It can be done, but the system must be linearized about some operating point and the range of operation constrained about that point. Devarokonda et al. [16] and Na et al. [22] used linearized models for SCR state estimation and controls. In general, a linear state estimation technique applied to a non linear system results in large errors with increasing non linearities. To decrease the estimation errors, a non linear state estimation strategy should be used.

Recent work on Extended Kalman Filter (EKF) estimator design in diesel aftertreatment systems includes the $NH_3$ storage estimator [23] and $NO_X$ sensor cross-sensitivity estimator [24] for SCR catalysts by Hsieh et al. The authors also designed a $NO-NO_2$ concentration observer for both the DOC and CPF [25]. The main objective of the study was to estimate the $NO$ and $NO_2$ concentrations into the SCR. It should be noted that hydrocarbon and $CO$ oxidation reactions were not considered in the estimator design. The presence of large concentrations of hydrocarbons during CPF active regeneration inhibits the $NO$ oxidation reaction in the DOC [26,27]. Without modeling the $CO$ and HC oxidation and
the inhibition effects, the $NO$ and $NO_2$ prediction during active regeneration condition will be not accurate.

### 2.3 Reduced Order Models and Controls

In order to develop state estimators, an accurate model of the system is necessary. The high fidelity models for the DOC\cite{28-32} and the SCR\cite{33,34}, perform very well in predicting the performance characteristics, but these models are complex and implementing them on an ECU would require more computational resources\cite{35}. So to implement control and OBD strategies, reduced order models are needed.

For a DOC, the important states that need to be estimated include the $NO$, $NO_2$, hydrocarbon and temperatures states at the outlet of the DOC. The $NO$, $NO_2$ and temperature states are useful to predict passive PM oxidation in the CPF. The HC and temperature states during active regeneration are useful to predict the thermal oxidation of the retained PM, prevent CPF failures\cite{36} and also give better control over the regeneration process itself\cite{37}.

There have been several approaches to develop reduced order models for the DOC. Singh et al.\cite{38} developed a lumped parameter reduced order model to predict the DOC outlet hydrocarbon concentration and temperature during active regeneration. The DOC model was used along with a CPF model to evaluate control strategies. Birkby et al.\cite{39} developed model based controls using a reduced order model to predict the hydrocarbon concentration and temperature out of the DOC. The objective of the research was to control the DOC outlet temperature during active regeneration conditions. Researchers in refer-
ences [40,41] developed a reduced order model to predict the $C_3H_6$ oxidation across the DOC and the corresponding energy release. The authors also discuss the possibility of using the temperature response of the DOC for OBD.

In an SCR, the outlet $NH_3$, $NO$, $NO_2$ and $NH_3$ storage are the important states to estimate. Chi et al. [42] developed a 1D SCR model. The model consists of gas phase and surface phases for the species and energy balance. The objective of the study was to develop a urea injection control system to maintain the high $NO_X$ conversion efficiency of the SCR. Deverakonda et al. [16,43] developed SCR reduced order models for the purpose of $NO_X$ control. The research describes a 3-state and a 4-state SCR model. The models were compared to a more complex model and the experimental data. The authors concluded that a 4-state model is sufficient to predict the $NO_X$ conversion across the SCR and is suitable for the implementation of urea injection control strategy. Devarokonda et al. [16] developed a linear state estimator based on the 4 state SCR model. A control strategy was implemented using the SCR state estimator and a NOx sensor down stream of the SCR. Similarly Cho et al. [44] developed a 3 state SCR model with $NO_X$, $NH_3$ and $NH_3$ storage as states. Herman et al. [45] developed a 1D SCR model to predict the $NO_X$ conversion efficiency and the $NH_3$ slip across the SCR. A control system was developed using a SCR model along with a $NO_X$ sensor upstream of the SCR and a $NH_3$ sensor downstream of the SCR. Oliveira Costa et al. [46] developed diagnostic strategies to detect changes in the performance of the SCR using a reduced order model. The $NO_X$ conversion efficiency of the SCR model was compared with the actual SCR in real time to determine the changes in the conversion efficiency performance. Hollauf et al. [47] developed a reduced order model to implement a $NH_3$ based control strategy to minimize the $NH_3$ slip across the SCR. Mallouh et al. [48] used a combination of a linear and non linear SCR model to develop an adaptive proportional-integral(PI) control to prevent $NO_X$ and $NH_3$ slip at the
SCR outlet. The stored $NH_3$, SCR outlet $NO_X$ and SCR outlet $NH_3$ was assumed to be known to implement the control strategy. Na et al. [22] developed a reduced order model to implement control strategies. A linearized state space model was developed based on the reduced order model. McKinley et al [49] developed an eigen value based approach for controls oriented models. Stevens et al [50] developed a data driven model for the SCR and used the model to develop a urea injection profile for a HD-FTP test cycle which improved the $NO_X$ conversion efficiency and reduced the amount of urea injected.

### 2.4 Extended Kalman Filter (EKF) Based State Estimator

The Extended Kalman Filter (EKF) is a nonlinear Kalman filter which linearizes about the current mean and covariance [51]. To implement an extended Kalman filter, the equations describing the model must be differentiable functions. A general discrete non-linear system with states $\bar{x}_k$, inputs $\bar{u}_k$ and noises $\bar{w}_k$ and $\bar{v}_k$ can be represented as [52].

\[
\bar{x}_k = f_{k-1}(\bar{x}_{k-1}, \bar{u}_{k-1}, \bar{w}_{k-1}) \tag{2.1}
\]

\[
\bar{y}_k = h_k(\bar{x}_k, \bar{v}_k) \tag{2.2}
\]

The function $f$ is used to predict the state estimate and the function $h$ is used to compute the predicted measurement. $\bar{w}_k$ and $\bar{v}_k$ are the process and observation noises, which are assumed to be zero mean multivariate Gaussian noises with covariance $Q_k$ and $R_k$ respectively. Implementation of EKF on such a system involves the following steps: [52].
Compute the matrices $F_k$ and $L_k$ from $f_{k-1}$

$$F_k = \frac{\partial f_{k-1}}{\partial x}|_{\hat{x}_{k-1}, \hat{u}_{k-1}} \quad (2.3)$$

$$L_k = \frac{\partial f_{k-1}}{\partial w}|_{\hat{x}_{k-1}, \hat{u}_{k-1}} \quad (2.4)$$

Update the state estimate and estimation error covariance

$$\hat{x}_k^- = f_{k-1}(\hat{x}_{k-1}^+, \hat{u}_{k-1}, 0) \quad (2.5)$$

$$P_k^- = F_k^-P_{k-1}^+F_k^{T} + L_k^-Q_{k-1}L_k^{T} \quad (2.6)$$

Compute the matrices $H_k$ and $M_k$ from $h_k$

$$H_k = \frac{\partial h_k}{\partial x}|_{\hat{x}_k^-} \quad (2.7)$$

$$M_k = \frac{\partial h_k}{\partial v}|_{\hat{x}_k^-} \quad (2.8)$$

Calculate the optimal Kalman gain

$$K_k = P_k^-H_k^{T}(H_kP_k^-H_k^{T} + M_kR_k^-M_k^{T})^{-1} \quad (2.9)$$

Perform the measurement update of the state estimate and estimation error covariance

$$\hat{x}_k^+ = \hat{x}_k^- + K_k(y_k - h_k(\hat{x}_k^-, 0)) \quad (2.10)$$

These steps are followed at each time step and the covariance and gain matrices are updated with new values of the optimal Kalman gain matrix. An optimal estimator minimizes the estimation error by using the measured states and the knowledge of the known system. For
the Kalman Filter to be optimal, the system should satisfy the following conditions:

1. The process and observation noises $\vec{w}_k$ and $\vec{v}_k$ are known and are zero mean multi-variate Gaussian noises

2. The covariances of the noise are exactly known

3. For an EKF, the state transition and observation functions are not needed to be linear but must be differentiable functions

The literature review of the control systems have shown that accurate estimate of $NH_3$ storage is very important for the performance of both an open loop and control loop system. Both $NO_X$ and $NH_3$ sensors can be used as feedback to a closed loop control system. The $NH_3$ sensor used with feedback controls not only provides the high $NO_X$ conversion efficiencies of $NO_X$ sensor based control system but also reduces the $NH_3$ slip at the SCR outlet. A model used to estimate the $NH_3$ storage would be accurate during normal operation of the SCR, but when used with an aged SCR the model will fail to simulate the $NH_3$ storage and $NO$, $NO_2$ and $NH_3$ concentrations. State estimators with sensors can be used to estimate $NH_3$ storage in realtime and can also be used to estimate $NO$ and $NO_2$ concentrations which can be used to develop better control strategies. In this dissertation, development of reduced order models and estimators for the DOC and SCR is described. The estimators are simulated on the experimental data and the effect of $NO_X$ and $NH_3$ sensors on SCR estimator performance is described.
This section describes the experimental setup and the test matrices used to acquire the experimental data. The data to simulate both the DOC and SCR model were acquired using a 2010 Cummins ISB engine with Cummins production aftertreatment system.

### 3.1 Experimental Test Setup

The testing for the DOC and SCR was done using a 2010 cummins ISB engine with a 2010 Cummins ISB production system consisting of the DOC, CPF and SCR aftertreatment system. Table 3.1 shows the details and dimensions of the DOC, CPF, SCR and AMOX components. The DOC substrate is made of cordierite, has a diameter of 9.5in, length of 4in and celldensity of 400 cpsi. The DPF is substrate is made of cordierite, has a diameter of 9.5in, length of 12in and celldensity of 200 cpsi. The Cu-Zeolite SCR is made of cordierite, has a diameter of 10.5in, length of 12in and celldensity of 400 cpsi. The AMOX is made of cordierite, has a diameter of 10.5in, length of 4in and celldensity of 400 cpsi.
Table 3.1
Aftertreatment system specifications

<table>
<thead>
<tr>
<th>Material</th>
<th>DOC</th>
<th>DPF</th>
<th>SCR</th>
<th>AMOX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter (inch)</td>
<td>9.5</td>
<td>9.5</td>
<td>10.5</td>
<td>10.5</td>
</tr>
<tr>
<td>Length (inch)</td>
<td>4</td>
<td>12</td>
<td>12</td>
<td>4</td>
</tr>
<tr>
<td>Cell Geometry</td>
<td>Square</td>
<td>Square</td>
<td>Square</td>
<td>Square</td>
</tr>
<tr>
<td>Total Volume (L)</td>
<td>4.65</td>
<td>13.94</td>
<td>17.03</td>
<td>5.68</td>
</tr>
<tr>
<td>Cell Density $\frac{1}{in^2}$</td>
<td>400</td>
<td>200</td>
<td>400</td>
<td>400</td>
</tr>
<tr>
<td>Cell Width (mil)</td>
<td>46</td>
<td>59</td>
<td>46</td>
<td>46</td>
</tr>
<tr>
<td>Filtration Area ($in^2$)</td>
<td>NA</td>
<td>19975</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>Open Frontal Area ($in^2$)</td>
<td>60</td>
<td>24</td>
<td>73</td>
<td>73</td>
</tr>
<tr>
<td>Channel Wall Thickness (mil)</td>
<td>4</td>
<td>12</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Wall density $\frac{g}{cm^3}$</td>
<td>1.2</td>
<td>1.2</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.35</td>
<td>0.59</td>
<td>0.35</td>
<td>0.35</td>
</tr>
<tr>
<td>Mean Pore Size ($\mu m$)</td>
<td>NA</td>
<td>15</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>Number of inlet cells</td>
<td>28353</td>
<td>7088</td>
<td>34636</td>
<td>34636</td>
</tr>
</tbody>
</table>

The test cell is equipped with a 2010 Cummins ISB engine coupled with an eddy current dynamometer. A schematic of the test cell setup is shown in Figure 3.1. The exhaust from the engine can be routed through two lines: baseline and trapline. Baseline is used to warm up the engine. When the exhaust is routed through the base line, the exhaust gas bypasses the aftertreatment system and goes directly to the building exhaust. This capability provides the ability to warm up and condition the engine before starting the experiments. When the exhaust is routed through the trap line the exhaust from the engine flows through the DOC, CPF and SCR aftertreatment system. The trapline is equipped with thermocouples and pressure drop transducers to measure the temperature and pressure drop across the DOC, CPF and SCR. The trapline is also equipped with the sample probes which can be used to sample the gaseous emissions upstream of the DOC, downstream of the DOC/upstream of CPF, downstream of CPF, upstream of the SCR and downstream of the SCR. The pressure drop sensor in the Laminar Flow Element(LFE) measures the air flow into the engine. The
fuel flow measurement from the AVL fuel flow meter along with the air flow rate is used to estimate the exhaust mass flow rate. The exhaust temperatures in the DOC, CPF and SCR are measured using K type thermocouples. The list of all the emission measurements, measurement locations and the instruments used are tabulated in Table 3.2.

**Table 3.2**  
Measurements and measurement locations in the test cell

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Measurement Location</th>
<th>Instruments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure Drop</td>
<td>Upstream DOC</td>
<td>$\Delta P$ Transducer</td>
</tr>
<tr>
<td></td>
<td>Downstream DOC</td>
<td>$\Delta P$ Transducer</td>
</tr>
<tr>
<td></td>
<td>Downstream CPF</td>
<td>$\Delta P$ Transducer</td>
</tr>
<tr>
<td></td>
<td>Upstream SCR</td>
<td>$\Delta P$ Transducer</td>
</tr>
<tr>
<td></td>
<td>Downstream SCR</td>
<td>$\Delta P$ Transducer</td>
</tr>
<tr>
<td>Gaseous measurement</td>
<td>Upstream DOC</td>
<td>Mass Spectrometer/5 Gas Analyzer</td>
</tr>
<tr>
<td></td>
<td>Downstream DOC</td>
<td>Mass Spectrometer/5 Gas Analyzer</td>
</tr>
<tr>
<td></td>
<td>Downstream CPF</td>
<td>Mass Spectrometer/5 Gas Analyzer</td>
</tr>
<tr>
<td></td>
<td>Upstream SCR</td>
<td>Mass Spectrometer/5 Gas Analyzer</td>
</tr>
<tr>
<td></td>
<td>Downstream SCR</td>
<td>Mass Spectrometer/5 Gas Analyzer</td>
</tr>
</tbody>
</table>

| Temperature         | Upstream DOC                          | K Type Thermocouples              |
|                     | Downstream DOC                        | K Type Thermocouples              |
|                     | Downstream CPF                        | K Type Thermocouples              |
|                     | Upstream SCR                          | K Type Thermocouples              |
|                     | Downstream SCR                        | K Type Thermocouples              |
|                     | In the DOC,CPF & SCR                  | K Type Thermocouples              |

| Sensors             | Upstream DOC                          | $NO_X$ Sensor                     |
|                     | Downstream SCR                        | $NO_X$ and $NH_3$ sensor          |

| PM concentration   | Upstream DOC                          | Stack Sampler                     |
| measurement        | Downstream CPF                        | Stack Sampler                     |

| PM particle size   | Upstream DOC                          | Scanning Mobility Particle Sizer  |
| measurement        | Downstream DOC                        | Scanning Mobility Particle Sizer  |
|                    | Downstream CPF                        | Scanning Mobility Particle Sizer  |
|                    | Upstream SCR                          | Scanning Mobility Particle Sizer  |
|                    | Downstream SCR                        | Scanning Mobility Particle Sizer  |

| Engine airflow     | Engine Inlet                          | Laminar Flow Element             |
| Engine fuel flow   | Engine Inlet                          | AVL Fuel Flow Meter              |
3.2 DOC Test Data

The goal of the experimental studies of the DOC was to collect data to use for identification of the kinetic parameters in the DOC model. To achieve this, the tests were divided into steady state, active regeneration and transient tests. The steady state experiments were designed to identify the kinetic parameters during normal engine operating conditions. The active regeneration experiments were designed to identify kinetic parameters during active regeneration conditions and the transient tests were developed to identify the transient behavior of the DOC including the transient temperature response of the substrate due to the thermal inertia and the heat transfer to the ambien.

3.2.1 DOC Steady State Data

The objective of the DOC steady state experiments was to acquire performance data that can be used to identify the kinetic parameters in the DOC model. The performance of the DOC is a function of DOC inlet temperature and the inlet space velocities. To capture the effect of both space velocity and the temperature, the tests were developed such that the DOC inlet temperatures and space velocities were varied. To capture the effect of space velocity three space velocities of 162 k, 235 k and 281 k hr$^{-1}$ were selected as shown in table 3.3. The space velocity of the exhaust is calculated at the actual temperature and pressure and the equation to calculate the actual space velocities are calculated using Equation 3.1.

$$\text{SpaceVelocity(Actual) } = \frac{\text{MassFlowRate}}{\text{ExhaustGasDensity(ActualTemperature)}}$$ (3.1)
These space velocities were selected to cover the range of space velocities observed by the DOC during normal engine operation. At each of these space velocities the DOC inlet temperature was varied from 237 to $474^0C$ as shown in table 3.3. The engine speed and load were varied to achieve different DOC inlet temperatures while keeping the DOC inlet space velocity constant.

Table 3.3 shows the tabulated values of DOC inlet and outlet $CO$, $NO$, $NO_2$ and hydrocarbon ($HC$) concentrations and DOC inlet temperature for the steady state testing. The first column in the table is the DOC inlet space velocities at actual temperatures and the second column shows the DOC inlet mass flow rate in $kg/min$. The rest of the table is divided into DOC inlet and outlet concentrations and temperatures. The first column under the DOC inlet shows the DOC inlet temperature in $^0C$, the second, third and fourth columns show the DOC inlet $CO$, $NO$, $NO_2$ concentrations in $ppm$ and the fifth column shows the DOC inlet $HC$ concentrations in $ppmC$. The columns under DOC outlet shows $CO$, $NO$ and $NO_2$ concentrations in $ppm$ and the $HC$ concentrations in $ppmC$. 
Table 3.3
Test matrix for the steady state data showing the DOC inlet and outlet $CO$, $NO$, $NO_2$ and $HC$ concentrations and the DOC inlet temperature and space velocities (SV)

<table>
<thead>
<tr>
<th>SV *</th>
<th>$\dot{M}_{kg}^{-1}$</th>
<th>$T_{in}$ $^\circ C$</th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\dot{M}$ $\frac{kg}{min}$</td>
<td>$CO$ ppm</td>
<td>$NO$ ppm</td>
<td>$NO_2$ ppm</td>
</tr>
<tr>
<td>162k</td>
<td>7.4</td>
<td>237</td>
<td>83</td>
<td>287</td>
</tr>
<tr>
<td></td>
<td>6.6</td>
<td>296</td>
<td>63</td>
<td>301</td>
</tr>
<tr>
<td></td>
<td>6.4</td>
<td>315</td>
<td>56</td>
<td>395</td>
</tr>
<tr>
<td></td>
<td>6.2</td>
<td>352</td>
<td>53</td>
<td>434</td>
</tr>
<tr>
<td></td>
<td>5.5</td>
<td>399</td>
<td>73</td>
<td>587</td>
</tr>
<tr>
<td></td>
<td>5.8</td>
<td>374</td>
<td>81</td>
<td>480</td>
</tr>
<tr>
<td></td>
<td>5.4</td>
<td>431</td>
<td>81</td>
<td>669</td>
</tr>
<tr>
<td></td>
<td>5.2</td>
<td>457</td>
<td>96</td>
<td>970</td>
</tr>
<tr>
<td></td>
<td>7.0</td>
<td>272</td>
<td>69</td>
<td>283</td>
</tr>
<tr>
<td>235k</td>
<td>10.0</td>
<td>252</td>
<td>88</td>
<td>206</td>
</tr>
<tr>
<td></td>
<td>10.1</td>
<td>275</td>
<td>82</td>
<td>242</td>
</tr>
<tr>
<td></td>
<td>8.3</td>
<td>390</td>
<td>61</td>
<td>331</td>
</tr>
<tr>
<td></td>
<td>8.9</td>
<td>345</td>
<td>67</td>
<td>282</td>
</tr>
<tr>
<td></td>
<td>8.3</td>
<td>369</td>
<td>63</td>
<td>306</td>
</tr>
<tr>
<td></td>
<td>7.9</td>
<td>439</td>
<td>107</td>
<td>497</td>
</tr>
<tr>
<td></td>
<td>7.3</td>
<td>462</td>
<td>205</td>
<td>490</td>
</tr>
<tr>
<td></td>
<td>7.0</td>
<td>492</td>
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</tr>
<tr>
<td></td>
<td>8.2</td>
<td>413</td>
<td>58</td>
<td>451</td>
</tr>
<tr>
<td></td>
<td>9.3</td>
<td>369</td>
<td>69</td>
<td>306</td>
</tr>
<tr>
<td></td>
<td>9.3</td>
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<td>308</td>
</tr>
<tr>
<td></td>
<td>9.7</td>
<td>402</td>
<td>69</td>
<td>274</td>
</tr>
<tr>
<td></td>
<td>10.6</td>
<td>356</td>
<td>61</td>
<td>281</td>
</tr>
<tr>
<td></td>
<td>8.7</td>
<td>474</td>
<td>212</td>
<td>484</td>
</tr>
<tr>
<td>281k</td>
<td>12.1</td>
<td>273</td>
<td>91</td>
<td>204</td>
</tr>
<tr>
<td></td>
<td>10.2</td>
<td>378</td>
<td>63</td>
<td>284</td>
</tr>
<tr>
<td></td>
<td>11.4</td>
<td>302</td>
<td>78</td>
<td>247</td>
</tr>
<tr>
<td></td>
<td>9.5</td>
<td>424</td>
<td>57</td>
<td>420</td>
</tr>
<tr>
<td></td>
<td>11.1</td>
<td>323</td>
<td>68</td>
<td>269</td>
</tr>
<tr>
<td></td>
<td>8.9</td>
<td>446</td>
<td>103</td>
<td>482</td>
</tr>
<tr>
<td></td>
<td>8.6</td>
<td>507</td>
<td>293</td>
<td>700</td>
</tr>
<tr>
<td></td>
<td>10.6</td>
<td>356</td>
<td>59</td>
<td>289</td>
</tr>
</tbody>
</table>
The space velocity (SV) of the exhaust is calculated at actual temperature and pressure and is calculated using equation 3.1.

Figure 3.2 shows a plot of the experimental CO, NO and HC conversion efficiencies for the three space velocities plotted against temperature in °C along the x axis. The conversion efficiencies for 162 khr⁻¹ are plotted in red 'X', 235 khr⁻¹ space velocities are plotted in green 'X' and 281 khr⁻¹ are plotted with blue 'X'. The first subplot shows the NO conversion efficiencies, the plot shows that between 200 – 350 °C the NO conversion efficiency decreases with the increasing DOC space velocities. At temperatures higher than 350 °C data shows similar NO conversion efficiencies for all space velocities. The second subplot shows the DOC CO conversion efficiencies plotted as a function of the temperature. It can be observed from the plot that the experimental data shows 100% conversion of CO across the DOC for all temperatures. The third subplot shows the HC conversion efficiencies as a function of temperature. The plot shows that the HC conversion efficiencies for 235 and 281 khr⁻¹ space velocities are similar. Compared to the 162 khr⁻¹ space velocity, HC conversion efficiencies for both 235 and 281 khr⁻¹ shows lower conversion efficiencies.
Figure 3.2. Experimental measured DOC conversion efficiencies of NO, CO and HC during steady state conditions at three DOC inlet space velocities
3.2.2 DOC Active Regeneration Data

The active regeneration condition in the DOC represents a special case in the operation of the DOC. The active regeneration condition exposes the DOC to high temperatures and high concentration of HCs. The high HC concentrations in the exhaust results in the inhibition of the other reactions in the DOC. To capture the effects of the high temperature and high HC concentrations in the exhaust, three data points from the steady state testing test matrix were selected. The test conditions were selected such that the DOC inlet temperature was above 320°C. This was done to ensure the DOC light off for the HC oxidation reaction was achieved. At each of these conditions the HC injection (post injection in the cylinder) was varied to achieve different DOC inlet HC concentrations and DOC outlet temperatures. The DOC inlet and outlet CO, NO, NO₂ and HC concentrations and temperatures were measured using the mass spectrometer emission measurement instrument described in Figure 3.1. Table 3.4 shows the tabulated values of DOC inlet and outlet concentrations and temperatures for the three space velocities. In the table the CO, NO and NO₂ concentration are in ppm, the HC concentrations are in ppmC and the temperatures are in °C. From the table it can be observed that the DOC inlet concentration of CO, NO and NO₂ and DOC inlet temperatures are constant, while the the DOC inlet HC concentration is varied depending on the desired DOC outlet temperature.
Table 3.4
Test matrix for the active regeneration tests showing the DOC inlet and outlet $CO$, $NO$, $NO_2$ and $HC$ concentrations and the DOC inlet temperatures and space velocities. The $HC$ injection was achieved through in cylinder post injection.

| SV $hr^{-1}$ | Inlet | | | | Outlet |
|--------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $C^0 C$ ppm | $CO$ ppm | $NO$ ppm | $NO_2$ ppm | $HC$ ppm | $CO$ ppm | $NO$ ppm | $NO_2$ ppm | $HC$ ppm |
| 162k         | 344   | 83    | 499   | 18    | 132   | 348   | 0     | 183   | 334   | 16    | 497   | 3     | 481   | 36    | 305   |
|              | 344   | 83    | 499   | 18    | 8340  | 348   | 0     | 183   | 334   | 16    | 497   | 3     | 481   | 36    | 305   |
|              | 344   | 83    | 499   | 18    | 9896  | 526   | 4     | 497   | 20    | 319   | 547   | 6     | 507   | 10    | 313   |
|              | 344   | 83    | 499   | 18    | 11021 | 547   | 6     | 507   | 10    | 313   | 599   | 12    | 517   | 0     | 330   |
|              | 344   | 83    | 499   | 18    | 13620 | 599   | 12    | 517   | 0     | 330   | 599   | 12    | 517   | 0     | 330   |
| 235k         | 344   | 71    | 296   | 13    | 185   | 350   | 0     | 124   | 185   | 18    | 504   | 12    | 305   | 7     | 468   |
|              | 344   | 71    | 296   | 16    | 7875  | 504   | 12    | 305   | 7     | 468   | 524   | 17    | 307   | 5     | 516   |
|              | 344   | 71    | 296   | 16    | 9069  | 524   | 17    | 307   | 5     | 516   | 548   | 23    | 320   | 3     | 930   |
|              | 344   | 71    | 296   | 27    | 10791 | 548   | 23    | 320   | 3     | 930   | 615   | 75    | 325   | 4     | 1104  |
|              | 344   | 71    | 296   | 33    | 14259 | 615   | 75    | 325   | 4     | 1104  | 615   | 75    | 325   | 4     | 1104  |
| 281k         | 320   | 75    | 285   | 21    | 215   | 326   | 0     | 130   | 175   | 34    | 509   | 58    | 301   | 8     | 1323  |
|              | 320   | 75    | 285   | 24    | 10550 | 509   | 58    | 301   | 8     | 1323  | 533   | 65    | 306   | 6     | 1426  |
|              | 320   | 75    | 285   | 27    | 11687 | 533   | 65    | 306   | 6     | 1426  | 557   | 80    | 310   | 5     | 1550  |
|              | 320   | 75    | 285   | 34    | 15199 | 557   | 80    | 310   | 5     | 1550  | 597   | 140   | 312   | 7     | 1695  |

Figure 3.3 shows the plot of the experimental $NO$, $CO$ and $HC$ conversion efficiencies plotted against the DOC outlet temperature. The conversion efficiencies for $162khr^{-1}$ are plotted in red ‘X’, $235khr^{-1}$ are plotted in green ‘X’ and $281khr^{-1}$ are plotted with blue ‘X’. The conversion efficiencies between temperatures of $300 – 350^0C$ indicate the $NO$ conversion efficiencies without $HC$ injection. The conversion efficiencies at temperatures higher than $500^0C$ show conversion efficiencies with $HC$ injection. The first subplot shows the $NO$ conversion efficiencies plotted against the DOC outlet temperature. The plot shows that at temperatures greater than $500^0C$ the $NO$ conversion efficiency shows negative values indicating the conversion of $NO_2$ to $NO$. The second plot shows the $CO$
conversion efficiencies of DOC plotted against DOC outlet temperature. It can be observed from the plot that the $CO$ conversion efficiency decreases with an increase in the DOC inlet $HC$ concentration. The $281khr^{-1}$ space velocity $CO$ conversion efficiency shows negative conversion at temperatures greater than $550^0C$. The negative $CO$ conversion indicates the production of $CO$ across the DOC. The third subplot shows $HC$ conversion efficiencies plotted against the DOC outlet temperatures. The plot shows that for the temperatures tested, the $HC$ conversion efficiency remains more than 80% and there is no significant difference between the $HC$ conversion for three space velocities.
Figure 3.3. Experimental measured DOC conversion efficiencies of NO, CO and HC during active regeneration conditions at three DOC inlet space velocities.
3.2.3 DOC Transient Data

To understand the transient performance of the DOC, a surrogate FTP cycle based on a standard Heavy-Duty FTP cycle was developed[53]. The surrogate FTP cycle captures the important transient features of the standard FTP cycle. But eliminates the speed load points that are beyond the capability of the test cell.

Figure 3.4. Experimental measured DOC inlet and outlet concentrations of $NO$, $CO$ and $HC$ and temperatures during transient test
Figure 3.4 shows the DOC inlet and outlet concentrations of \( NO \), \( NO_2 \), \( CO \) and 
\( HC \) and the temperatures during the transient FTP test. In the figure, the curves in black
represents the DOC inlet concentrations and temperatures and the curves in red represent
the DOC outlet concentrations and temperatures. The first subplot shows the DOC inlet
and outlet temperature in °C plotted as a function of time in minutes along the x axis.
It can be observed that the DOC inlet and outlet temperatures vary from 200 to 405°C
and consist of regions where the DOC inlet temperature increases and decreases, which
simulates the heating and cooling of the DOC. The second subplot shows the DOC inlet
and outlet \( NO \) concentrations in ppm plotted against time in minutes along the x axis.
It can be observed that the DOC inlet \( NO \) concentrations vary from 0 to 770 ppm. The
\( NO \) concentrations show fast transients where the inlet concentrations change from greater
than 700 ppm to less than 100 ppm. The third subplot shows the DOC inlet and outlet
\( NO_2 \) concentrations in ppm plotted against time in minutes along the x axis. Compared to
the DOC inlet \( NO \) concentration the DOC inlet \( NO_2 \) concentration is much lower which
indicates that most of the engine out \( NO_X \) is composed of \( NO \). The DOC outlet \( NO_2 
concentration profile is higher than the DOC inlet \( NO_2 \) concentration which represents
the oxidation of \( NO \) to \( NO_2 \) across the DOC. The fourth subplot shows the DOC inlet
and outlet \( CO \) concentration in ppm plotted against time in minutes along the x axis. The
DOC inlet \( CO \) concentration does not change and remains constant except for the spikes
observed at 1 minute and between 15 and 16 minutes. For the entire test, the DOC outlet
\( CO \) shows almost 100% conversion of \( CO \) across the DOC except at 1 minute. The fifth
subplot shows the DOC inlet and outlet \( HC \) concentrations in ppmC plotted against time
in minutes along the x axis. The DOC inlet \( HC \) concentration is less than 50 ppmC for the
entire test. The DOC outlet \( HC \) is less than 10 ppmC which shows that for the entire test
conditions the DOC light off is achieved.
The DOC high fidelity model was simulated using the steady state, active regeneration and transient data. The DOC reduced order model was simulated on steady state and active regeneration data and the reduced order DOC estimator was simulated on the transient FTP data.

3.3 SCR Test Data

To simulate and validate the SCR reduced order model and reduced order estimator, steady state and transient tests were conducted. Both the data sets were generated on a 2010 Cummins ISB engine with a 2010 Cummins production aftertreatment system. This section briefly describes the experimental data for the SCR tests. More detailed analysis of the data and details on the test setup can be found in the reference[1].

3.3.1 SCR Steady State Data

The objective of the SCR steady state tests was to identify the kinetic parameters to simulate the SCR on an engine. The steady state data was collected at 8 different SCR inlet temperatures. The engine speed and load points were selected to achieve different SCR inlet temperatures and \( NO_2/NO_X \) ratios. Table 3.5 shows the test matrix for the light test points for the steady state tests. The SCR inlet temperatures were varied from 250 – 299°C. At each of the SCR inlet temperatures, the inlet \( NO \) and \( NO_2 \) concentrations were maintained constant. For the eight tests the SCR inlet \( NO \) and \( NO_2 \) concentration varied between 78 to 462 ppm and 120 to 295 ppm respectively. During each of these tests, different \( NH_3/NO_X \) ratios were achieved by varying the urea injection rate.
Table 3.5
Test matrix for the SCR steady state tests showing the SCR inlet $NO$, $NO_2$ and $NH_3$ concentrations along with the SCR inlet temperatures

<table>
<thead>
<tr>
<th>Test Point</th>
<th>SCR inlet Temp C</th>
<th>SCR SV $khr^{-1}$</th>
<th>SCR Inlet $NO$ ppm</th>
<th>SCR Inlet $NO_2$ ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>399</td>
<td>58.9</td>
<td>462</td>
<td>295</td>
</tr>
<tr>
<td>2</td>
<td>376</td>
<td>60.1</td>
<td>185</td>
<td>160</td>
</tr>
<tr>
<td>3</td>
<td>353</td>
<td>61.5</td>
<td>115</td>
<td>187</td>
</tr>
<tr>
<td>4</td>
<td>331</td>
<td>59.8</td>
<td>97</td>
<td>176</td>
</tr>
<tr>
<td>5</td>
<td>301</td>
<td>60.6</td>
<td>78</td>
<td>220</td>
</tr>
<tr>
<td>6</td>
<td>278</td>
<td>60.8</td>
<td>80</td>
<td>199</td>
</tr>
<tr>
<td>7</td>
<td>252</td>
<td>60.2</td>
<td>110</td>
<td>120</td>
</tr>
<tr>
<td>8</td>
<td>366</td>
<td>53.5</td>
<td>197</td>
<td>208</td>
</tr>
</tbody>
</table>

Figure 3.5. Experimental measured SCR inlet concentrations of $NO$, $NO_2$ and $NH_3$ during steady state test
Figure 3.5 shows the SCR inlet concentrations of $NO$, $NO_2$ and $NH_3$ plotted against time for test number 8. The plot shows that the SCR inlet $NO$ and $NO_2$ concentrations are maintained constant for the entire test and the SCR inlet $NH_3$ concentration varies to achieve different SCR inlet $NH_3 / NO_X$ ratios. The SCR inlet $NH_3$ concentrations are calculated using the DEF injector flow rate, urea properties and the exhaust flow rate. More details on the $NH_3$ concentration calculation can be found in Appendix A. More detailed analysis of the data and details on the test setup can be found in the reference[1].

3.3.2 SCR Transient Data

To simulate the SCR transients, the surrogate FTP test was created [1]. The surrogate FTP test is based on a standard heavy duty FTP test. The standard heavy duty FTP test was modified to remove some of the test conditions which are beyond the capability of the test cell. Figure 3.6 shows the SCR inlet $NO$, $NO_2$ and $NH_3$ concentrations and the SCR inlet and outlet temperatures during the surrogate FTP test. The first subplot shows the SCR inlet $NO$, $NO_2$ and $NH_3$ concentrations plotted against time in minutes. The plots show that the inlet concentrations show fast transients similar to the standard FTP cycle. The second subplot shows a plot of the SCR inlet and outlet temperatures against time in minutes. The SCR inlet temperature varies from 250 to 375°C. The plot also shows that the SCR inlet and outlet temperature profiles are similar but the SCR outlet temperature lags the inlet temperature.
Figure 3.6. Experimental measured SCR inlet concentrations of $NO$, $NO_2$ and $NH_3$ and the SCR inlet and outlet temperatures during surrogate FTP test.

The SCR steady state test data were used to compare to the reduced order model simulation and the transient test data were used to compare to the SCR reduced order estimator simulation.
4. DOC AND SCR HIGH FIDELITY MODELS

Aftertreatment system modeling has been used in the design process to improve the performance and to reduce the cost of the system including the development cost and to understand the performance characteristics of these systems. The 1D single channel modeling approach is the most commonly used approach, since 3D and 2D modeling of an aftertreatment system is very complex and requires significant computational resources. The 1D modeling approach requires less computational resources and is still relatively accurate. This section describes the 1D modeling approach as applied to the DOC and SCR aftertreatment devices as used in the dissertation.

4.1 DOC High Fidelity Model

The DOC model developed for this dissertation is a 1D single square channel approximation of the DOC. The DOC model simulates three important reactions for $CO$, $HC$ and $NO$ oxidation. The DOC model assumes that a single channel can be used to represent a DOC and simulates the gas and surface phase mass and energy balance equations. The heat and mass transfer between the gas and surface phase are limited by the heat and mass transfer coefficients. The important assumptions made in the development of the
DOC model are:

1. Exhaust gas is assumed to be ideal.
2. Reaction rate constants are of the Arrhenius form.
3. Convection heat transfer is assumed to ambient.

![Diagram of DOC](image)

**Figure 4.1.** Schematic showing the exhaust flow through the DOC

### 4.1.1 Reactions in the DOC

The DOC model simulates the oxidation of $CO$, $NO$ and $HC$ in the exhaust. $HC$ and $CO$ oxidation are considered as forward only reactions and $NO$ oxidation is considered as a reversible reaction. The $NO \leftrightarrow NO_2$ oxidation is a reversible reaction which is kinetics limited at low temperatures and thermodynamically limited at higher temperatures [28–30, 55]. $NO \leftrightarrow NO_2$ equilibrium is used to determine the direction of the $NO$ oxidation reaction and is based on the Gibbs free energy function [28, 80, 55]. Some modeling studies such as OH et al [56] have used $C_3H_6$ to represent fast oxidizing hydrocarbons and $CH_4$. 


methane to represent the slow oxidizing hydrocarbons. But several research studies \cite{28-30,55,57,58} involving modeling of the DOC have concluded that \(C_3H_6\) is sufficient to represent the exhaust of a heavy duty diesel engine. Hence, in the DOC model used in this study, \(C_3H_6\) is considered to be a representative hydrocarbon in the DOC. This reduces the number of differential equations to be solved in the model and improves the speed of the model. The reactions considered in the model are shown below:

NO oxidation:

\[
NO + \frac{1}{2}O_2 \leftrightarrow NO_2 \tag{4.1}
\]

CO oxidation:

\[
CO + \frac{1}{2}O_2 \rightarrow CO_2 \tag{4.2}
\]

Hydrocarbon oxidation:

\[
C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O \tag{4.3}
\]

\textbf{Figure 4.2.} Schematic of the DOC high fidelity model showing the gas and surface phase concentrations and temperatures
4.1.2 Mass and Energy Balance Equations

The species balance equations for $CO$, $NO$, $NO_2$ and $C_3H_6$ are represented as:

$$
\epsilon \frac{\partial C_{g,i}}{\partial t} = -\epsilon u \frac{\partial C_{g,i}}{\partial x} - \beta_i A_g (C_{g,i} - C_{s,i}) \quad (4.4)
$$

$$(1 - \epsilon) \frac{\partial C_{s,i}}{\partial t} = -\beta_i A_g (C_{s,i} - C_{g,i}) - R_i \quad (4.5)
$$

$i = CO, NO, NO_2, C_3H_6$

Where, $C_{g,i}$ and $C_{s,i}$ are the gas and surface concentration of $i^{th}$ species, $\epsilon$ is the void fraction and $u$ is the exhaust gas velocity. The energy balance equation is represented as:

$$
\rho C_v \frac{\partial T_g}{\partial t} = -\rho u C_p \frac{\partial T_g}{\partial t} - h_g \frac{4}{a_w} (T_g - T_w)
$$

$i = CO, NO, NO_2, C_3H_6

$$
(\rho_s c_{p,s}) \frac{\partial T_w}{\partial t} = h_g \frac{4a_w}{\alpha_p^2 - \alpha_w^2} (T_g - T_w) - h_a \frac{4\alpha_p}{\alpha_p^2 - \alpha_w^2} (T_g - T_w) + \frac{A_g}{1 - \epsilon} \sum_{i=CO}^{HC} \frac{\Delta h_i r_i}{MW_i} \quad (4.7)
$$

Where, $T_g$ and $T_w$ are the gas and substrate temperatures, $h_g$ and $h_a$ are the heat transfer coefficients between gas and surface phase and the between the outer surface of the channel and the atmosphere, $\rho_s$ and $c_{p,s}$ are the density and specific heats, $\rho$ is the density of the exhaust gas, $c_p$ and $c_v$ are specific heats of the exhaust gas, $\Delta h_i$ is the enthalpy of the $CO$, $NO$ and $C_3H_6$ oxidation reactions, $MW_i$ is the molecular weight of $i^{th}$ species and $A_g$ is the geometric surface area. The heat transfer to the ambient is an empirical approximation.

The reaction rate for the $CO$, $NO$ and $C_3H_6$ oxidation reactions are defined as:

$$
r_{CO} = \frac{k_{CO,s} c_{CO,s} c_{O_2}}{G_1} \quad (4.8)
$$
\[ r_{NO} = \frac{k_{NO} \left( c_{NO,s} c_{O_2,0}^{0.5} - \frac{c_{NO_2,s}}{K_p} \right)}{G_2} \] (4.9)

\[ r_{C_3H_6} = \frac{k_{C_3H_6} c_{C_3H_6} c_{O_2}}{G_3 G_4} \] (4.10)

where \( k_{CO}, k_{NO} \) and \( k_{C_3H_6} \) are the Arrhenius reaction rate constants given by Eq. 4.11.

\[ k_i = A_i e^{-\left( \frac{E_i}{R T_s} \right)} \] (4.11)

\[ i = CO, NO, NO_2, C_3H_6 \]

where the \( A_i \) are the pre exponential factors, \( E_i \) are the activation energies and \( T_s \) is the substrate temperature. The quantity \( K_p \) is the thermodynamic equilibrium constant and is calculated as:

\[ K_p = \frac{RT_s e^{\left( \frac{\Delta G}{RT_s} \right)}}{P} \] (4.12)

where, \( \Delta G \) is the Gibbs free energy for a mixture of \( NO, NO_2 \) and \( O_2 \) at temperature \( T_s \), \( R \) is the universal gas constant and \( P \) is exhaust gas pressure. \( G_1, G_2, G_3 \) and \( G_4 \) are the inhibition terms to account for the inhibition of the oxidation reactions due to the availability of catalyst sites.

\[ G_1 = G_2 = G_3 = (1 + K_{a,1} C_{s,CO} + K_{a,2} C_{s,C_3H_6})^2 (1 + K_{a,3} C_{s,CO}^2 C_{s,C_3H_6}^2) + K_{a,4} C_{s,NO}^{0.7} \]

\[ G_4 = (1 + K_{a,5} C_{s,O_2})^{1.5} \] (4.13)

Where \( K_{a,j} \) are of the Arrhenius form and are called inhibition factors:

\[ K_{a,j} = A_{a,j} e^{\frac{\Delta H_{a,j}}{RT_s}} \] (4.14)

\[ j = 1, 2, \ldots, 5 \]
Where, $A_{a,j}$ are the adsorption constants and $\Delta H_{a,j}$ are the adsorption heats.

### 4.1.3 High Fidelity Model Calibration

The DOC high fidelity model was simulated using the steady state and active regeneration data. The steady state data were used to identify the activation energies for $CO$, $NO$ and $HC$ oxidation reactions and the active regeneration data were used to identify the inhibition factors during active regeneration with diesel fuel being injected into the cylinder later in the expansion stroke. The activation energies reported in the reference [1] were used as initial values.

### 4.1.4 Steady State Simulation

The steady state data consists of $CO$, $NO$ and $HC$ concentrations upstream and downstream of the DOC at DOC inlet temperatures from 237 to 507°C at three different space velocities of 162, 235 and 281 $khr^{-1}$. The steady state data provides the data needed to identify the activation energies and pre exponential factors for the $CO$, $NO$ and $HC$ oxidation reactions.

To identify the activation energies and pre exponential factors, the adsorption factors in the inhibition terms were set to zero. The activation energies for each of the oxidation reactions were changed to simulate the shape of the conversion efficiency curves. Table 4.1 contains the kinetic parameters used in simulating the steady state data. As mentioned earlier, the inhibition factors were set to zero.
### Table 4.1
Kinetic parameters used to simulate steady state conditions

<table>
<thead>
<tr>
<th></th>
<th>CO Oxidation</th>
<th>HC Oxidation</th>
<th>NO Oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activation Energy</td>
<td>894000.0</td>
<td>10000.0</td>
<td>715000.0</td>
</tr>
<tr>
<td>Preexponential Factor</td>
<td>39.0</td>
<td>25.0</td>
<td>46.4</td>
</tr>
<tr>
<td>Inhibition</td>
<td>$A_{a,j}$</td>
<td>$\Delta H_{a,j}$</td>
<td>$A_{a,j}$</td>
</tr>
<tr>
<td>$A_{a,1}$</td>
<td>0.0</td>
<td>7990.0</td>
<td>0.0</td>
</tr>
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<td>$A_{a,2}$</td>
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<td>75000.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,3}$</td>
<td>0.0</td>
<td>96534.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,4}$</td>
<td>0.0</td>
<td>31036.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,5}$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Figure 4.3. Comparison of the simulated and experimental DOC CO conversion efficiencies

Figure 4.3 shows the comparison of the experimental and simulated CO conversion efficiency for 162, 235 and 281khr\(^{-1}\) space velocities. The experimental (measured) CO conversion efficiencies are plotted with symbol ‘O’ in red and the simulated CO conversion efficiencies are plotted with symbol ‘△’ in black. The experimental CO conversion efficiency was more than 99% for all the temperatures. Hence, to simulate the conversion efficiency profile, the activation energy used to simulate the model was lowered to 39 J/kmol for the CO oxidation reaction. With the lower activation energy, the model is able...
to simulate the experimental $CO$ conversion efficiencies observed in the experimental data.

Figure 4.4 shows the comparison of the experimental and simulated $HC$ conversion efficiencies for 162, 235 and 281 $khr^{-1}$ space velocities. The experimental (measured) $HC$ conversion efficiencies are plotted with symbol ’O’ in red and the simulated $HC$ conversion efficiencies are plotted with symbol ’△’ in black. At 235 $khr^{-1}$ space velocity, the experimental data shows a decrease in conversion efficiency with increasing temperature. This trend is not seen in the other space velocities and when the measurement uncertainty of ±5 ppm$C$ is considered, it can be concluded that the trend is not a real phenomenon. The experimental $HC$ conversion efficiency curve shows more than 98% conversion efficiency for temperatures above 350$^0C$. To simulate the conversion efficiency profile, the activation energy used to simulate the model was lowered to 25 $J/kmol$ for the $HC$ oxidation reaction. With the lower activation energy, the model is able to simulate the experimental $HC$ conversion efficiencies.
Figure 4.4. Comparison of the experimental and simulated HC conversion efficiencies

Figure 4.5 shows a comparison of the simulated and experimental DOC outlet $NO_2/NO_X$ ratios for three space velocities. The $NO_2/NO_X$ ratio is plotted as a function of temperature along the x axis. The experimental (measured) $NO_2/NO_X$ ratios are plotted with symbol ‘O’ in red and the simulated $NO_2/NO_X$ ratios are plotted with symbol ‘Δ’ in black. With the activation energy of 46.4 $J/kmol$, the model follows the shape of the experimental $NO_2/NO_X$ ratio. There are slight differences in the $NO_2/NO_X$ ratios at a given temperature, but these differences fall within the limits of measurement uncertainty.
Figure 4.5. Comparison of the simulated and experimental DOC outlet $NO_2/NO_X$ ratio

4.1.5 Active Regeneration Simulation

The active regeneration data consists of in cylinder $HC$ dosing which results in increased $HC$ concentrations at the inlet of the DOC. The data consists of $HC$, $NO$ and $CO$ conversion across the DOC at three space velocities and different HC injection levels and corresponding DOC outlet temperatures. The important difference between the steady
Table 4.2
Kinetic parameters used to simulate active regeneration

<table>
<thead>
<tr>
<th></th>
<th>CO Oxidation</th>
<th>HC Oxidation</th>
<th>NO Oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preexponential Factor</td>
<td>894000.0</td>
<td>10000.0</td>
<td>715000.0</td>
</tr>
<tr>
<td>Activation Energy</td>
<td>39.0</td>
<td>25.0</td>
<td>46.4</td>
</tr>
<tr>
<td>Inhibition</td>
<td>$A_{a,j}$ $\Delta H_{a,j}$</td>
<td>$A_{a,j}$ $\Delta H_{a,j}$</td>
<td>$A_{a,j}$ $\Delta H_{a,j}$</td>
</tr>
<tr>
<td>$A_{a,1}$</td>
<td>0.0</td>
<td>7990.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,2}$</td>
<td>7.0E+07</td>
<td>75000.0</td>
<td>20.5</td>
</tr>
<tr>
<td>$A_{a,3}$</td>
<td>0.0</td>
<td>96534.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,4}$</td>
<td>0.0</td>
<td>31036.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,5}$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

state and active regeneration tests is the presence of high hydrocarbon concentrations and the large temperature increase across the DOC. This provides an opportunity to identify the inhibition factors and adsorption heats for inhibition due to the hydrocarbons affecting the reaction rates. To simulate the DOC outlet species measurements, the inhibition factor associated with the affect of the $HC$ concentrations on oxidation reactions ($A_{a,2}$ and $\Delta H_{a,2}$) were changed to simulate the DOC outlet concentrations and temperatures. Table 4.2 contains the kinetic parameters used in simulating the active regeneration data. The main difference from the Table 4.1 is that the inhibition factors are non-zero and are different between HC, CO and NO oxidation reactions.

Figure 4.6 shows the comparison of the experimental and simulated DOC $HC$ conversion efficiencies for 162, 235 and 281 $k/hr$ space velocities. To simulate the DOC outlet CO conversion efficiency, the inhibition factor for $A_{a,2}$ and adsorption heat $\Delta H_{a,2}$ were changed to $6.8 \times 10^{+08}$ and 75000 for the $CO$ oxidation reaction. With the new values for inhibition, the model is able to simulate the shape of experimental DOC $CO$ conversion efficiency curve for most of the 162 and 235 $k/hr$ space velocities. The model is not able to simulate the 550°C and higher temperature points and the 281 $k/hr$ space velocity points.
This is due to the presence of CO production in the DOC from incomplete HC oxidation and the model does not have the capability to model this phenomenon.

Figure 4.6. Comparison of the simulated and experimental DOC CO conversion efficiencies during active regeneration

Figure 4.7 shows the comparison of the experimental and simulated HC conversion efficiencies for 162, 235 and 281 \( khr^{-1} \) space velocities. With the inhibition factor for the HC inhibition, the model is able to simulate the experimental HC conversion efficiencies. At temperatures less than 350\(^0\)C, the model predicts lower conversion of HC across the DOC. But when the measurement uncertainty of \( \pm 5 \text{ ppmC} \) is considered, the simulated conversion efficiency falls within the error.
Figure 4.7. Comparison of the experimental and simulated DOC HC conversion efficiencies during active regeneration
Figure 4.8 shows the comparison of the experimental and simulated DOC outlet $NO_2/NO_X$ ratios for the 162, 235 and 281 $khr^{-1}$ space velocities. To simulate the DOC outlet $NO_2/NO_X$ ratios, the inhibition factor for $A_{a,2}$ and adsorption heat $\Delta H_{a,2}$ were changed to $7.0 \times 10^{+07}$ and 75000 for the NO oxidation reaction. With the new values for the inhibition factor, the model is able to simulate the experimental DOC outlet $NO_2/NO_X$ ratios.

Figure 4.8. Comparison of the simulated and experimental DOC outlet $NO_2/NO_X$ ratio during active regeneration

Figure 4.9 shows the comparison of the experimental and simulated DOC outlet temperatures for 162, 235 and 281 $khr^{-1}$ space velocities. To simulate the DOC outlet tem-
perature profile, the inhibition factor for $A_{0,2}$ was changed to 20.5 for the HC oxidation reaction. With this inhibition factor, the model is able to simulate the experimental DOC outlet temperature.

![Comparison of experimental and simulated DOC outlet temperatures](image)

**Figure 4.9.** Comparison of the experimental and simulated DOC outlet temperatures

### 4.1.6 Transient Simulation

The kinetic constants tabulated in Table 4.2 were used to simulate the transient FTP data. From the initial simulation results, it was observed that there was a lag in the response of simulated DOC outlet temperature compared to the experimental DOC outlet tempera-
tures. To improve the thermal response of the DOC model, the density of the substrate ($ρ_{s,i}$) was reduced. However, the resulting effect of reduced density of the substrate was not sufficient to simulate the experimental temperature. To simulate the experimental DOC outlet temperature, the heat transfer coefficient to ambient was set to $'ha = 0.11 \frac{W}{m^2\cdot K}$.
Figure 4.10. Comparison of the DOC outlet temperature, $HC$ concentration, $NO_2/NO_X$ ratio and $CO$ concentration for the surrogate FTP cycle.

Figure 4.10 shows the simulation results. The experimental DOC inlet and outlet val-
ues are plotted in black and red and the simulated DOC outlet values are plotted in blue. The first subplot in Figure 4.10 shows the comparison of the experimental and simulated temperatures. With the heat transfer to ambient added to the model, the model is able to simulate the response of the DOC experimental data except between 4-6 minutes. The second subplot shows the comparison of the DOC outlet HC concentrations. The experimental data shows complete conversion of HC across the DOC, but the model results show HC slip of up to 50 ppmC across the DOC. The third subplot shows the comparison of the NO$_2$/NO$_X$ ratios. The simulated NO$_2$/NO$_X$ ratio follows the experimental DOC outlet NO$_2$/NO$_X$ ratio. The fourth subplot shows the comparison of the DOC outlet CO concentration. The experimental data shows complete conversion of CO across the DOC and the model is able to simulate the outlet CO concentration.

### 4.1.7 Aged Data Simulation

To evaluate the capability of the DOC model to simulate aging of the catalyst, the experimental data was carried out at Johnson Matthey USA. The engine and the DOC used for testing was similar in size to the specification DOC used in this research and is described in chapter 3. The test data consists of several engine speed load points to achieve different DOC inlet temperatures. The DOC inlet temperatures for the fresh (degreened) data ranged from 312 to 504°C. The DOC inlet CO concentrations varied from 23 to 169 ppm, NO concentrations varied from 140 to 571 ppm, NO$_2$ concentrations varied from 15 to 28 ppm and HC concentrations varied from 75 to 1380 ppmC. To simulate the DOC, the kinetic parameters identified (Table 4.2) from simulating the steady state and active regeneration data in this dissertation was used as the starting point for simulating the degreened data. The activation energy for the CO oxidation reaction was changed from
39J/kmol to 55J/kmol, the activation energy for the NO oxidation reaction was changed from 46.4J/kmol to 55J/kmol and activation energy for the HC oxidation reaction was changed from 25J/kmol to 55J/kmol. The activation energies were changed to simulate the shape of the conversion efficiency curves.

Figure 4.11. Comparison of the experimental and simulated DOC outlet HC, NO2 and CO concentrations for the degreened data
Figure 4.11 shows a comparison between the experimental and simulated DOC outlet $HC$, $NO_2$ and $CO$ concentrations for the fresh data. The DOC outlet $HC$, $NO_2$ and $CO$ concentrations are plotted against temperature. The $HC$ concentrations are plotted in ppm and the $CO$ and $NO_2$ concentrations are plotted in ppm. The experimental data is plotted with an error bar of $\pm 5$ppm. The simulated $HC$ concentrations are within the error bars except for the $311^0C$ and $390^0C$ cases and the simulated $CO$ concentration falls within the experimental error bars except for the $311^0C$ condition where the experimental measured $CO$ concentration is 3 ppm and the simulated concentration is 12 ppm. The simulated $NO_2$ concentration falls within the experimental error bars except for temperatures between 390 to $410^0C$ and at $310^0C$. The kinetic parameters used in the simulation are tabulated in Table 4.3.

### Table 4.3

Kinetic parameters used to simulate Johnson Matthey degreened data

<table>
<thead>
<tr>
<th></th>
<th>CO Oxidation</th>
<th>HC Oxidation</th>
<th>NO Oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$(fresh)</td>
<td>1500000.0</td>
<td>1500000.0</td>
<td>4600000.0</td>
</tr>
<tr>
<td>$A$(aged)</td>
<td>1500000.0</td>
<td>1500000.0</td>
<td>1000000.0</td>
</tr>
<tr>
<td>$E_a$(fresh)</td>
<td>55.0</td>
<td>55.0</td>
<td>55.0</td>
</tr>
<tr>
<td>$E_a$(aged)</td>
<td>55.0</td>
<td>55.0</td>
<td>55.0</td>
</tr>
<tr>
<td>Inhibition</td>
<td>$A_{a,j}$</td>
<td>$\Delta H_{a,j}$</td>
<td>$A_{a,j}$</td>
</tr>
<tr>
<td>$A_{a,1}$</td>
<td>0.0</td>
<td>7990.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,2}$</td>
<td>7.0E+07</td>
<td>75000.0</td>
<td>20.5</td>
</tr>
<tr>
<td>$A_{a,3}$</td>
<td>0.0</td>
<td>96534.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,4}$</td>
<td>0.0</td>
<td>31036.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$A_{a,5}$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

The test data for the aged DOC consists of several engine speed load points to achieve different DOC inlet temperatures. To simulate the effect of aging, the DOC was aged at $700^0C$ for 100 hrs. The DOC inlet temperatures for the degreened data ranged from 275
to 413°C. The DOC inlet CO concentration varied from 79 to 159 ppm, NO concentrations varied from 165 to 637 ppm, NO₂ concentrations varied from 9 to 29 ppm and HC concentrations varied from 28 to 46 ppm. Figure 4.12 shows a comparison between the experimental and simulated DOC outlet HC, NO₂ and CO concentration for the aged data.

**Figure 4.12.** Comparison of the experimental and simulated DOC outlet HC, NO₂ and CO concentrations for the aged data
To simulate the aged DOC data, the kinetic parameters from the degreened data simulation was used as the starting point. The experimental CO and HC conversion efficiencies for the degreened and aged DOC were similar and to simulate the aged data the kinetic parameters for CO and HC oxidation reactions were not changed. The NO conversion efficiencies for the aged DOC was significantly lower compared to the degreened data. Hence, to simulate the aged data the pre exponential factor for the NO oxidation reaction was changed from 4.6E06 to 1.5E06. Figure 4.12 shows a comparison between the experimental and simulated DOC outlet HC, NO2 and CO concentration for the aged DOC data. The DOC outlet HC, NO2 and CO concentrations are plotted against temperature. The HC concentrations are plotted in ppmC and the CO and NO2 concentrations are plotted in ppm. The experimental data is plotted with an error bar of ±5 ppm. The simulated HC concentration are within the error bars and the simulated CO concentration falls within the experimental error bars except for the 250°C condition where the experimental measured CO concentration is zero and the simulated concentration is 8 ppm. The simulated NO2 concentration falls within the experimental error bars except for the 390°C temperature condition. The kinetic parameters used to simulate both the degreened and aged data are tabulated in Table 4.4. It can be observed that the kinetic parameters for the degreened and aged data are similar except for the NO oxidation reaction pre exponential factor. The results show that with aging, the reactions still have the similar activation energies but the pre exponential factor for NO oxidation is lower. In a OBD model for the DOC, this effect would be important to include since the NO2 into the CPF affects the rate of NO2 production assisted PM oxidation and it would in turn affect the SCR reactions. Since the NO2/NOx ratio is an important parameter for the NOx conversion efficiencies and the NH3 slip [1].
Table 4.4
Kinetic parameters used to simulate Johnson Matthey degreened and aged data

<table>
<thead>
<tr>
<th></th>
<th>CO Oxidation</th>
<th>HC Oxidation</th>
<th>NO Oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ (degreened)</td>
<td>1500000.0</td>
<td>1500000.0</td>
<td>4600000.0</td>
</tr>
<tr>
<td>$A$ (aged)</td>
<td>1500000.0</td>
<td>1500000.0</td>
<td>1000000.0</td>
</tr>
<tr>
<td>$E_a$ (degreened)</td>
<td>55.0</td>
<td>55.0</td>
<td>55.0</td>
</tr>
<tr>
<td>$E_a$ (aged)</td>
<td>55.0</td>
<td>55.0</td>
<td>55.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Inhibition*</th>
<th>$A_{a,j}$</th>
<th>$\Delta H_{a,j}$</th>
<th>$A_{a,j}$</th>
<th>$\Delta H_{a,j}$</th>
<th>$A_{a,j}$</th>
<th>$\Delta H_{a,j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{a,1}$</td>
<td>0.0</td>
<td>7990.0</td>
<td>0.0</td>
<td>7990.0</td>
<td>0.0</td>
<td>7990.0</td>
</tr>
<tr>
<td>$A_{a,2}$</td>
<td>7.0E+07</td>
<td>75000.0</td>
<td>20.5</td>
<td>3000.0</td>
<td>6.8E+08</td>
<td>75000.0</td>
</tr>
<tr>
<td>$A_{a,3}$</td>
<td>0.0</td>
<td>96534.0</td>
<td>0.0</td>
<td>96534.0</td>
<td>0.0</td>
<td>96534.0</td>
</tr>
<tr>
<td>$A_{a,4}$</td>
<td>0.0</td>
<td>31036.0</td>
<td>0.0</td>
<td>31036.0</td>
<td>0.0</td>
<td>31036.0</td>
</tr>
<tr>
<td>$A_{a,5}$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

*Both degreened and aged data.

4.2 SCR High Fidelity Model

A metal based Zeolite SCR catalyst is commonly for heavy duty diesel application. The function of the SCR is to reduce the $NO_X$ in the exhaust to $N_2$ and $H_2O$. To achieve this, urea is injected into the exhaust upstream of the SCR. The urea thermally decomposes to $NH_3$ and adsorbs onto the surface of the catalyst. The urea decomposition is a complex function which depends on the SCR inlet temperature, flowrates and injection profile\[59\]. The urea decomposes in the exhaust and on the catalyst surface[60]. Some of the $NH_3$ reacts with the $NO$ and $NO_2$ on the catalyst surface to form $N_2$ and $H_2O$ and the rest of the $NH_3$ is stored in the catalyst through adsorption. In addition, $NH_3$ slip occurs which is oxidized by the AMOX catalyst brick at the SCR outlet. The stored ammonia either reacts with the $NO_X$ or desorbs from the catalyst surface to the exhaust. Several 1D high-fidelity
models similar to the model described in this study have been reported in the literature\cite{34, 54, 61, 62}.

The model described in this section was developed by Song et al in reference\cite{1}. The model was developed to simulate the copper-Zeolite SCR used in the aftertreatment system Cummins ISB 2010 engine described in section \cite{3}. The bench reactor \cite{63} and engine dynamometer\cite{64} data were used to calibrate the model. The model and the calibration is briefly described in this dissertation since it is used in the developing the SCR reduced order model.

4.2.1 Reactions in the SCR

The $NH_3$ storage is modeled using two storage sites, site 1 participates in the $NH_3$ storage and $NO_X$ reduction where as site 2 participates only in the storage of $NH_3$ \cite{63, 64}. The reduction of the $NO_X$ take place through three main reaction mechanisms\cite{61, 62, 65}: standard, fast and slow SCR reactions as shown in equations \cite{4.20, 4.21, 4.22, 4.23} in reference \cite{61}.

$NH_3$ adsorption:

\begin{align*}
Site1 & : NH_3 + S_1 \rightarrow NH_{3,1}^* \\
Site2 & : NH_3 + S_2 \rightarrow NH_{3,2}^* 
\end{align*}

\hspace{1cm} (4.15)

\hspace{1cm} (4.16)

$NH_3$ desorption:

\begin{align*}
Site1 & : NH_{3,1}^* \rightarrow NH_3 + S_1 \\
Site2 & : NH_{3,2}^* \rightarrow NH_3 + S_2 
\end{align*}

\hspace{1cm} (4.17)

\hspace{1cm} (4.18)
$NH_3$ oxidation:

$$NH_{3,1}^* + \frac{3}{4}O_2 \rightarrow \frac{1}{2}N_2 + \frac{3}{2}H_2O \quad (4.19)$$

Standard SCR 1:

$$Site1: \ NH_{3,1}^* + NO + \frac{1}{4}O_2 \rightarrow N_2 + \frac{3}{2}H_2O \quad (4.20)$$

Standard SCR 2:

$$Site1: \ NH_{3,1}^* + \frac{3}{5}NO + \frac{9}{20}O_2 \rightarrow \frac{4}{5}N_2 + \frac{3}{2}H_2O \quad (4.21)$$

Fast SCR:

$$Site1: \ NH_{3,1}^* + \frac{1}{2}NO + \frac{1}{2}NO_2 \rightarrow N_2 + \frac{3}{2}H_2O \quad (4.22)$$

Slow SCR:

$$Site1: \ NH_{3,1}^* + \frac{3}{4}NO_2 \rightarrow \frac{7}{8}N_2 + \frac{3}{2}H_2O \quad (4.23)$$

NO oxidation:

$$Site1: \ NO + \frac{1}{2}O_2 \leftrightarrow NO_2 \quad (4.24)$$

$N_2O$ formation:

$$Site1: \ NH_{3,1}^* + \frac{4}{3}NO_2 \rightarrow \frac{7}{6}N_2O + \frac{3}{2}H_2O \quad (4.25)$$

These reactions are exponential functions in temperature, hence the $NO_X$ reduction performance of the SCR is also a function of the temperature. There are two main types of the commercially available Zeolite based SCR’s in production in the U.S depending on the catalyst formulation: Iron-Zeolite(Fe-Ze) and Copper-Zeolite(Cu-Ze). Among the two SCR catalysts, the Cu-Zeolite SCR performs better at low temperatures\[66–68\]. Several studies\[61,66\] have shown that the maximum $NO_X$ conversion efficiency can be achieved at $\frac{NO_2}{NO_X} = 0.5$ for both Fe-Zeolite and Cu-Zeolite catalysts.
4.2.2 Mass and Energy Balance Equations

The differential equations describing the high-fidelity SCR model are shown in Equations 4.26 to 4.29. Equations 4.26 and 4.27 is the species balance equation for NH$_3$, NO, NO$_2$, and N$_2$O.

\[
\epsilon \frac{\partial C_{g,i}}{\partial t} = -u \frac{\partial C_{g,i}}{\partial x} - \beta_i A_g (C_{g,i} - C_{s,i}) \quad (4.26)
\]

\[
(1 - \epsilon) \frac{\partial C_{s,i}}{\partial t} = \beta_i A_g (C_{g,i} - C_{s,i}) - \sum_{i=NH_3}^{N_2O} n_{i,j} R_j \quad (4.27)
\]

\[i = NH_3, NO, NO_2, N_2O \quad \text{&} \quad j = \text{Ads, Des, Std, Fst, Slo, Oxi}\]

The symbol u is the velocity of the exhaust gas in m/s, the $C_i$ are the concentrations of NH$_3$, NO, NO$_2$, and N$_2$O, $n_{i,j}$ is the stoichiometric coefficient and the $R_j$ are the reaction rates. Equations 4.28 and 4.29 describe the NH$_3$ balance equations for NH$_3$ storage sites 1 and site 2 in the two site model [69].

\[
\Omega_1 \dot{\theta}_1 = R_{\text{Ads},1} - R_{\text{Des},1} - 4R_{\text{Oxi}} - 4R_{\text{Std}} - 4R_{\text{Fst}} - 4R_{\text{Slo}} \quad (4.28)
\]

\[
\Omega_2 \dot{\theta}_2 = R_{\text{Ads},2} - R_{\text{Des},2} \quad (4.29)
\]

where, $\theta_i$ are NH$_3$ storage fractions and $\Omega_i$ are storage capacities. The quantities $R_{R_{\text{Ads},1}}$, $R_{R_{\text{Ads},2}}$, $R_{R_{\text{Des},1}}$ and $R_{R_{\text{Des},2}}$ are the adsorption and desorption rates. $R_{\text{Oxi}}$, $R_{\text{Std}}$, $R_{\text{Fst}}$ and $R_{\text{Slo}}$ are the reaction rates for NH$_3$ oxidation, standard SCR, fast SCR and slow
SCR reactions. The rate equations for all the reactions in the SCR are shown below:

\[ R_{\text{Ads},1} = k_{\text{Ads},1} C_{\text{NH}_3,s}(1 - \theta_1) \Omega_1 \]  
\[ R_{\text{Des},1} = k_{\text{Des},1} \theta_1 \Omega_1 \]  
\[ R_{\text{Ads},2} = k_{\text{Ads},2} C_{\text{NH}_3,s}(1 - \theta_2) \Omega_2 \]  
\[ R_{\text{Des},2} = k_{\text{Des},2} \theta_2 \Omega_2 \]  
\[ R_{\text{Oxi,NH}_3} = k_{\text{Oxi,NH}_3} \eta_2 \theta_1 \Omega_1 \]  
\[ R_{\text{Std}} = k_{\text{Std}} C_{\text{NO}_2,s} \eta_2 \theta_1 \Omega_1 \]  
\[ R_{\text{Std}2} = k_{\text{Std}2} C_{\text{NO}_2,s} \eta_2 \theta_1 \Omega_1 \]  
\[ R_{\text{Fst}} = k_{\text{Fst}} C_{\text{NO}_2,s} \theta_1 \Omega_1 \]  
\[ R_{\text{Slo}} = k_{\text{Slo}} C_{\text{NO}_2,s} \theta_1 \Omega_1 \]  
\[ R_{\text{NO}} = k_{\text{NO}} \left( c_{\text{NO}_2,s}^{0.5} \frac{c_{\text{O}_2}}{K_p} \right) \]  
\[ R_{\text{N}_2\text{O}} = k_{\text{N}_2\text{O}} C_{\text{NO}_2,s} \theta_1 \Omega_1 \]

The reaction rate coefficients \( k_i \) are of the Arrhenius form and are expressed as:

\[ k_i = A_i e^{-\frac{E_{a,i}}{RT}} \]

\[ i = \text{Ads}_1, \text{Des}_1, \text{Ads}_2, \text{Des}_2, \text{Std}_1, \text{Std}_2, \text{Fast, Slow, NOoxidation&N}_2\text{O Formation} \]

Where, \( A_i \) is the pre exponential factor and \( E_{a,i} \) is the activation energies for the \( i^{th} \) reaction.
4.2.3 High Fidelity Model Calibration

The SCR high fidelity model was calibrated to both the engine and the reactor data. The details of the calibration process and the data are described in references \[1,63,64\]. This section shows the results for one of the test cases (test point 8) in Table 3.5.

Figure 4.13. Comparison of the SCR outlet NO, NO\(_2\), and NH\(_3\) concentrations between the experimental and the high-fidelity model corrected for sample line effects\[1\].

Figure 4.13 shows a comparison of the SCR outlet NO, NO\(_2\), and NH\(_3\) concentration between the mass spectrometer experimental data and the high-fidelity model. The first
subplot shows the SCR inlet $NH_3$, $NO$ and $NO_2$ concentrations. The $NO$ and $NO_2$ concentrations are maintained constant for the entire test and the inlet $NH_3$ concentration is varied by controlling the urea injector located upstream of the SCR to achieve different levels of $NH_3/NO_X$ ratio. The second subplot shows the comparison of the SCR outlet $NO$ concentration. It is observed that the high fidelity model simulates the experimental $NO$ concentration profile with less than ± 30 ppm error. The third subplot shows the comparison of the SCR outlet $NO_2$ concentration. Similar to $NO$ the that the high fidelity model simulates the experimental $NO_2$ concentration profile with less than ±/-20 ppm error. The fourth subplot shows the comparison of the SCR outlet $NH_3$ concentration. An exhaust sample line model described in reference[1,64] was used to simulate the effect of adsorption of the $NH_3$ in the sample line. The high-fidelity model follows the experimental $NH_3$ concentration profile with less than ±/-48 ppm error when the simulation results are corrected for the sample line adsorption/desorption effects.

4.3 SCR Aged Data Simulation

The testing for the aged SCR was conducted at Oak Ridge National Laboratories on an SCR core sample of 8 cm length and 2 cm diameter. The data for both degreened and aged core samples were acquired on a reactor setup and Spaci-IR measurement technique was used to measure the emissions. The cores were degreened for 4 hours at $700^0C$ and aged core was aged at $800^0C$ for 16 hours. The simulation of the degreened and aged SCR with the SCR highfidelity model was done by Xiaobo Song as part of his PhD research work and detailed description of the test setup and the core samples is described in reference [1]. The experimental results showed the aging process does not change the overall $NO_X$
conversion efficiencies but changes the axial concentration profiles. The experimental data also showed that the $NH_3$ storage capacity for aged SCR is 30% lower compared to the degreened SCR.

The SCR high fidelity model was used to simulate both the degreened and aged SCR data. The kinetic parameters simulate the axial $NH_3$ storage and axial $NO$, $NO_2$ and $NH_3$ concentration profiles were identified. Table 4.5 shows the important kinetic parameters that were different between the degreened and aged SCR data. The table shows that the $NH_3$ storage capacity for the aged SCR is lower compared to the degreened SCR. The table also shows the activation energies for the $NH_3$ desorption, $NH_3$ oxidation, fast SCR and standard SCR reactions for aged SCR are lower compared to the degreened SCR.

### Table 4.5

<table>
<thead>
<tr>
<th>Parameter</th>
<th>De-greened</th>
<th>Aged</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Omega$</td>
<td>138</td>
<td>94.6</td>
<td>$gmol/m^3$</td>
</tr>
<tr>
<td>$E_{ads}$</td>
<td>0</td>
<td>0</td>
<td>$kJ/gmol$</td>
</tr>
<tr>
<td>$E_{des}$</td>
<td>38.2</td>
<td>28.6</td>
<td>$kJ/gmol$</td>
</tr>
<tr>
<td>$A_{NH_3Oxi}$</td>
<td>1.35E+04</td>
<td>5.81E+02</td>
<td>$1/s$</td>
</tr>
<tr>
<td>$E_{NH_3Oxi}$</td>
<td>86</td>
<td>66.3</td>
<td>$kJ/gmol$</td>
</tr>
<tr>
<td>$A_{Fast}$</td>
<td>1.40E+08</td>
<td>6.13E+06</td>
<td>$m^6/gmol^2.s$</td>
</tr>
<tr>
<td>$E_{Fast}$</td>
<td>52.8</td>
<td>41.6</td>
<td>$kJ/gmol$</td>
</tr>
<tr>
<td>$A_{Std}$</td>
<td>9.99E+04</td>
<td>2.33E+04</td>
<td>$m^3/gmol.s$</td>
</tr>
<tr>
<td>$A_{Std}$</td>
<td>47.3</td>
<td>39.9</td>
<td>$kJ/gmol$</td>
</tr>
</tbody>
</table>

It was concluded that the aging of the SCR results in 30% lower $NH_3$ storage capacity and the aging also decreases the activation energies for $NH_3$ desorption, $NH_3$ oxidation, fast SCR and standard SCR reactions. The results showed that the SCR aging does not change the overall $NO_X$ conversion efficiency of the SCR but changes the axial $NH_3$ storage and $NO$, $NO_2$ and $NH_3$ concentration profiles.
5. **DOC and SCR Reduced Order Models**

The high fidelity models are accurate in predicting the outlet concentrations and temperatures from a DOC and a SCR. But these models are computationally demanding and state estimation strategies are difficult to implement with them. Hence, reduced order models are an important part of state estimation which is the focus of this dissertation. The reduced order models are often based on the complex models, but some assumptions are made to reduce the computational resources needed. This section describes the development of the reduced order models for the DOC and the SCR. To reduce the order of the model, the following assumptions were made:

1. The reactions are instantaneous \( \Rightarrow \frac{\partial C_g}{\partial t} = \frac{\partial C_s}{\partial t} = 0 \)

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, \( T = T_g = T_s \).

The assumption 2 results in the elimination of the mass transfer coefficients from the mass balance equations and the assumption 3 results in the elimination of the heat transfer coefficients from the energy balance equations. If the DOC and SCR operates in a space
velocity range where the reactions are mass transfer limited, then the reduced order model will not be able to simulate the reactions. The mass transfer coefficients could be simulated but it would make reduced order model and the estimator significantly more complex computationally.

5.1 DOC Reduced Order Model Development

A reduced order DOC model to capture the non linear behavior of the DOC was developed based on the high fidelity model in references [28,53]. 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 as used in many high fidelity model studies. This reduces the complexity and reduces the simulation time and computational requirements to simulate the DOC. A schematic highlighting the important differences between the high fidelity and reduced order model is shown in Figure 5.1. A 1-D, single channel representation was developed using MATLAB/Simulink. A discrete time step solver is used to solve the species and energy conservation equations.

Using assumptions 1 and 2, the equations (4.4) and (4.5) reduce to equation (5.1), an ODE for the reduced order model species balance.

\[ \epsilon u \frac{dC_i}{dx} = -r_i \]  
\[ i = CO, NO, NO_2, C_3H_6 \]  

(5.1)

Using the assumption 3, the equations (4.6) and (4.7) reduce to equation (5.2) for the re-
Figure 5.1. Schematic showing the differences between high fidelity and reduced order DOC model energy balance.

\[
\left(\rho_s c_{p,s} + \rho c_v\right) \frac{\partial T}{\partial t} = -\rho u c_p \frac{\partial T}{\partial x} + \frac{A_g}{1 - \epsilon} \sum_{i=1}^{3} \frac{\Delta h_i r_i}{MW_i}
\]

(5.2)

\[i = CO, NO, NO_2, C_3H_6\]

where, \(\rho_s\) and \(c_{p,s}\) are the density and specific heats of the substrate, \(\rho\) is the density of the exhaust gas, \(c_p\) and \(c_v\) are specific heats of the exhaust gas, \(\Delta h_i\) is the enthalpy of the \(CO\), \(NO\) and \(C_3H_6\) oxidation reactions, \(MW_i\) is the molecular weight of \(i^{th}\) species and \(A_g\) is the geometric surface area.
5.2 SCR Reduced Order Model Development

The SCR reduced order model is based on the 1D high-fidelity model \[63,64\]. The SCR model is similar to several models reported in the published literature. The high fidelity model simulates gas and surface phase along with $NH_3$ storage. The model uses two $NH_3$ storage sites to simulate $NH_3$ adsorption and desorption. The important difference between the reduced order and hi-fidelity model is the absence of the separate gas and surface phase in the reduced order model. In the reduced order model, the gas and surface phase are combined to form a representative bulk phase. Figure 5.2 highlights the important differences between the high-fidelity and reduced order SCR model.

![Figure 5.2. Schematic showing the differences between high fidelity and reduced order SCR model](image)

The SCR model consists of adsorption and desorption of $NH_3$ on site 1 and 2. Site 2 also consists of $NH_3$ oxidation, standard SCR, fast SCR, slow SCR, $NO$ oxidation and...
$N_2O$ production reactions. The chemical balance equations describing these reactions are shown in Equations 4.15 through 4.25.

Using the assumption 1 and 2, Equations (4.26) and (4.27) reduces to Equation (5.3), the species balance equation for $NH_3$, $NO$, $NO_2$ and $N_2O$.

\[
\frac{\partial C_i}{\partial t} = -u \frac{\partial C_i}{\partial x} - \sum_j n_{i,j} R_j
\]

\[i = NH_3, NO, NO_2, N_2O \quad & \quad j = Ads, Des, Std, Fst, Slo, Oxi\]

The symbol $u$ is the velocity of the exhaust gas, the $C_i$ are the concentrations of $NH_3$, $NO$, $NO_2$ and $N_2O$, $n_{i,j}$ is the stoichiometric coefficient and the $R_j$ are the reaction rates. The $NH_3$ balance equations for the high fidelity and reduced order models are the same. Equations (5.4) and (5.5) are the $NH_3$ balance equations for storage site 1 and 2 respectively.

\[
\Omega_1 \dot{\theta}_1 = R_{Ads,1} - R_{Des,1} - 4R_{Oxi} - 4R_{Std} - 4R_{Fst} - 4R_{Slo}
\]

\[
\Omega_2 \dot{\theta}_2 = R_{Ads,2} - R_{Des,2}
\]

where, $\theta_i$ are $NH_3$ storage fractions and $\Omega_i$ are storage capacities. The quantities $RR_{Ads,1}$, $RR_{Ads,2}$, $RR_{Des,1}$ and $RR_{Des,2}$ are the adsorption and desorption rates. $R_{Oxi}$, $R_{Std}$, $R_{Fst}$ and $R_{Slow}$ are the reaction rates for $NH_3$ oxidation, standard SCR, fast SCR and slow SCR reactions. The reaction rate and rate coefficients are the same as the hi-fidelity model and are described in Equations 4.30 to 4.40.
5.3 DOC Reduced Order Model Calibration

The DOC reduced order model was simulated with the steady state and active regeneration data and compared to the high fidelity model and the experimental data. The steady state data was collected for three different space velocities $162k$, $235k$ and $281khr^{-1}$. At each of these space velocities the DOC inlet temperatures were varied. The active regeneration tests was collected for three space velocities of $162k$, $235k$ and $281khr^{-1}$ at a DOC inlet temperature of greater than $320^0C$. The incylinder hydrocarbon injection at the DOC inlet was varied to achieve different DOC outlet temperatures.

5.3.1 Steady State Simulation

The test matrix for steady state testing consists of three space velocities of $162k$, $235k$ and $281khr^{-1}$. The DOC inlet temperature was varied and the $NO$, $CO$ and $HC$ conversion across the DOC was measured. Table 5.1 shows the space velocities and the DOC inlet temperatures used for the steady state testing conditions. More details about the test setup, test conditions and calibration of high fidelity model to the data can be found in reference[53].

<table>
<thead>
<tr>
<th>Space Velocities($hr^{-1}$)</th>
<th>Inlet Temperature($^0C$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>162k</td>
<td>237-457</td>
</tr>
<tr>
<td>235k</td>
<td>252-492</td>
</tr>
<tr>
<td>281k</td>
<td>273-507</td>
</tr>
</tbody>
</table>

Table 5.1

Steady state testing conditions
To simulate the experimental data with the reduced order model, some of the calibration constants were changed from the high fidelity model in Table 4.2. With the high fidelity $NO$ oxidation kinetic parameters, the reduced order model was predicting higher $NO_2/NO_X$ ratios at temperatures $450^\circ C$ and above. To simulate the DOC outlet $NO_2/NO_X$ at higher temperatures, the inhibition factor associated with $NO$ concentrations was set to $15.0E05$ and the pre exponential for $NO$ oxidation was changed to $10.15E05$. The complete list of calibration constants are given in Table 5.2.

### Table 5.2

Kinetic parameters used to simulate steady state data

<table>
<thead>
<tr>
<th></th>
<th>CO Oxidation</th>
<th>HC Oxidation</th>
<th>NO Oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activation Energy</td>
<td>894000.0</td>
<td>10000.0</td>
<td>715000.0</td>
</tr>
<tr>
<td>Preexponential Factor</td>
<td>39.0</td>
<td>25.0</td>
<td>46.4</td>
</tr>
<tr>
<td>Inhibition</td>
<td>$A_{a,j}$, $\Delta H_{a,j}$</td>
<td>$A_{a,j}$, $\Delta H_{a,j}$</td>
<td>$A_{a,j}$, $\delta H_{a,j}$</td>
</tr>
<tr>
<td>$A_{a,1}$</td>
<td>0.0, 7990.0</td>
<td>0.0, 7990.0</td>
<td>0.0, 7990.0</td>
</tr>
<tr>
<td>$A_{a,2}$</td>
<td>7.0E+07, 75000.0</td>
<td>20.5, 3000.0</td>
<td>6.8E+08, 75000.0</td>
</tr>
<tr>
<td>$A_{a,3}$</td>
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<td>0.0, 96534.0</td>
<td>0.0, 96534.0</td>
</tr>
<tr>
<td>$A_{a,4}$</td>
<td>0.0, 31036.0</td>
<td>0.0, 31036.0</td>
<td>150000.0, 31036.0</td>
</tr>
<tr>
<td>$A_{a,5}$</td>
<td>0.0, 0.0</td>
<td>0.0, 0.0</td>
<td>0.0, 0.0</td>
</tr>
</tbody>
</table>
Figure 5.3 shows the comparison of the HC conversion efficiencies between the measured experimental, high fidelity model and the reduced order model for three space velocities. The reduced order model agrees with the experimental and high fidelity model DOC HC conversion efficiencies within ±12%. The CO conversion plot is not shown here since the CO conversion across the DOC during steady state conditions were close to 100% for all the space velocities and the reduced order model agrees with the experimental data.
Figure 5.4. Comparison of DOC outlet $NO_2/NO_X$ ratios between the high fidelity and reduced order model for the steady state data

Figure 5.4 shows a comparison of the DOC outlet $NO_2/NO_X$ ratios from the high fidelity and reduced order model with the experimental measurements for the three space velocities. The reduced order model agrees with the experimental and the high fidelity model DOC outlet $NO_2/NO_X$ ratios generally within maximum error of ± 30%. Table 5.3 shows the tabulated values of the comparison of the experimental and simulated CO, NO, NO2 and HC concentrations for the steady state testing. The table also shows the error between the simulated and experimental DOC outlet NO2 concentration in ppm and percent which ranged from −50 to 15 ppm and −60 to 10%. Typically the NO2 concentrations were within ±20 ppm.
Table 5.3
Comparison of the reduced order simulated and the experimental DOC outlet CO, NO, NO$_2$ and HC concentrations for the steady state data

<table>
<thead>
<tr>
<th>$T_{inlet}$</th>
<th>Experimental</th>
<th></th>
<th>Simulated</th>
<th>$\Delta NO_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CO ppm</td>
<td>NO ppm</td>
<td>NO$_2$ ppm</td>
<td>HC ppm</td>
</tr>
<tr>
<td>237</td>
<td>0</td>
<td>150</td>
<td>182</td>
<td>13</td>
</tr>
<tr>
<td>296</td>
<td>0</td>
<td>102</td>
<td>232</td>
<td>9</td>
</tr>
<tr>
<td>315</td>
<td>0</td>
<td>128</td>
<td>298</td>
<td>8</td>
</tr>
<tr>
<td>352</td>
<td>1</td>
<td>170</td>
<td>288</td>
<td>6</td>
</tr>
<tr>
<td>399</td>
<td>0</td>
<td>329</td>
<td>276</td>
<td>4</td>
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<td>374</td>
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<td>288</td>
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<td>431</td>
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<td>457</td>
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<td>4</td>
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<td>272</td>
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<td>111</td>
<td>209</td>
<td>11</td>
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<td>252</td>
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<td>275</td>
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<td>131</td>
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<td>23</td>
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<td>182</td>
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<tr>
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<td>148</td>
<td>179</td>
<td>11</td>
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<td>142</td>
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<tr>
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<td>83</td>
<td>7</td>
</tr>
<tr>
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<td>1</td>
<td>299</td>
<td>170</td>
<td>8</td>
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<td>110</td>
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<td>5</td>
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<td>109</td>
<td>192</td>
<td>14</td>
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<td>375</td>
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<td>71</td>
<td>4</td>
</tr>
<tr>
<td>356</td>
<td>0</td>
<td>132</td>
<td>181</td>
<td>12</td>
</tr>
</tbody>
</table>
5.3.2 Active Regeneration Simulation

The active regeneration experiments were done on the test setup described in chapter 3. Three test points corresponding to different space velocities with the DOC inlet temperatures of greater than 320°C were selected. The hydrocarbon injection was varied to achieve DOC outlet temperatures from 500-600°C. Table 4 shows the engine conditions used for active regeneration testing. The DOC inlet and outlet concentrations and the temperatures were measured during the experiments. The hydrocarbon concentrations downstream of the DOC were measured and the hydrocarbon concentrations upstream of the DOC were estimated using an energy balance across the DOC. A detailed description of this procedure is given in Reference [4].

Figure 5.5 shows the comparison of the CO conversion efficiencies between the measured, high fidelity model and the reduced order model for three space velocities. The measured CO conversion efficiency shows CO production across the DOC and both the reduced order model and the high fidelity model are not able to simulate this due to the absence of CO production reaction in the model.
Figure 5.5. Comparison of DOC outlet CO conversion efficiencies between the high fidelity and reduced order model for the active regeneration experiments

Figure 5.6 shows the comparison of the $HC$ conversion efficiencies between the measured, high fidelity model and the reduced order model for three space velocities. The observed experimental $HC$ conversion efficiency is always greater than 90% and the reduced order model agrees with the measured and high fidelity model DOC $HC$ conversion efficiencies within +/-6%.
Figure 5.6. Comparison of DOC outlet HC conversion efficiencies between the high fidelity and reduced order model for the active regeneration experiments.

Figure 5.7 shows the comparison of the DOC outlet $NO_2/NO_X$ ratios between the measured, high fidelity model and the reduced order model for three space velocities. The DOC outlet $NO_2/NO_X$ ratios are plotted against the experimental DOC outlet temperatures. The experimental data shows lower $NO$ conversion with the increase in the DOC outlet temperature. The reduced order model agrees with the experimental and high fidelity model DOC $NO_2/NO_X$ ratios within +/-20%.
Figure 5.7. Comparison of DOC outlet $NO_2/NO_X$ ratios between the high fidelity and reduced order model for the active regeneration experiments.

Figure 5.8 shows the comparison of the DOC outlet temperatures between the measured, high fidelity model and the reduced order model for three space velocities. The DOC outlet temperatures are plotted against the experimental DOC outlet temperature along the x axis. The reduced order model agrees with the experimental and high fidelity model DOC outlet temperatures within +/-3%. Table 5.4 shows the tabulated values of the comparison of the experimental and simulated $CO$, $NO$, $NO_2$ and $HC$ concentrations for the active regeneration experiments. The table also shows the error between the simulated and
experimental DOC outlet $NO_2$ concentration in ppm and percent.

![Figure 5.8](image)

**Figure 5.8.** Comparison of DOC outlet temperature between the high fidelity and reduced order model with respect to experimental DOC outlet temperature for the active regeneration experiments.

Table 5.4 shows the tabulated values of the comparison of the experimental and simulated $CO$, $NO$, $NO_2$ and $HC$ concentrations for the steady state testing. The table also shows the error between the simulated and experimental DOC outlet $NO_2$ concentration in ppm and percent which ranged from $-27$ to $43$ ppm and $-100$ to $33\%$. 

85
Table 5.4
Comparison of the reduced order simulated and the experimental DOC outlet CO, NO, NO₂ and HC concentrations for the active regeneration data

<table>
<thead>
<tr>
<th>Experimental DOC Outlet</th>
<th>Simulated DOC Outlet</th>
<th>Δ NO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>T °C</td>
<td>CO ppm</td>
<td>NO ppm</td>
</tr>
<tr>
<td>348</td>
<td>0</td>
<td>183</td>
</tr>
<tr>
<td>497</td>
<td>3</td>
<td>481</td>
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<td>526</td>
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<td>497</td>
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<td>350</td>
<td>0</td>
<td>124</td>
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<td>504</td>
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<td>305</td>
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<tr>
<td>524</td>
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<td>548</td>
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<td>615</td>
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</tr>
<tr>
<td>597</td>
<td>140</td>
<td>312</td>
</tr>
</tbody>
</table>

5.4 SCR Reduced Order Model Calibration

The SCR reduced order model was simulated using the test point 8 to compare the reduced order model to the high fidelity model. The kinetic parameters identified in the high fidelity model [1,64] were used in the reduced order model. More details on the high fidelity model calibration and parameter identification process can be found in reference [1,63,64].

Figure 5.9 shows a comparison of the SCR outlet NO, NO₂ and NH₃ concentrations between the experimental, high-fidelity model and the reduced order model. The first sub-
Figure 5.9. Comparison of the reduced order model with the experimental and high fidelity model results for test 8

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plot shows the SCR inlet $NH_3$, $NO$ and $NO_2$ concentrations. The $NO$ and $NO_2$ concentrations are maintained constant for the entire test and the inlet $NH_3$ concentration is varied by controlling the urea injector located upstream of the SCR to achieve different levels of the $NH_3/NO_X$ ratio. The second subplot shows the comparison of the SCR outlet $NO$ concentration. It is observed that the reduced order model follows the experimental measured $NO$ concentration profile with less than $\pm 30$ ppm error. The third subplot shows the comparison of the SCR outlet $NO_2$ concentration. Similar to $NO$ the reduced order model follows the experimental measured $NO_2$ concentration profile with less than $\pm 20$ ppm error. The fourth subplot shows the comparison of the SCR outlet $NH_3$ concentration. An exhaust sample line model described in reference [1164] was used to simulate the effect of adsorption of the $NH_3$ in the sample line. The reduced order model follows the experimental measured $NH_3$ concentration profile with less than $\pm 48$ ppm error.

5.10 shows a comparison of the SCR outlet $NO_2$, $NO_2$ and $NH_3$ concentration between the experimental and the reduced order model for test point 2. The first subplot shows the SCR inlet $NO_2$, $NO_2$ and $NH_3$ concentrations. The second subplot shows the comparison of the SCR outlet $NO$ concentration. It is observed that the reduced order model follows the experimental measured $NO$ concentration profile with less than $\pm 40$ ppm error. The third subplot shows the comparison of the SCR outlet $NO_2$ concentration. Similar to $NO$, the reduced order model follows the experimental measured $NO_2$ concentration profile with less than $\pm 20$ ppm error. The fourth subplot shows the comparison of the SCR outlet $NH_3$ concentration. The reduced order model follows the experimental measured $NH_3$ concentration profile with a maximum error of $\pm 10$ ppm.
Figure 5.10. Comparison of the reduced order model with the experimental and high fidelity model results for test 2.
6. Extended Kalman Filter (EKF) Estimator Development

This chapter describes the development of the EKF estimators for the DOC and SCR. To develop the EKF estimator, the reduced order DOC and SCR models described in Chapter 5 were used. An EKF estimator for a typical nonlinear discrete system and the implementation of the EKF strategy on the DOC and SCR reduced order models is described in chapter 2. The DOC and SCR EKF estimators are simulated on the surrogate FTP test described in Chapter 3 and the results are quantified.

6.1 DOC Estimator Development

An EKF state estimator, based on an ‘N’ axial element DOC model was developed. To implement the EKF on the DOC reduced order model, the species and energy balance equations were discretized using Euler expansion. The discretized species and energy balance
The states vector for the discrete system was defined as:

\[
\vec{x}_k = \begin{bmatrix}
T_{1,k} \\
T_{2,k} \\
\vdots \\
T_{r-1,k} \\
T_{r,k}
\end{bmatrix}
\]  

(6.3)

The process noise\((\vec{w}_k)\) was neglected and the covariance matrix \((R_k)\) for the observation noise\((\vec{v}_k)\) was constructed using a standard deviation of 0.1. To estimate the covariance matrix \(P_k^-\) the jacobian \(F_k\) was calculated by differentiating equation (6.3)

### 6.2 DOC Estimator Simulation

The DOC estimator was simulated on active regeneration and transient data. The test setup, test matrix and the details of the testing are explained in the Experimental setup section of Chapter 3. The parameters needed for the estimator and their measurement
location and source of measurement is shown in Figure 6.1. The estimator uses the inlet mass flow rate, temperature, pressure, $CO$, $NO$, $NO_2$, $C_3H_6$ and $O_2$ concentrations from the ECU maps along with the upstream $NO_X$ and temperature measurements to estimate the $CO$, $NO$, $NO_2$, $C_3H_6$ and temperature states in the catalyst. For the results shown here, the number of axial elements in both the model and the estimator were fixed at $N=15$. The DOC state estimator and reduced order model use the same set of species balance and energy balance equations.

Figure 6.1. Schematic showing the inputs to the estimator from the sensors and ECU maps

6.2.1 Active Regeneration Test Case Simulation

The estimation goal is to compute $NO$, $NO_2$ and $C_3H_6$ concentrations within the DOC during active regeneration of the CPF when the DOC inlet HC concentrations are between
9000 to 16000 ppm and the temperature increase through the DOC is $200 - 300^\circ C$. Hence a test case representative of the active regeneration condition was used to simulate the estimator. A test case was constructed using an inlet mass flow rate of 0.95 kg/s, inlet temperature of 300°C and inlet concentrations of 434 ppm NO, 24 ppm NO$_2$, 53 ppm CO and 4500 ppm of C$_3$H$_6$. Along with these inputs, the estimator uses the downstream DOC temperature sensor measurement to estimate the states in the DOC. A simulated temperature sensor measurement was constructed using the DOC outlet temperature from the reduced order model. Figure 6.2 shows the simulated temperature sensor measurement with added Gaussian noise.

![Temperature Sensor Measurement](image)

**Figure 6.2.** Simulated temperature sensor measurement with Gaussian noise for test case

The pre exponential factor for HC oxidation used in the estimator is 10% higher than the model. With 10% high pre exponential the initial temperature estimate of the estimator is higher than the model simulated DOC outlet temperature. The estimator uses the temperature signal generated using DOC reduced order model (Figure 6.2) and corrects the
estimated temperature. Figure 6.3 shows the comparison between the simulated and estimated hydrocarbon concentration and temperature at the 10th axial element of the DOC. The 10th element was selected to illustrate the ability of the estimator to predict concentrations and temperatures inside the DOC. In the following figures, simulated concentrations are plotted as a continuous line and the estimated concentrations are plotted with ‘+’ symbols. The estimated hydrocarbon concentration closely follows the simulated hydrocarbon concentration with the maximum error of less than 1.5%. In Figure 6.3, the estimated temperature follows the simulated temperature with the maximum error of less than 0.5%.

**Figure 6.3.** DOC inlet hydrocarbon concentration and a comparison between the simulated and estimated HC concentration and temperature at the 10th element
6.2.2 FTP Transient Cycle Simulation

The performance of the DOC estimator was also evaluated using a engine run with a surrogate FTP cycle. The surrogate FTP test [53] is a simplified FTP cycle which recreates the transients similar to that in an FTP cycle as explained in Chapter 3. For the estimator, the constants identified with the reduced order model were used to simulate the test. The performance of the estimator in open and closed loop is compared. When operated in open loop the estimator does not use the DOC outlet temperature measurement and performs as a DOC model. When operated in closed loop the estimator uses the DOC outlet temperature to correct the temperatures in the DOC.

![Graph](image.png)

**Figure 6.4.** Comparison of the DOC outlet $NO_2$ concentrations and temperatures with the estimator in open loop for the FTP cycle
Figure 6.4 shows the comparison of the DOC outlet $NO_2$ concentrations and the outlet temperature for the surrogate FTP data. The estimator was operated in open loop by setting the optimal Kalman gain to zero. From the figure it can be observed that the estimator DOC outlet temperature does not follow the measured DOC outlet temperature. The temperature has a maximum error of 51%. The error in the temperatures translates to large errors (maximum of 50%) in the estimated DOC outlet $NO_2/NO_X$ ratio. Clearly there is a need to operate in the closed loop.

![Figure 6.4](image)

**Figure 6.5.** Comparison of the DOC outlet $NO_2$ concentrations and temperatures with the estimator in closed loop for the FTP cycle

Figure 6.5 shows the comparison of the DOC $NO_2$ concentrations 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 \( NO_2 \) concentrations for most parts of the test with a maximum error of 26% and a typical error of less than 20 ppm.

Simulation of the high fidelity model on the surrogate FTP test showed that the heat transfer to ambient is important to predict the DOC outlet temperature. Eliminating the heat transfer to ambient in the reduced order model introduced errors in the transient temperature response of the DOC observed in the open loop simulation. In the closed loop simulation the estimator accounts the absence of heat transfer to ambient and reduces the error in the temperature.

### 6.3 SCR Estimator Development

The reduced order SCR model was used as the basis to implement the EKF estimation strategy. The estimator consist of the \( NH_3 \) coverage fraction on site 1 an site 2 as the states and the concentration of \( NH_3 \), \( NO \), \( NO_2 \) and \( N_2O \) are outputs calculated based on the states. To implement the EKF estimation strategy, SCR the states for the SCR system is defined as:

\[
\bar{x}_k = \begin{bmatrix}
\theta_{1,k} \\
\theta_{2,k} \\
\vdots \\
\theta_{r-1,k} \\
\theta_{r,k}
\end{bmatrix}
\]  

(6.4)
To calculate the Jacobian matrix the relationship of $\theta_1$ and $\theta_2$ with $NH_3$, $NO$ and $NO_2$ concentration was used. The details of the Jacobian matrix calculation is found in Appendix C. To implement an EKF on the SCR reduced order model, the process noise ($w_k$) was neglected and a standard deviation of 0.1 was used to construct the covariance matrix ($R_k$). Figure 6.6 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 $NO_X$ sensor upstream (or $NO_X$ 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. Figure 6.6 shows a schematic of the state estimator along with the inputs needed.

![Figure 6.6. Schematic of the inputs to the SCR state estimator with the sensors downstream of the SCR](image)

The model for the $NO_X$ and $NH_3$ sensors were developed using the experimental
measured concentrations of NO, NO₂ and NH₃. The model for the NOₓ sensor was developed based on the NOₓ sensor model described in reference[70]. The equation 6.5 describes the NOₓ sensor model.

\[ NO_x \text{ sensor} = a_0 + a_1 \times NO + a_2 \times NO_2 + a_3 \times NH_3 \] (6.5)

The constants \( a_0, a_1, a_2 \) and \( a_3 \) were identified using the surrogate FTP data described in chapter 3. More detailed description of the model and the calibration procedure is described in Appendix A. The NH₃ sensor model is similar to the NOₓ sensor model and is described in reference[1] and equation 6.6.

\[ NH_3 \text{ sensor} = b_0 + b_1 \times NO + b_2 \times NO_2 + b_3 \times NH_3 \] (6.6)

NH₃ sensor sensitivity to NO and NO₂ was found to be zero. Hence the constants \( b_0, b_1 \) and \( b_2 \) were set to zero. The constant \( b_3 \) was found to be 1.17.

## 6.4 SCR Estimator Simulation and the Effect of NOₓ and NH₃ Sensors on State Estimation Quality

The performance of the SCR estimator was evaluated using engine data from the surrogate FTP cycle and three different SCR outlet sensor configurations: NOₓ only, NH₃ only and both NOₓ and NH₃. The surrogate FTP test [1,64] is a simplified FTP cycle which recreates the transients similar to that in an FTP cycle as explained in Chapter 3. For the estimator, the constants identified with the reduced order model were used to simulate the
test. The $NO_X$ and $NH_3$ sensor signals along with the measured inputs to the SCR were used as estimator model inputs.

Figure 6.7 shows a comparison of the SCR outlet $NO$ and $NO_2$ concentrations and $NH_3$ sensor signal with the estimator in open loop. The estimator was operated in open
loop by setting the optimal Kalman gain to zero (the estimator does not use either the $NO_X$ or $NH_3$ sensor measurements). The SCR outlet $NH_3$ sensor signal predicted by the estimator is lower than the measured value with the maximum error of $\pm 226 \text{ ppm}$ and the fit for SCR outlet $NO$ and $NO_2$ concentration has a maximum error of $\pm 150 \text{ ppm}$.

![Figure 6.8. Comparison of the measured and estimated SCR outlet $NO$ and $NO_2$ concentrations and $NH_3$ sensor signal for the FTP cycle with the estimator in closed loop - with both $NO_X$ and $NH_3$ sensor downstream of the SCR](image)

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The estimator was operated in closed loop and Figure 6.8 shows a comparison of the SCR outlet $NO$ and $NO_2$ concentrations and $NH_3$ sensor signal. From the figure it can be observed that the estimator in closed loop simulates the SCR outlet $NH_3$ sensor with a maximum error of $\pm 24$ ppm. To reduce the error in the $NO_X$ and $NH_3$ sensor signals, the estimator changes the $NH_3$ storage states. The open loop simulation of the estimator shows that the SCR estimator does not simulate the $NH_3$ desorption accurately. When operated in closed loop, the estimator uses the sensor measurements to correct the $NH_3$ desorption such that the error in the SCR outlet $NO_X$ and $NH_3$ sensors are reduced.

![Comparison of the $NH_3$ storage between an open loop and closed loop estimator for the FTP cycle - with both $NO_X$ and $NH_3$ sensor downstream.](image)

**Figure 6.9.** Comparison of the $NH_3$ storage between an open loop and closed loop estimator for the FTP cycle - with both $NO_X$ and $NH_3$ sensor downstream.
Figure 6.9 shows a comparison of the \(NH_3\) storage estimate from the open loop and closed loop estimator. The figure shows the \(NH_3\) storage plotted as a function of time. The first subplot shows the total stored \(NH_3\) and the second and third subplot shows the \(NH_3\) stored for site 1 and site 2. The plot shows that the estimated \(NH_3\) storage is similar to that of the reduced order model. With the improved \(NH_3\) storage estimate, the estimator reduced the error in the \(NO\ NO_2\) and \(NH_3\) concentrations at the SCR outlet.

With the improved estimate of the \(NH_3\) storage the error in the \(NO\) and \(NO_2\) concentration is reduced from ±150 ppm to ±75 ppm and the error in \(NH_3\) concentration is reduced from ±226 ppm to ±24 ppm.

### 6.4.1 Effect of \(NO_X\) and \(NH_3\) Sensors on State Estimator

The objective of this part of the study is to evaluate the effect of sensors on the state estimation quality. Based on the available sensors there are three possible sensor combinations that can be used for the SCR state estimator at the outlet of the SCR. The possible sensor combinations are:

1. Both \(NH_3\) and \(NO_X\) sensors.
2. \(NO_X\) sensor only.
3. \(NH_3\) sensor only.

Figure 6.8 showed the results from case 1, with both \(NH_3\) and \(NO_X\) sensors at the SCR outlet. With both \(NH_3\) and \(NO_X\) sensors at the SCR outlet, the error in the SCR outlet \(NH_3\) sensor is less than ±26 ppm.
Figure 6.10. Comparison of the measured and estimated SCR outlet $NO$ and $NO_2$ concentrations and $NH_3$ sensor signal for the FTP cycle - with just $NO_X$ sensor downstream.

Figure 6.10 shows the plot of SCR outlet $NO$, $NO_2$ concentrations and $NH_3$ sensor signal for case 2 where the estimator uses only the $NO_X$ sensor at the SCR outlet. The plot shows that with just the $NO_X$ sensor downstream of SCR, the maximum error in the esti-
mate of the \(NH_3\) sensor signal of \(\pm 216 \text{ ppm}\) which is seven times the error observed in case 1. The maximum errors are as follows \(NO\) concentration \(\pm 177 \text{ ppm}\), \(NO_2\) concentration \(\pm 192 \text{ ppm}\) and \(NH_3\) sensor signal \(\pm 216 \text{ ppm}\).

Figure 6.11. Comparison of the measured and estimated SCR outlet \(NO\) and \(NO_2\) concentrations and \(NH_3\) sensor signal for the FTP cycle - with just \(NH_3\) sensor downstream.
Figure 6.11 shows the plot of SCR outlet $NO$, $NO_2$ concentrations and $NH_3$ sensor signal for case 3 where the estimator uses only the $NH_3$ sensor at the SCR outlet. The plot shows that with just the $NH_3$ sensor downstream of SCR, the maximum error in the estimate of the $NH_3$ sensor signal is $\pm 40$ ppm which is higher than case 1 but lower than case 2. The maximum error in the NO concentration is $\pm 72$ ppm and the $NO_2$ concentration is $\pm 125$ ppm.

Table 6.1
Maximum errors and the standard deviation of the errors between the measured and estimated SCR outlet concentrations with $NO_X$ sensor, $NH_3$ sensor and both $NO_X$ and $NH_3$ sensors for the surrogate FTP cycle.

<table>
<thead>
<tr>
<th>Sensors</th>
<th>$NO_X$</th>
<th>$NH_3$</th>
<th>$NO_X$ and $NH_3$</th>
<th>$NO_X$</th>
<th>$NH_3$</th>
<th>$NO_X$ and $NH_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Error</td>
<td>$NO$</td>
<td>177</td>
<td>72</td>
<td>75</td>
<td>27</td>
<td>19</td>
</tr>
<tr>
<td>Error</td>
<td>$NO_2$</td>
<td>193</td>
<td>125</td>
<td>80</td>
<td>46</td>
<td>40</td>
</tr>
<tr>
<td>Error</td>
<td>$NH_3$</td>
<td>216</td>
<td>76</td>
<td>24</td>
<td>38</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 6.1 shows the tabulated values of the maximum errors in the $NO$, $NO_2$ concentrations and $NH_3$ sensor signal along with standard deviation in the errors for the three sensor combinations of $NO_X$ sensor only, $NH_3$ sensor only and both $NO_X$ and $NH_3$ sensors. The case with the just the $NO_X$ sensor at the SCR outlet has the maximum errors in $NO$, $NO_2$ concentrations and $NH_3$ sensor signal and the case with both $NO_X$ and $NH_3$ sensors at the SCR outlet has the least error and the case with just the $NH_3$ sensor has errors in the middle. The standard deviation in the errors is maximum for $NO_X$ sensor only situation and minimum for both the $NO_X$ and $NH_3$ sensor case.

The possible reason for the poor performance of the $NO_X$ sensor only case is the presence of the $NH_3$ in the exhaust after 12 minutes. $NO_X$ sensor model results in Appendix A also show that the $NO_X$ sensor model does not perform well in presence of the $NH_3$. 

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in the exhaust. So to further evaluate the performance of the sensors the test is separated to two sections: no $NH_3$ at the SCR outlet and $NH_3$ at the SCR outlet. Table 6.2 shows the comparison of the maximum errors and the standard deviation in the error when the test is divided to two sections. The table shows that for the $0 - 12$ minutes section of the test the maximum and standard deviation of the errors in $NO$ and $NO_2$ concentrations between the $NO_X$ and $NH_3$ sensor only cases are the same, but the $NH_3$ sensor only case has maximum error of $15ppm$ in $NH_3$ sensor signal compared to $44ppm$ for the $NO_X$ sensor only case. In the $NH_3$ sensor case even though the estimator is correcting the storage based on the $NH_3$ sensor measurement, the magnitude of the corrections are small and do not affect the $NO$ and $NO_2$ conversion across the SCR. But with the information from the $NH_3$ sensor the estimator does reduce the error in $NH_3$ concentration to $15ppm$. This can be observed in Table 6.2 where the $NO_X$ sensor and $NH_3$ sensor cases both have the same maximum error and standard deviation in the error in the $NO$ and $NO_2$ concentrations.

The results between $12 - 20$ minutes show that the maximum and standard deviation of the errors in $NO$, $NO_2$ concentrations and $NH_3$ sensor signal for the $NO_X$ sensor only case is higher than the $NH_3$ sensor only and both $NH_3$ and $NO_X$ sensor case. Based on the results it can be concluded that the under lower $NH_3$ slip conditions both $NO_X$ and $NH_3$ sensor performance is similar and cross sensitivity of the $NO_X$ sensor to $NH_3$ at higher $NH_3$ concentrations is responsible for the higher errors in the $NO_X$ sensor only case.
Table 6.2
Maximum errors and the standard deviation of the errors between the measured and estimated SCR outlet concentrations with $NO_X$ sensor, $NH_3$ sensor and both $NO_X$ and $NH_3$ sensors for the surrogate FTP cycle for two sections of the test

<table>
<thead>
<tr>
<th></th>
<th>Maximum Error (ppm)</th>
<th>Standard Deviation of Error (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$NO_X$ Sensor</td>
<td>$NH_3$ Sensor</td>
</tr>
<tr>
<td>0-12 minutes</td>
<td>NO</td>
<td>76</td>
</tr>
<tr>
<td></td>
<td>NO$_2$</td>
<td>135</td>
</tr>
<tr>
<td></td>
<td>$NH_3$</td>
<td>44</td>
</tr>
<tr>
<td>12-20 minutes</td>
<td>NO</td>
<td>177</td>
</tr>
<tr>
<td></td>
<td>NO$_2$</td>
<td>193</td>
</tr>
<tr>
<td></td>
<td>$NH_3$</td>
<td>216</td>
</tr>
</tbody>
</table>
7. Summary and Conclusions

The DOC high fidelity model was developed to simulate the DOC during steady-state and active regeneration conditions. The DOC model simulates the oxidation of CO, NO and HC across the DOC. The DOC model simulates the gas and surface phase, mass and energy balance equations, which are limited by the mass and heat transfer coefficients. The DOC model was simulated to the steady state test data for three space velocities and active regeneration data with different DOC inlet HC concentrations. The model is unable to match the CO production during active regeneration due to the absence of a CO production reaction in the model. The kinetic parameters for the CO, NO and HC oxidation reactions were identified. The inhibition factors associated with HC oxidized were needed to simulate the experimental data from the active regeneration experiments. The DOC model was simulated on the transient surrogate FTP test. To simulate the DOC model on the transient surrogate FTP test, the heat transfer to ambient was necessary in order to simulate the outlet temperature. The model results shows higher HC concentration at the DOC outlet during the transient test compared to the experimental data. To simulate the DOC on the aged DOC data, the pre exponential factor for NO oxidation was reduced to 78% lower. A procedure to calibrate the DOC model was developed and is described.

DOC reduced order was developed based on the high fidelity model. The assumptions
used in the model reduction resulted in the elimination of the heat and mass transfer co-
efficients from the differential equations. The DOC reduced order model simulates the
oxidation of $CO$, $NO$ and $HC$ in the exhaust. The reduced order model was simulated on
the steady state and active regeneration data. The results showed that including the inhib-
iton effect of $NO$ on the oxidation reactions is sufficient to simulate the experimentally
observed $CO$, $NO$ and $HC$ conversion efficiencies.

The DOC estimator was developed by applying EKF state estimation strategy to the
DOC reduced order model. The DOC estimator uses the DOC inlet $CO$, $NO$, $NO_2$ and
$HC$ concentrations, DOC inlet temperature, mass flow rate, inlet pressure and the DOC
outlet temperature to estimate the concentrations of $CO$, $NO$, $NO_2$ and $HC$ and the tem-
peratures in the DOC. The DOC estimator was simulated on the surrogate FTP test. The
errors in the estimator performance with and without the DOC outlet temperature measure-
ments were quantified.

An SCR reduced order model was derived from the SCR high fidelity model [1]. The
SCR reduced order model simulates the $NH_3$ storage and $NO_X$ reduction reactions. The
SCR reduced order model was simulated on the steady state engine data and compared to
the high fidelity model and the experimental data. The results from the simulation were
quantified in terms of error in the SCR outlet $NO$, $NO_2$ and $NH_3$ concentrations.

The SCR reduced order model was used to develop an EKF estimator for the SCR. The
EKF estimator uses the SCR inlet $NO$, $NO_2$, $O_2$ and $NH_3$ concentrations, temperature,
exhaust mass flow rate and pressure along with the $NO_X$ and/or $NH_3$ sensor at the SCR
outlet to estimate the $NH_3$ storage and $NO$, $NO_2$ and $NH_3$ concentrations in the SCR. The
SCR estimator was simulated on the surrogate FTP data. The estimator is able to correct
for the $NH_3$ concentration measured at the SCR outlet and estimate the $NO$, $NO_2$, $NH_3$
and $NH_3$ storage states of the SCR. The effect of the $NO_X$ and $NH_3$ sensors on the state estimation quality were quantified in terms of the maximum error and standard deviation in the SCR outlet concentrations.

### 7.1 DOC Estimation

Based on the results of simulating the DOC high fidelity model, reduced order model and estimator on the experimental data the following conclusions can be made:

1. The DOC high fidelity and reduced order model is able to simulate the experimental $HC$, $CO$ and $NO$ conversion across the DOC during steady state and active regeneration conditions.

2. To simulate the DOC outlet temperature, $\frac{NO_x}{NO_X}$ ratio and $CO$ concentration the transient cycle, heat transfer to the ambient was added.

3. The results for aged data high fidelity model simulation shows that reactions in an aged DOC have activation energies similar to the degreened DOC, but the pre exponential factors are $78\%$ lower for the $NO$ oxidation reaction.

4. The reduced order DOC model simulation results show that the effect of order reduction on $HC$, $CO$ and $NO$ conversion is not significant.

5. The DOC estimator simulation on active regeneration data shows that it is possible to estimate the DOC outlet $HC$ concentration with a temperature measurement at the DOC outlet.
6. The results from simulating the closed loop estimator simulation on the surrogate FTP cycle shows that the DOC estimator is able to reduce the error in temperatures to less than 0.1%.

7. The improved temperature estimate from the closed loop estimator results in a reduced error (maximum error reduced from 50% to 26%) in the NO$_2$ concentration estimate compared to the open loop estimator on the surrogate FTP cycle test.

### 7.2 SCR Estimation

Based on the results of simulating the SCR high fidelity model, reduced order model and estimator on the experimental data, the following conclusions can be made:

1. The reduced order SCR model agrees with the experimental and high fidelity model NO, NO$_2$ and NH$_3$ concentrations at the SCR outlet within ±40 ppm for NO and NO$_2$ and ±10 ppm for NH$_3$.

2. The closed loop estimator using a NO$_X$ and NH$_3$ sensor downstream is able to provide an accurate estimate of the NO, NO$_2$, NH$_3$ and NH$_3$ storage in the SCR with less than ±80 ppm error in NO, NO$_2$ and NH$_3$ concentrations.

3. With NH$_3$ and NO$_X$ sensors at the SCR outlet, the estimator is able to estimate the NH$_3$ concentration at the SCR outlet with a maximum error of 24 ppm. With only a NO$_X$ sensor at the SCR outlet, the estimator has 9 times higher error in the estimated NH$_3$ concentration at the SCR outlet compared to the NH$_3$ and NO$_X$ sensor combination with a maximum error of 216 ppm. With just the NH$_3$ sensor at
the SCR outlet, the estimator is able to estimate the \( NH_3 \) concentrations at the SCR outlet with a maximum error of 76 ppm. The \( NH_3 \) sensor improves the ability of the SCR EKF estimator to estimate \( NH_3 \) storage.

4. Under lower \( NH_3 \) slip conditions both \( NO_X \) and \( NH_3 \) sensor performance is similar and cross sensitivity of the \( NO_X \) sensor to \( NH_3 \) at higher \( NH_3 \) concentrations is responsible for the higher errors in the \( NO_X \) sensor only case.
REFERENCES


(6) Ronny Allansson and Philip G. Blakeman and Barry J. Cooper and Howard Hess and Peter J. Silcock and Andrew P. Walker, “Optimising the Low Temperature Performance and Regeneration Efficiency of the Continuously Regenerating Diesel Partic-


APPENDIX A. \(NH_3\) Concentration Calculation from DEF Injector Flowrate

The SCR inlet \(NH_3\) cannot be measured directly due to partial decomposition of urea and the limitations of the mass spectrometer. Hence the SCR inlet \(NH_3\) concentrations are estimated using the DEF injector flow rate, urea properties and the exhaust flow rate. DEF is an aqueous solution consisting of 32.5% urea blended with 67.5% of deionized water by weight. The SCR inlet \(NH_3\) concentration is calculated using the equation [A.1]

\[
NH_3 (ppm) = \frac{NH_3 \text{ molar flowrate (kmol/s)}}{\text{exhaust molar flowrate (kmol/s)}} \tag{A.1}
\]

The molar flow rate of \(NH_3\) is calculated with equation [A.2] using the DEF flow rate, density of DEF and the molecular weight of the urea.

\[
NH_3 \text{ molar flowrate (kmol/s)} = \frac{\text{DEF mass flowrate (kg/s)}_{\text{Act}} \cdot \rho_{\text{DEF,Act}} \cdot 0.325 \cdot 2}{MW_{\text{Urea}}} \tag{A.2}
\]
The exhaust molar flow rate is calculated with equation [A.2] using the exhaust mass flow rate, the exhaust gas density and the molecular weight of exhaust.

\[
\text{Exhaust molar flowrate (kmol/s)} = \frac{\text{Exhaust mass flowrate (kg/s)}_{\text{Act}} \times \rho_{\text{Exh,Act}}}{MW_{\text{Exh,Act}}} \quad (A.3)
\]
APPENDIX B. $NO_X$ SENSOR MODEL

The $NO_X$ sensor model was developed based on the model described in reference [70]. The model is an algebraic equation with sensitivities to $NO$, $NO_2$ and $NH_3$ and is described using equation B.1

$$NO_X \text{ sensor} = a_0 + a_1 \cdot NO + a_2 \cdot NO_2 + a_3 \cdot NH_3$$  \hspace{1cm} (B.1)

The parameters $a_1$, $a_2$ and $a_3$ in the model are constants which define the sensitivity of $NO_X$ sensor to $NO$, $NO_2$ and $NH_3$ in the exhaust. To identify these parameters the data from the surrogate FTP test was used. Figure B.1 shows the fit of the $NO_X$ sensor model to the experimental data. The first subplot shows the experimental SCR outlet concentrations of $NO$, $NO_2$ and $NH_3$ in ppm at the SCR outlet against time along the x axis. The second subplot shows the experimentally measured $NO_X$ sensor measurement and the simulated $NO_X$ sensor measurement from the $NO_X$ sensor model in equation B.1. The $NO_X$ sensor model follows the experimental $NO_X$ sensor measurement generally with less than $\pm 20$ ppm error and a maximum error of $\pm 116$ ppm at 40 secs. The constants $a_0$, $a_1$, $a_2$ and $a_3$ for the model are tabulated in table B.1. The magnitude of the parameter $a_0$ was very small compared to the other parameters in equation B.1 and was set to zero.
Figure B.1. Comparison of the $NO_X$ sensor model with the $NO_X$ sensor measurement

Table B.1
Kinetic parameters used to simulate steady state conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>0</td>
</tr>
<tr>
<td>$a_1$</td>
<td>1.23</td>
</tr>
<tr>
<td>$a_2$</td>
<td>0.85</td>
</tr>
<tr>
<td>$a_3$</td>
<td>0.49</td>
</tr>
</tbody>
</table>
APPENDIX C. SCR JACOBIAN

CALCULATIONS

One of the requirements for the EKF estimator is that the differential equations that describe the nonlinear system must be differentiable. The differentiability property of the system equations are used to calculate the state transition matrix for the EKF estimator. Hence calculating the Jacobian matrix for the system is an important calculation in the EKF estimator development. For the SCR EKF estimator developed in this study, the states for the estimator are the \( NH_3 \) storage on site 1 and site 2 for each axial element. The differential equations [5.4] and [5.5] in Chapter 5 describe the mass balance for the \( NH_3 \) storage states. The mass balance equations represented as functions for an SCR with 2 axial elements are tabulated in Table C.1.

Table C.1: States and outputs of an SCR with 2 axial elements

<table>
<thead>
<tr>
<th>Inlet</th>
<th>Axial Element 1 (( x_1 ))</th>
<th>Axial Element 2 (( x_2 ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( NH_3 ) in</td>
<td>( \theta_{1(x_1)}(NH_3, in, NO, in, NO_2, in, T, t) )</td>
<td>( \theta_{1(x_2)}(NH_3, x_1, NO, x_1, NO_2, x_1, T, t) )</td>
</tr>
<tr>
<td>( NO ) in</td>
<td>( \theta_{2(x_1)}(NH_3, in, T, t) )</td>
<td>( \theta_{2(x_2)}(NH_3, x_1, T, t) )</td>
</tr>
<tr>
<td>( NO_2 ) in</td>
<td>( NH_3, (x_1)(NH_3, in, \theta_{1(x_1)}, \theta_{2(x_1)}, T) )</td>
<td>( NH_3, (x_2)(NH_3, x_1, \theta_{1(x_2)}, \theta_{2(x_2)}, T) )</td>
</tr>
</tbody>
</table>

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The $NH_3$ storage of site 1 in the first element is a function of the inlet $NH_3$, $NO$ and $NO_2$ concentrations, temperature, and the $NH_3$ storage from previous time. Similarly the $NH_3$ storage of site 2 in the first element is a function of the inlet $NH_3$ concentration, temperature and the $NH_3$ storage from previous time. The $NH_3$ concentration is a function of the inlet $NH_3$ concentration, $NH_3$ storage in site 1 and site 2 and temperature. The $NO$ and $NO_2$ concentrations are functions of inlet $NO$ and $NO_2$ concentrations, $NH_3$ storage in site 1 and temperature. For the second axial element the $NH_3$ storage and $NO$, $NO_2$ and $NH_3$ concentrations are functions of the concentrations at axial element number 1 and the $NH_3$ storage at axial element 2.

If we observe the functions for the $NH_3$ storage states for element 1 and 2, the differential equations appear to be not differentiable with respect to states. This would mean that $NH_3$ storage for the second element would be unobservable with respect to $NH_3$ storage in element 1. However the observability can be established by using the output equations for $NH_3$, $NO$ and $NO_2$. For the second axial element the $NH_3$ storage for site 1 and 2 can be made differentiable by using chain rule and exploiting the relationship between storage and $NH_3$, $NO$ and $NO_2$ concentrations as shown from equation C.1 to C.4.

\[
\frac{\partial \theta_1(x_2)}{\partial \theta_1(x_1)} = \frac{\partial \theta_1(x_2)}{\partial NH_3(x_1)} \ast \frac{\partial NH_3(x_1)}{\partial \theta_1(x_1)} + \frac{\partial \theta_1(x_2)}{\partial NO(x_1)} \ast \frac{\partial NO(x_1)}{\partial \theta_1(x_1)} + \frac{\partial \theta_1(x_2)}{\partial NO_2(x_1)} \ast \frac{\partial NO_2(x_1)}{\partial \theta_1(x_1)}
\] (C.1)

\[
\frac{\partial \theta_1(x_2)}{\partial \theta_2(x_1)} = \frac{\partial \theta_1(x_2)}{\partial NH_3(x_1)} \ast \frac{\partial NH_3(x_1)}{\partial \theta_2(x_1)}
\] (C.2)
\[
\frac{\partial \theta_2(x_2)}{\partial \theta_2(x_1)} = \frac{\partial \theta_2(x_2)}{\partial NH_3(x_1)} \ast \frac{\partial NH_3(x_1)}{\partial \theta_2(x_1)}
\]  
(C.3)

\[
\frac{\partial \theta_1(x_2)}{\partial \theta_1(x_1)} = \frac{\partial \theta_2(x_2)}{\partial NH_3(x_1)} \ast \frac{\partial NH_3(x_1)}{\partial \theta_1(x_1)}
\]  
(C.4)