Adaptive PI Control of NO_x Emissions in a Urea Selective Catalytic Reduction System using System Identification Models

by

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Abstract

The Urea SCR System has shown great potential for implementation on diesel vehicles wanting to meet the upcoming emission regulations by the EPA. The objective of this thesis is to develop an adaptive controller that is capable of uniformly maintaining a high efficiency and a low ammonia slip in the presence of various uncertainties in the underlying mechanisms as well as the environment that significantly affect the SCR dynamics. Towards this end, the dynamics of the Urea SCR System was modeled using input-output data as a first order transfer function model.Using Stored NH_3 as the output, and Excess $NH_{3,in}$ as input, a systems identification approach was adopted to estimate the values of k and τ, the parameters for the transfer function. A family of these parameter values was determined as the operating conditions of $NH_{3,in}$ and $NO_{x,in}$ were varied. Using a full chemistry model developed in the literature, the model was tested and verified to ensure that an acceptable level of accuracy was being achieved. A closed-loop PI controller was first designed and tested using the Stored NH_3 as the system output. The closed-loop performance of the resulting system was evaluated using the full chemistry model, and was shown to result in an efficiency of 95% or higher, with a maximum NH_3 slip of less than 20 ppm. An adaptive PI controller was then designed and tested, and was shown to lead to comparable performance even as the operating conditions varied. Since Stored NH_3 is not measurable in an actual physical system, the next step was to use the combined state of NH_3 Slip and NO_x Slip as a system output. A novel adaptive PI-controller with nonlinear components and projection maps was developed in order to account for the nonlinear relationship between Stored NH_3 and the new system output. The same metrics of NO_x reduction efficiency and peak ammonia slip were computed for the resulting system during a typical FTP cycle. It was observed the nonlinear adaptive controller was capable of delivering at least 90% NOx efficiency and a peak NH_3 Slip of less than 20 ppm. In conclusion, the Non-Linear Adaptive PI Controller successfuly met the target requirements in the context of a full chemistry simulations.

Thesis Supervisor: Anuradha Annaswamy
Title: Senior Research Scientist

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First, I would like to thank Dr. Annaswamy for her guidance throughout the length of my research period. Her invaluable support and words of advice ensured smooth progress through the months. I would also like to thank Prof. Ghoniem for his insights and pointers that he provided from the start till the end. This research thesis would not have been possible without the support and guidance of the Ford team at the Research and Innovation Center, Ilya Kolmanovsky, Paul Laing, Jeong Kim, Dennis Reed and many others who have helped along the way. Finally, I would like to acknowledge my peers at the Active Adaptive Control Laboratory of MIT, whose comments and suggestions along the way made a world of difference.

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Chapter 1

Introduction

With oil prices soaring up to USD \$140 a barrel over the course of one summer in 2008, it has come to everyone's attention that we needed to find more ways to ease our dependence on fossil fuels, or at least to maximise the value that we get out of every drop. While the introduction of the electric engines and hybrid vehicles give a glimpse of what we might expect in the future, we are already in possession of techonology that is able to help us get the most out of our vehicles; the diesel engine. In order for the diesel engine to be competitive with the gasoline engine that is widely used in passenger vehicles, it needs to first be able to meet the emissions standards set out by the United States Enivironmental Protection Agency (EPA). The objective of this work is to present the use of the Urea Selective Catalytic Reduction (Urea SCR) system with an adaptive controller for the task of regulating the Nitrous Oxides (NO_x) emissions of a diesel engine.

1.1 Motivation

The United States EPA is responsible for the emissions regulations of land vehicles running on diesel engines. Pollutants like NO_x from diesel engines may give rise to air quality problems and human exposure to these can contribute to health issues. In the report of December 2008[1, 2], EPA set the emissions standards for vehicles running on diesel engines to meet the standard of 0.20 g/bhp-hr by the year 2010. In the years leading up to 2010, the emissions standards will be tightened based on a phase-in approach starting from 2004, as shown in Table 1.1.

Year	NO_x Emission Standard (g/bhp-hr)
2004	2.5
2007	1.2
2010	0.2

Table 1.1: NO_x Emissions Standards Phase-In

To meet the tightening emission standards, several aftertreatment systems were developed to be used with diesel engines, namely the Lean NO_x Trap (LNT) and the Urea Selective Catalytic Reduction (Urea SCR) systems. As tasked upon by Ford Motor Company, the Urea SCR system was selected to be the most cost-effective and suitable aftertreatment package to be implemented for the 2010 emissions goal. With the support of the research team at Ford Motor Company, we seek to implement a working adaptive control algorithm on the Urea SCR system.

1.2 Background

The diesel engine differs from the gasoline engine that is found in most passenger cars in the United States. In the gasoline engine, fuel is injected into the combustion chamber premixed with air at a stoichiometric ratio. The aftertreatment system on a gasoline engine, the catalytic convertor, is able to function very effectively as the air-to-fuel ratio is neither lean nor rich. This is not the case for diesel engines, where the normalised air-to-fuel ratio can vary between 0.3 to 1.0. A catalytic convertor will be unable to function efficiently, and a different aftertreatment system needs to be adapted.

1.2.1 Comparison of Diesel and Gasoline Engines

While the diesel engine and gasoline engine are both internal combustion engines, they differ on how the combustion of fuel is achieved. In the gasoline engine, fuel is premixed with air is compressed by the piston and subsequently ignited by sparks from spark plugs. In a diesel engine, the air is compressed first, and fuel is subsequently injected and combustion is achieved through self-ignition. Due to the differences in ignition mechanism, the diesel engine is able to achieve a much higher compression ratio than the gasoline engine. As efficiency of the engine is linked to the compression ratio of the air-fuel mix, the diesel engine is thus able to achieve an improvement in efficiency over the gasoline engine [3].

Lexus GS 450h
Cost: $56,550
Engine: 3.5L V6
HP: 340 (Total)
0 – 60 mph: 5.2 seconds
MPG: 22 (city), 25 (highway)
Cost per mile: $ 0.09 - $ 0.10 / mile

Mercedes-Benz E320 Bluetec
Cost: $54,200
Engine: 3.0L V6
HP: 210 (Net)
0 – 60 mph: 6.6 seconds
MPG: 23 (city), 32 (highway)
Cost per mile: $ 0.07 - $ 0.10 / mile

Figure 1-1: Comparison of Diesel and Hybrid Engine Vehicles[4, 5]

The diesel fuel also consists of longer-chained carbon molecules, as compared to gasoline, and thus has a higher energy density per unit mass. Combined with the more efficient diesel engine, diesel is thus able to achieve better mileage per gallon of fuel. As shown in Figure 1-1, the diesel engine vehicle is able to match the performance of the hybrid gasoline engine[4, 5].

1.2.2 Urea Selective Catalytic Reduction System

A series of aftertreatment systems are employed for cleaning up the exhaust of a diesel engine, and the Urea SCR aftertreatment system is part of it. It is responsible for the treatment of NO_x which consists of both Nitrogen Oxide (NO) and Nitrogen Dioxide (NO_2). The other aftertreatment systems include an upstream Diesel Oxidation Catalyst System (DOC), which removes the Carbon Monoxide (CO) and unburnt Hydrocarbons (HC). A Diesel Particulate Filter (DPF) is placed downstream to remove soot and other particulate matter from the exhaust. Figure 1-2 shows an overview of these three aftertreatment systems.

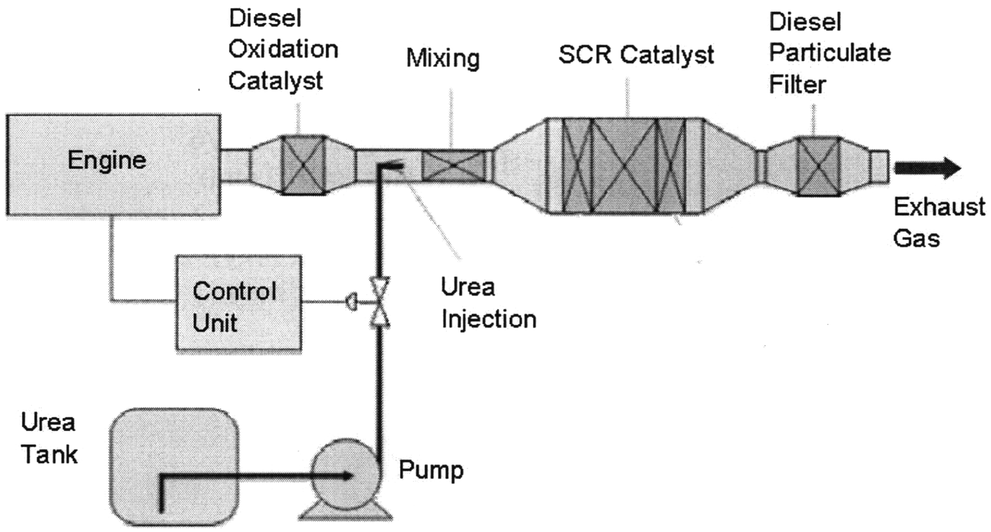


Figure 1-2: Exhaust Aftertreatment Systems

The Urea SCR system works by passing the exhaust through a fine comb of catalyst coating. Figure 1-3 shows a typical cross-sectional view of the catalyst honeycomb[6].

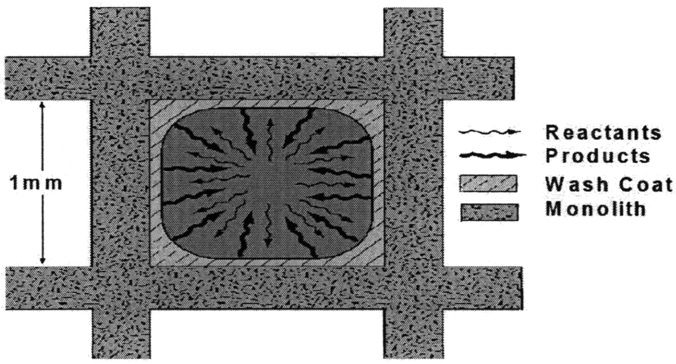


Figure 1-3: Cross-Section View of Urea SCR Catalyst[6]

Chemical reactions take place on the surface on the catalyst results in the converson of NO_x to harmless forms of Nitrogen (N_2) and Water (H_2O)[7]. These chemical reactions include:

Standard SCR Reaction:

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \tag{1.1}$$

Fast SCR Reaction:

$$4NH_3 + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O \tag{1.2}$$

NH_3 Oxidation:

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O \tag{1.3}$$

N_2O Formation:

$$4NH_3 + 4O_2 \rightarrow 2N_2O + 6H_2O \tag{1.4}$$

$$2NH_3 + 2NO_2 \rightarrow N_2O + N_2 + 3H_2O \tag{1.5}$$

$$4NH_3 + 4NO + 3O_2 \rightarrow 4N_2O + 6H_2O \tag{1.6}$$

Equlibrium Reaction:

$$2NO + O_2 \leftrightarrow 2NO_2 \tag{1.7}$$

The main reactions of concern are the Standard SCR Reaction and the Fast SCR Reaction where gaseous ammonia ($NH_{3,gas}$) molecules react with those of NO and NO_2 to form N_2 and H_2O. This is catalyzed by the surface coating via the Eley-Rideal mechanism [8].

$$NH_{3,g} + S_f \leftrightarrow S_{NH_3} \tag{1.8}$$

Free sites (S_f) on the surface of the catalyst coating reacts reversibly with gasous ammonia ($NH_{3,gas}$) to form occupied sites (S_{NH_3})as denoted by Eq. (1.8). This equilibrial process of adsorption and desorption is governed by the relative concentrations of $NH_{3,g}$ and S_{NH_3}. The occupied sites then react with the gaseous of NO and NO_2 to form other products, as shown in Figure 1-4. Molecule A represents the gaseous NO and NO_2, B represents the adsorbed NH_3 and C represents the products.

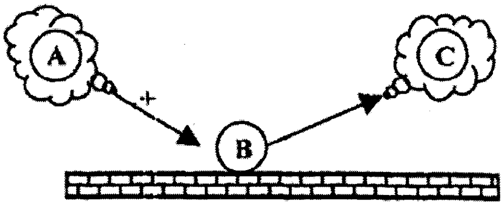


Figure 1-4: Eley-Rideal Mechanism[8]

Challenges

The main challenges of adapting the Urea SCR system are many, and the following lists some the main ones. While this thesis will not be able to address all of them, they have certainly been taken into consideration and when possible, tackled with our best efforts.

1. Need to Maximize NO_x reduction while minimizing NH_3 slip
   Gaseous NH_3 has a very strong, pungent smell that is easily detected even at low concentrations. It is extremely important that only the required amount is injected into the catalyst as any excess ammonia will slip through the tailpipe and present a unfavourable situation.

2. Inability of Catalyst to Control Exhaust Temperature
   The rates of reaction occuring within the catalyst are strong functions of temperature, thus resulting in a significant influence on the overall efficieny of the catalyst. Inability to control the exhaust temperature creates a problem in achieveing a good consistent efficiency of the system.

3. Site Availability is a Strong Function of Temperature

   As presented in the Eley-Rideal Mechanism, the availability of storages sites not only affect the rates of reactions, but fluctuations in temperature might also result in surface desorption that is unfavorable, and cause gaseous NH_3 to slip out of the tailpipe.

4. Undesirable Reactions at High Temperature

   NH_3 oxidation, as presented in Eq. (1.3) results in less available reactants to remove NO_x.

5. Catalyst Poisoning Presence of sulphur components in the exhaust might bind irreversibly with the surface coating and result in less available sites for adsorption gaseous NH_3.

1.2.3 Literature Search

Various approaches that have been reported in the literature was first explored in order to tackle the challenges of the Urea SCR system [6, 7, 8, 9, 10]. Various models that have been proposed in several automotive and mechanical engineering publications as well as their advantages and disadvantages were studied.

Full Chemistry Modeling of the Urea SCR Catalyst

In the SAE article authored by Jeong Kim et. al. [7], the team presented their full chemistry model where they tried to capture the behavior of the catalyst by modeling it as a one dimension single monolith channel. Using energy and mass balances, they formulated simple first order equations involving energy and mass transfer coefficients that were to be determined. These were in the form shown below.

$$\varepsilon \rho_g C_{p,g} V \left(\frac{\delta T_g}{\delta t} + u \frac{\delta T_g}{\delta x}\right) = -h_{in} A_{in} (T_g - T_s) \tag{1.9}$$

$$\varepsilon V \left(\frac{\delta C_{g,i}}{\delta t} + u \frac{\delta C_{g,i}}{\delta x}\right) = -k_m A_{in} (C_{g,i} - C_{s,i}) \tag{1.10}$$

with nomenclature as such:

ε	Channel Porosity
ρ	Density of Gas Phase
C_p	Heat Capacity
V	Catalyst brick Volume
T	Temperature
h_{in}	Heat Transfer Coefficient
A_{in}	Area
C	Concentration of each Species
k_m	Mass Transfer Coefficient

The reaction rates were modeled in the standard Arrhenius form with coefficients to be determined empirically from experimental data. A laboratory-scale flow reactor system was used to run the scale experiments.

$$R_{ad} = k_{ad} e^{\frac{-E_{ad}}{RT}} \tag{1.11}$$

$$R_{des} = K_{des} e^{\frac{-E_{des}(1-\gamma\theta)}{RT}} \tag{1.12}$$

In a demonstration of model application for control purposes, the full scale catalyst was modeled as four individual segments with the urea injections determined by the amount of Stored NH_3 in the second segment. As such, they were able to obtain a trade-off plot between NO_x reduction performance and NH_3 slip, as shown in Figure 1-5.

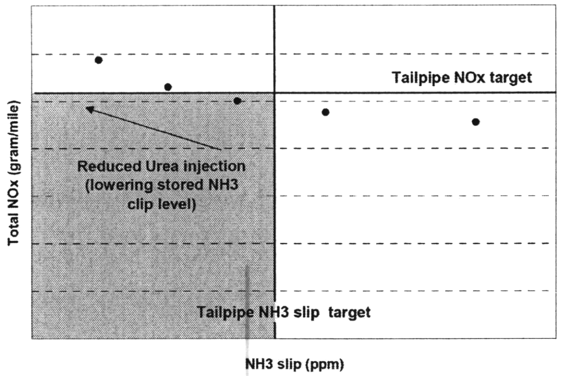


Figure 1-5: TradeOff plot between NO_x and NH_3

Modeling for Control - State Space Approach

In the ASME article by Devesh Upadhyay and Michiel Van Nieuwstadt [8], the authors presented a lumped parameter state space model for the Urea SCR system. In the control oriented model, three states were represented, namely the concentration of NO_x (C_{NO_x}), concentration of NH_3 (C_{NH_3}) and the surface coverage fraction of the catalyst (θ). While having similar conservation of energy and mass equations as Jeong Kim et. al., the model was of zero order and neglected the distribution gradient along the x-axis. Setting the boundary conditions as inputs, and using Orthogonal Collocation with the collocations points at the catalyst inlet and outlet, the state space model was presented as such:

$$\begin{bmatrix} \dot{C}_{NO_x} \\ \dot{\theta} \\ \dot{C}_{NH_3} \end{bmatrix} = \begin{bmatrix} -C_{NO_x}(\Theta_{sc}R_{red}\theta + \frac{F}{V}) + R_{ox}\Theta_{sc}\theta \\ -\theta(R_{ad}C_{NH_3} + R_{des} + R_{red}C_{NO_x} + R_{ox}) + R_{ad}C_{NH_3} \\ -C_{NH_3}(\Theta_{sc}R_{ad}(1-\theta) + \frac{F}{V}) + \Theta_{sc}R_{des}\theta \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{F}{V} \end{bmatrix} U + \begin{bmatrix} \frac{F}{V} \\ 0 \\ 0 \end{bmatrix} d \tag{1.13}$$

$$Y = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} C_{NO_x} \\ \theta \\ C_{NH_3} \end{bmatrix} \tag{1.14}$$

with nomenclature as such:

C	Concentration of each Species
θ	Surface Coverage Fraction of NH_3
Θ_{sc}	Total NH_3 Storage Capacity of Catalyst Coating
R	Reaction rates
F	Exhaust Flowrate
V	Catalyst Volume
U	Gaseous NH_3 injected
d	NO_x input disturbance
Y	Measured Output

Using experimental results to verify the model predictions, the authors concluded that the lumped parameter model was sufficient in capturing the chemical performance of the catalyst, and that it should provide an adequate framework for control design.

Modeling for Control - Systems Identification Approach

In their SAE article, John Chi and Herbert DaCosta [6] presented their work on modeling and control of a Urea SCR system. While their starting point was similar to that of Jeong and Devesh, they proposed a different method of controlling the urea injections. Using their catalyst test bed, they determined the Normalised Stoichiometric Ratio (NSR) $\left(\frac{NH_{3,in}}{NO_{x,in}}\right)$ required for different levels of NH_3 slip at different test conditions. Figure 1-6 shows the relationship between NH_3 slip and NO_x Reduction Efficiency at different NSR levels.

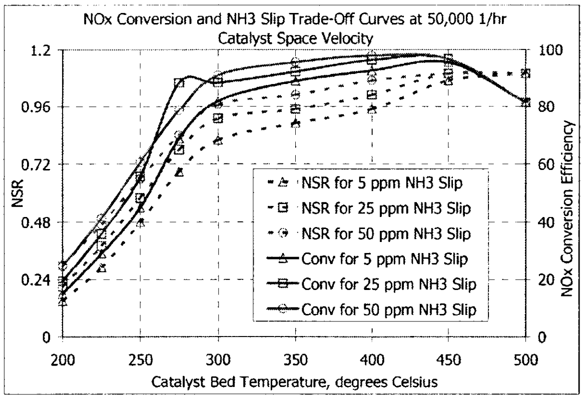


Figure 1-6: NH_3 Slip and NO_x Reduction Efficiency against NSR

A control algorithm was developed using the map of NH_3 Slip against NO_x Reduction Efficiency for a range of operating conditions. With the temperature, space velocity, target NH_3 slip level as inputs, the algorithm is thus able to estimate the achievable NO_x reduction efficieny, and the corresponding NSR for the injection. Subsequently, the response of the system to the range of NSR were captured and plotted in Figure 1-7 below.

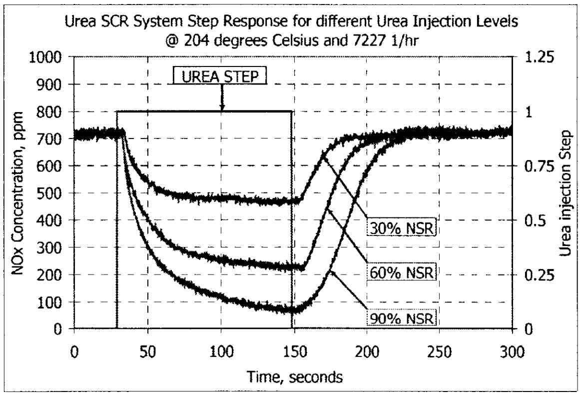


Figure 1-7: NO_x Response to Urea

The authors proposed that the behavior of the NO_x reduction can be modeled as a first-order system of the form shown below.

$$\frac{y(s)}{u(s)} = \frac{b_p}{s + a_p} \tag{1.15}$$

where the transfer function parameters are functions of the system operating conditions, namely inlet NO_x concentraion, inlet NH_3 concentration, amount of Stored NH_3 on the catalyst coat, catalyst space velocity and exhaust gas temperature. This meant that both a_p and b_p would be mapped by a five-dimension look-up table. Using the simplified first order transfer function, the authors then proposed to apply composite adaptive control with the following adaptive laws.

$$u = \hat{a}_r(t)r + \hat{a}_y(t)y \tag{1.16}$$

$$\dot{\hat{a}}_r = -sgn(b_p)\gamma er \tag{1.17}$$

$$\dot{\hat{a}}_y = -sgn(b_p)\gamma ey \tag{1.18}$$

where e is the error signal and γ is the adaptation gain.

Chapter 2

Approach

Results from the literature search yielded many approaches to tackling the problem of controlling a Urea SCR system. While all of them began with a full chemistry model of the catalyst, the simplification of the full chemistry model into a form more suitable for applying control algorithms were varied. In this thesis, we take an alternate approach where input-output data, together with a system-identification procedure is used to determine low-order models of the SCR. In particular, a first-order model is derived, whose accuracy is then compared using a full-chemistry model, using $NH_{3,in}$ as the input and Stored NH_3 as the output.

2.1 FTP Cycle

In order to understand the conditions under which to map the variables of the first order transfer model, the FTP-75 cycle was picked to be the benchmark [11] for vehicle operating conditions. The FTP-75 cycle is used for emission certification of diesel vehicles effective year 2000. It simulates different conditions of driving on the road, and consist of three phases: cold start phase, transient phase and hot start phase. Figure 2-1 shows the vehicle speed against time for the three phases[11].

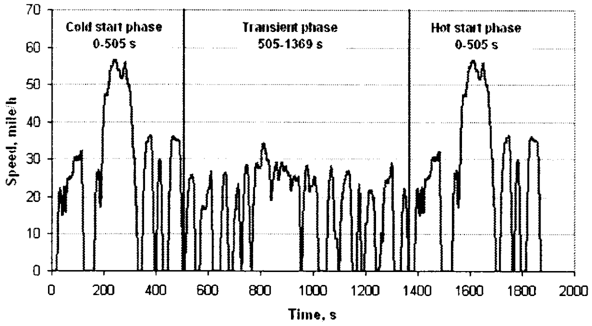


Figure 2-1: FTP-75 Cycle: Vehicle Speed against Time

Translating the FTP-75 cycle vehicle speed and vehicle load into profiles for NO_x in, Space Velocity and Temperature, we get a sense of the range of operating conditions that have to be mapped. Figure 2-2 shows the profiles for these catalyst inputs plotted against time.

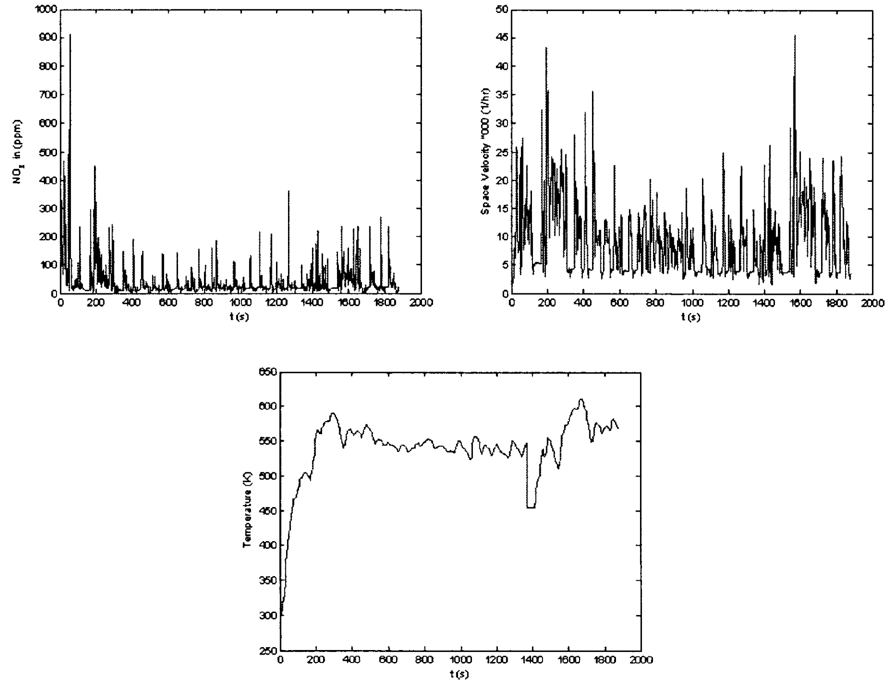


Figure 2-2: Input profiles for NO_x, Space Velocity and Temperature

2.2 Diesel Engine Operating Conditions

Based on the FTP-75 Cycle input profiles, the trim points for mapping the first order transfer function were selected to be as follows:

NO_x in (ppm) 87.5, 175, 262.5, 350

Space Velocity (1/hr) 10k, 30k, 45k

Temperature (K) 500, 550, 600

The number of trim points and spread between trim points were choosen based on a trial and error basis. Sufficient data points were selected such that the behavior of the state could be captured to an acceptable degree of accuracy, while minimizing the effort spent on capturing and calibrating the data points. A linear interpolation algorithm was used for all intermediate points.

2.3 First Order Linear Model for NH_3 Storage

Using input-output data from the full chemistry model in [7], with $NH_{3,in}$ as the input and Stored NH_3 as the output, a a transfer function model was developed. This was of the form:

$$\dot{x} = -\frac{1}{\tau}x + \frac{k}{\tau}u \tag{2.1}$$

where u denotes $NH_{3,in}$ and x denotes Stored NH_3. This model is shown in a transfer function form in Figure 2-3 with a transfer function $\frac{k}{\tau s+1}$.

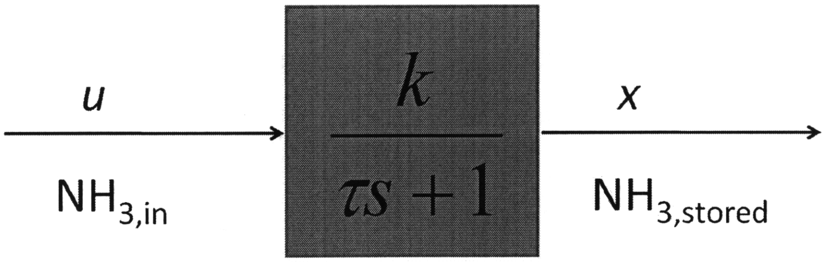


Figure 2-3: Block Diagram for Transfer Function Model

where k and τ are mapped by a 3-D or 4-D lookup table.

There are many ways to obtain the maps of k and τ and the following methods were tested to determine the best approach.

2.3.1 Method 1: Bode Plots

Different input profiles of NH_3 were introduced into the simulation, at different conditions as listed above. The input consists of both a step and sinusoidal wave. The sinusoidal frequency was changed over a suitable range determined by trial and error. The inputs were varied according to the following:

$$u = a_0 + a_1 sin(2\pi f t) \tag{2.2}$$

where

a_0	75 - 100% of $NO_{x,in}$
a_1	25 - 50% of $NO_{x,in}$
f	Frequency range from 5×10^{-5} - 1×10^{-2} Hz

For each trim point, the frequency was varied in order to estimate the values of k and τ through the unit gain and phase difference. Figure 2-4 below shows a summary of bode plots obtained for some of the trim points.

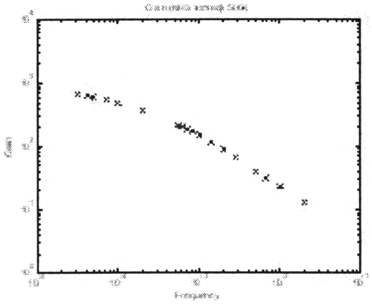
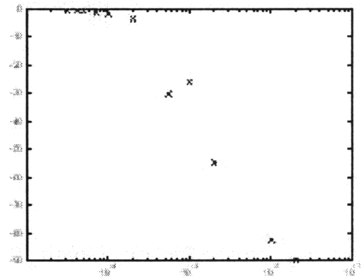
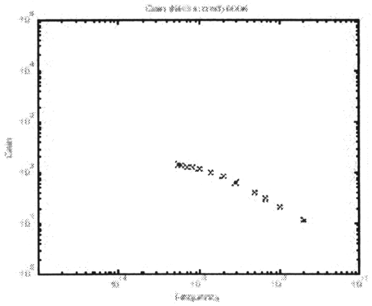
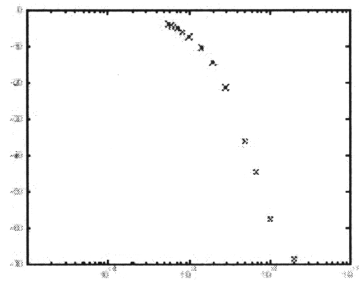
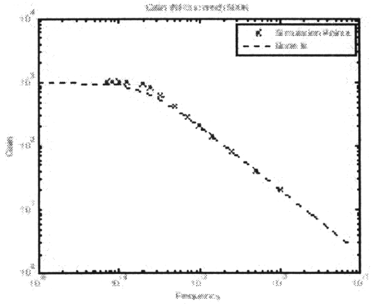
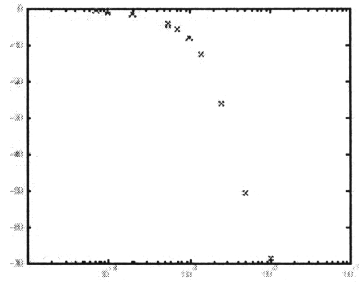
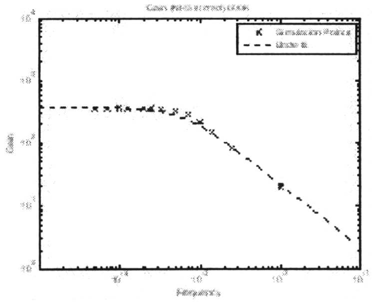
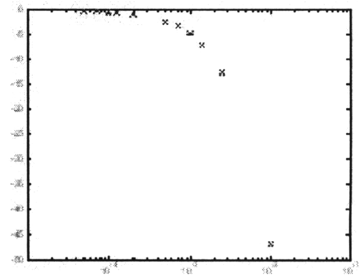
NO$_x$	**Temperature**	**Magnitude Plots**	**Phase Plots**
175 ppm	500 K		
175 ppm	600 K		
350 ppm	500 K		
350 ppm	600 K		

Figure 2-4: Bode Plot for determination of model paramters

By checking the the corner frequency and the DC gain of the magnitude and phase plots, the values of k and τ could be estimated. However, this was not easily done for all the plots. As seen in Figure 2-4, some of the behavior observed did not produce bode plots that were expected of a first order function. A quick verification of the k and τ values that were obtained also showed that the numbers did not reflect an accurate estimate of the state of NH_3 storage. As such, an alternate method was needed to map the k and τ values.

2.3.2 Method 2: Step Input

Using the full chemistry model in [7], a step input was applied to the system to trigger a response in NH_3 storage. Using the final steady state value, and the rise time to 63% of the final steady state value, the values of k and τ could be estimated. Figure 2-5 below shows a typical step response of the system.

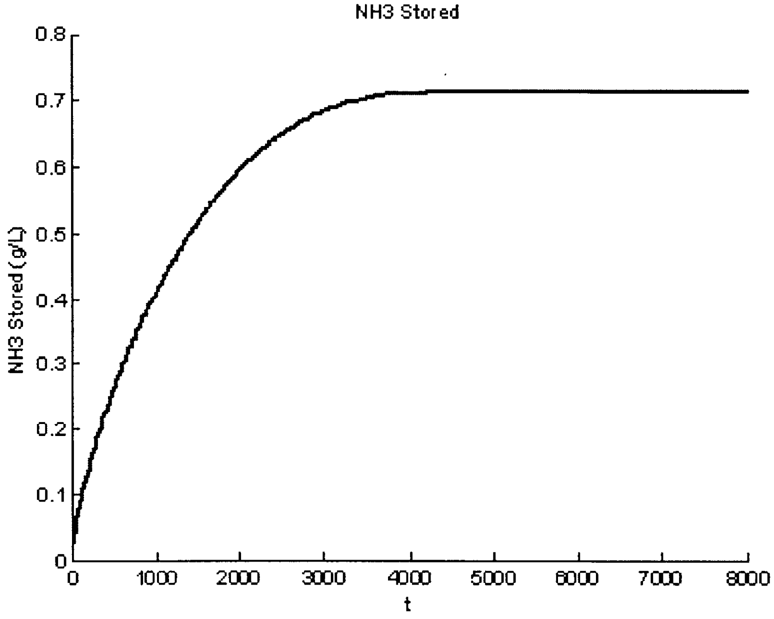


Figure 2-5: Step Response of NH_3 Storage to $NH_{3,in}$

However, depending on the initial condition of the NH_3 Storage, the k and τ values varied, and could not be adequately captured by a single value. A fourth dimension needed to be added to the map: NH_3 Storage level. Also, the amount of $NH_{3,in}$

injected also affected the gain and time delay constants, due to the chemical nature of the system. As higher concentrations of $NH_{3,in}$ were introducted, the system becomes less responsive to the injections and the gain values decrease. As such, two more dimensions were introduced to the mapping of k and τ.

NO_x in (ppm) 0, 87.5, 175, 262.5, 350

Space Velocity (1/hr) 10k, 30k, 45k

Temperature (K) 500, 550, 600

Excess $NH_{3,in}$ (ppm) 0, 87.5, 175, 262.5, 350

NH_3 Storage Level (g/L) 0, 0.01, 0.02, ..., 0.99, 1.00

Figure 2-6 shows the system responses to the same input with different initial conditions, and Figure 2-7 shows the system responses when overlapped.

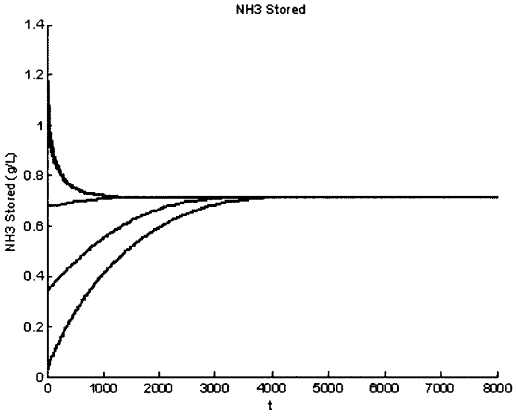


Figure 2-6: Family of System Responses with different Inital Conditions

As such, in order to capture the system response througout the whole range of NH_3 storage, only two simulation runs needed to be conducted; one from zero initial storage, and one from about 30% initial storage. Using the two system responses, the NH_3 Storage Level is broken down into steps of 0.01, and the values of k and τ estimated for each step. Figure 2-8 shows the system response broken down into a family of step responses with incremental initial conditions.

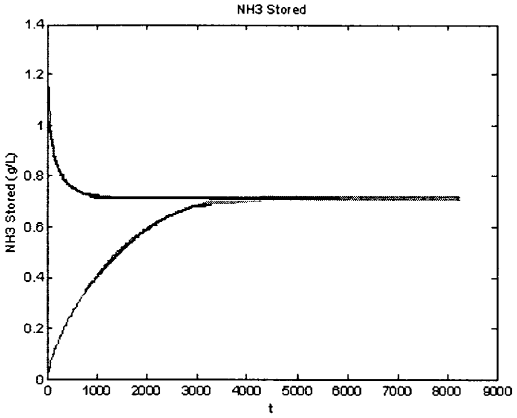


Figure 2-7: Family of System Responses when Overlapped

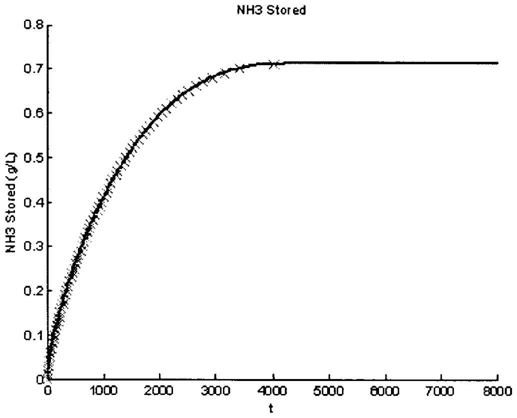


Figure 2-8: Single Step Response used to estimate k and τ values for different of Initial Conditions

To evaluate the accuracy of the k and τ values obtained, the output of the transfer function model was compared to that of the full chemistry on a few sets of simulations. Within the boundaries of the mapping dimensions, the transfer function model was able to capture the NH_3 Storage behavior to a very good degree of accuracy.

2.3.3 Method 3: Small Step Disturbance

Instead of expressing the state of Stored NH_3 as x, it can also be broken down into the following form:

$$x = x_{nominal} + \Delta x \tag{2.3}$$

where $x_{nominal}$ is the equilibrium value of Stored NH_3, and Δx is the deviation from the equilibrium. The transfer function model can then be applied to the deviation from equilibrium as such:

$$\frac{\Delta x}{u}(s) = \frac{k}{\tau s + 1} \tag{2.4}$$

The values of k and τ can be determined from small perturbations from the equilibrium value. While an additional map for $x_{nominal}$ needs to be obtained, it reduces the number of dimensions on the maps for the k and τ values. Figure 2-9 shows a simulation run where the system was allowed to reach equilibrium, and small step perturbations of +/- 5 ppm of $NH_{3,in}$ were introduced. Similarly, the k and τ values in this case could be estimated by the D.C. gain and the 63% percent rise time.

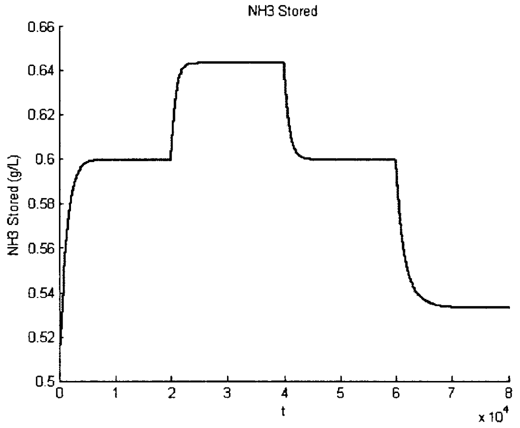


Figure 2-9: Small Step Perturbations

Using the Full Chemistry Model to map the values of $x_{nominal}$, k and τ with small step perturbations, this format proved to be the easiest to implement and calibrate. The maps obtained were saved using Microsoft Excel and imported by Matlab into a Simulink environment model. Model verification and subsequent control algorithm implementation were developed using this Simulink model as a base. A table of the k and τ values are included in Appendix B, and $x_{steadystate}$ in Appendix C.

2.4 NH_3 Slip as a Function of NH_3 Storage

In order to complete the transfer function model for the Urea SCR system, two more states needed to be captured. These were the NH_3 Slip and the NO_x Slip of the system. Based on information obtained from the literature search, it was known that the adsorption of $NH_{3,in}$ by the catalyst surface coating was highly efficient. Expressed in equation form

$$R_{ad} = k_{ad} e^{\frac{-E_{ad}}{RT}} \tag{2.5}$$

where the activation energy in the equation (E_{ad}) was set to zero in some full chemistry models. As such, it was logical to assume that any of the $NH_{3,in}$ injected will be adsorped by the catalyst surface coating, and the NH_3 Slip was a result of desorption

$$R_{des} = K_{des} e^{\frac{-E_{des}(1-\gamma\theta)}{RT}} \tag{2.6}$$

which was dependent on the surface coverage fraction of the system (θ). As the surface coverage fraction is related to the state of Stored NH_3 in the transfer funciton model, it was proposed that the state of NH_3 Slip (y_1) could be obtained as a function of Stored NH_3 (x).

$$y_1 = f(x) \tag{2.7}$$

Using the Full Chemistry SCR model, simulation runs were designed such that NH_3 Slip due to desorption was isolated and captured for the operating range as presented in the mapping stages. The Urea SCR System was first allowed to saturate with Stored NH_3 until a suitably high equilibrium level was reached. The flowrate of the simulation was then sustained, but with $NH_{3,in}$ reduced to zero. The Stored NH_3 was noted to drop to zero gradually, while the amount of NH_3 Slip per second was monitored and captured. Figure 2-10 shows a typical plot of the simulation run.

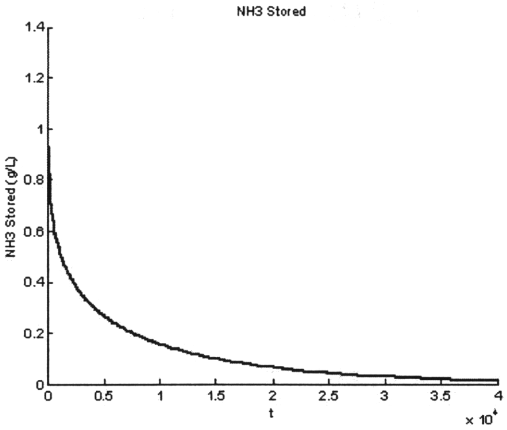


Figure 2-10: NH_3 Slip due to Catalyst Desorption

Using the data captured for Stored NH_3 and NH_3 Slip, the amount of NH_3 Slip at each level of NH_3 Storage could be matched and plotted. Figure 2-11 show the plot for one of the operating conditions, where Temperature, $T = 600$ (K), and Space Velocity, $u_in = 45{,}000$ (1/hr).

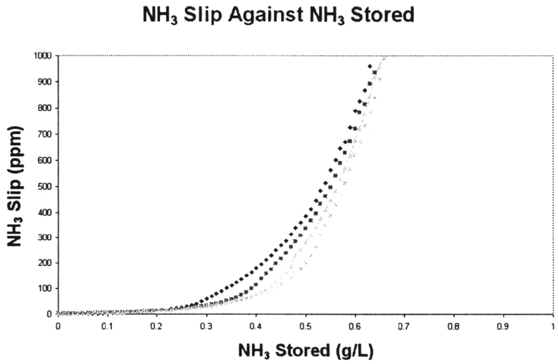


Figure 2-11: Plot of NH_3 Slip against Stored NH_3

Repeating the NH_3 Slip simulation runs across the range of mapping conditions, NH_3 Slip could be mapped entirely as a function of Stored NH_3, as as shown in Eq. (2.7). The complete map is included in a table format in Appendix D.

2.5 NO_x Slip as a Function of NH_3 Storage

Similar the the mapping of NH_3 Slip, the NO_x slip can be derived from the efficiency level of the Urea SCR System, as a function of the level of Stored NH_3.

$$y_2 = g(x) \tag{2.8}$$

Using the Full Chemistry SCR model, simulation runs were designed such that NO_x Slip for different levels of NH_3 Storage were captured. In order to capture the full range of data, two initial levels of Stored NH_3 were used; 0 (g/L) and 1.4 (g/L). Starting from zero NH_3 Storage, the Urea SCR System NH_3 Storage Level was slowly built up, while a constant flow of $NO_{x,in}$ was introduced. The amount of NO_x Slip, together with the amount of Stored NH_3 were measured at each instant throughout the experiment. In order to determine the data for storage levels above equilibrium, the setup was repeated for a initial level of NH_3 Storage that was higher than equilibrium. Figures 2-12 and 2-13 shows a typical plot of Stored NH_3 and NO_x Slip for the setup.

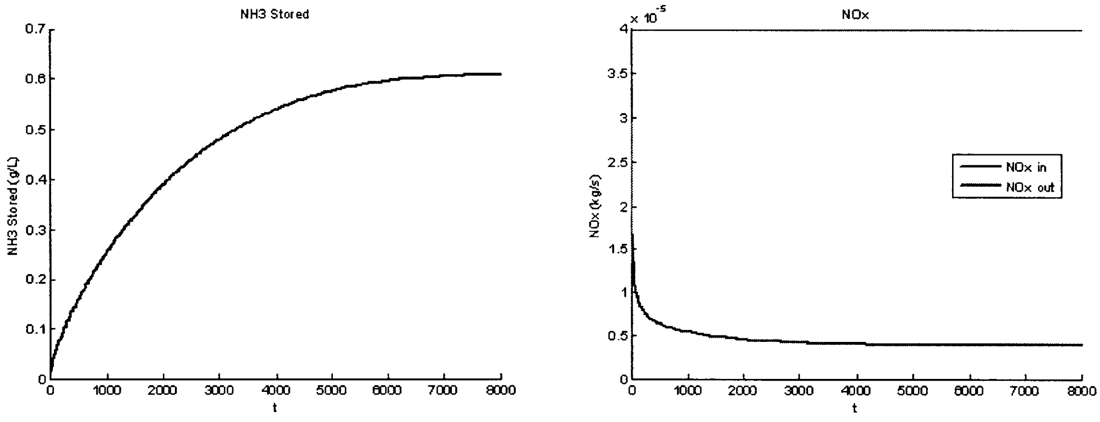


Figure 2-12: Plots for Stored NH_3 and NO_x Slip with 0 (g/L) Initial Condition

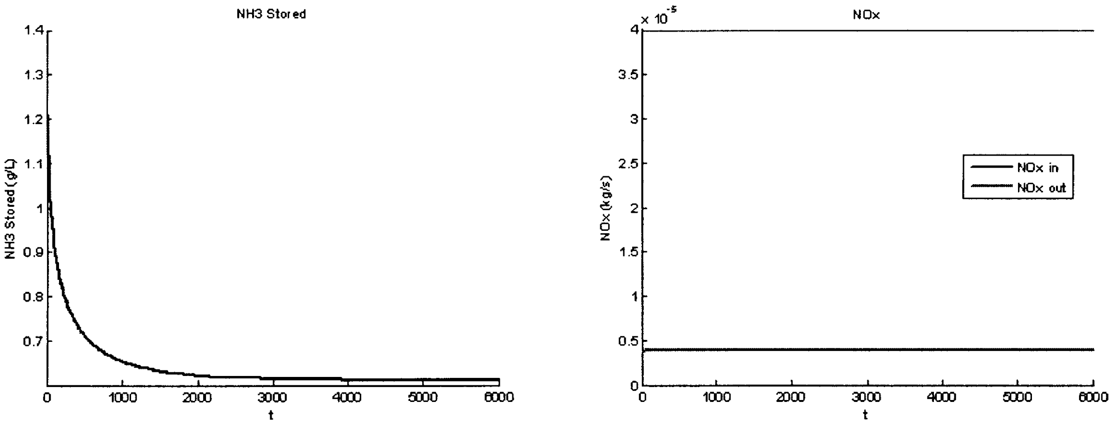


Figure 2-13: Plots for Stored NH_3 and NO_x Slip with 1.4 (g/L) Initial Condition

The setups were repeated for the operating range presented above. Using the data captured for Stored NH_3 and NO_x Slip, the amount of NO_x Slip at each level of NH_3 Storage could be matched and plotted. Expressed as a percentage of $NO_{x,in}$, the NO_x Slip fraction is plotted on the y-axis against the Stored NH_3 on the x-axis. Figure 2-14 show the plot for one of the operating conditions; T = 600 (K), u_in = 45,000 (1/hr).

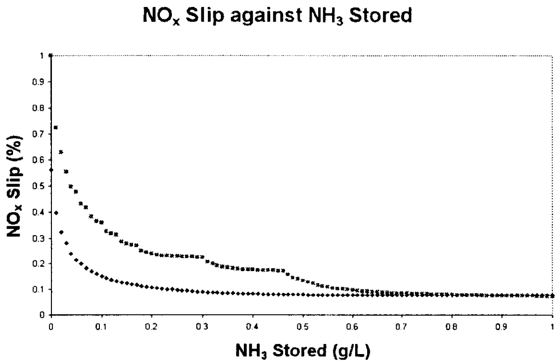


Figure 2-14: Plot of NO_x Slip Fraction against NH_3 Stored

Through examination of the simulation results, it was observed that the NO_x Slip fraction was the same for varying values of excess $NH_{3,in}$. Only when insufficient $NH_{3,in}$ were injected did the NO_x Slip fraction have a different value. In the Figure 2-14 above, the line with the poorer performance (shown in pink) was when insufficient $NH_{3,in}$ was injected, while the line shown in blue was when excess $NH_{3,in}$ was injected.

Repeating the NO_x Slip simulation runs across the range of mapping conditions, the NO_x Slip fraction could be mapped entirely as a function of NH_3 Stored, as proposed by the Eq. (2.8). The complete map is included in a table format in Appendix E.

Chapter 3

Control Using NH_3 Storage Feedback

With the transfer function model fully determined, the next step was to start implementing control algorithms on the system. This took place in several steps. Control algorithms were first tested on the linear transfer model to ensure that minimal performance standards were achieved. Subsequently, the full chemistry model was introduced as the plant, with the transfer function model acting as the plant model, and the control algorithms were tested again. Since the amount of NH_3 Slip and NO_x Slip were functions of Stored NH_3, setting a reference value for Stored NH_3 and having the system track the reference would give the best chance of minimizing both NH_3 Slip and NO_x Slip. Starting with a Proportional-Integral (PI) Controller on the NH_3 Storage, the closed loop system was first tested on a $NO_{x,in}$ profile of random steps and length, and subsequently proceeded more complicated profiles with variations in Temperature and Space Velocity. Building on a working PI Controller, an Adaptive PI Controller was also developed, implemented and tested.

3.1 PI Control

From the linear model proposed in Section 2.3.3, the transfer function model, as given by Eq. (2.3) and Eq. (2.4) were

$$x = x_{nominal} + \Delta x \tag{3.1}$$

$$\frac{\Delta x}{u}(s) = \frac{k}{\tau s + 1} \tag{3.2}$$

Rewriting the above equations in a simpler format, we have

$$X = x_{nominal} + x \tag{3.3}$$

$$\frac{x}{u}(s) = \frac{k}{\tau s + 1} \tag{3.4}$$

Figure 3-1 belows illustrates the Block Diagram of the transfer function model with a PI Controller added.

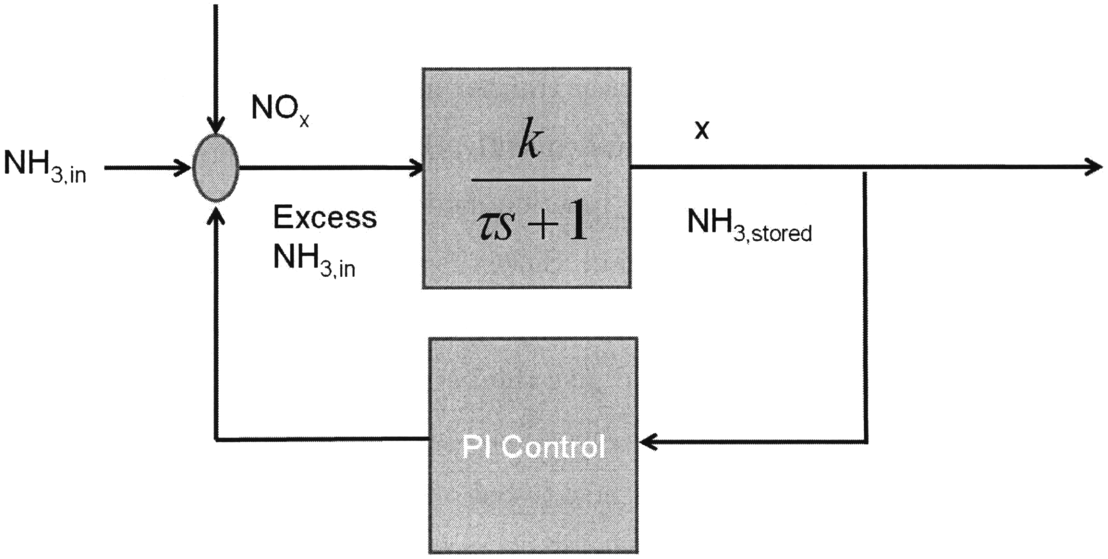


Figure 3-1: Block Diagram for Transfer Function Model with PI Control

Setting the reference signal for X to be $x_{nominal}$, it can be observed that the controller needs to maintain value of x at zero. Using PI control on a linear transfer function model, this can be easily achieved via the selection of the proportional gain(K_p) and integral gain (K_i) values, with the controller signal as such

$$u = -\left(K_p + \frac{K_i}{s}\right)x \tag{3.5}$$

From Eq. (3.5) for the control input, the complete closed loop transfer function model for the system becomes

$$\begin{aligned}
x &= \frac{k}{\tau s + 1}u & (3.6)\\
x &= -\frac{k}{\tau s + 1}\left(K_p + \frac{K_i}{s}\right)x & (3.7)\\
(\tau s + 1)x &= -k\left(K_p + \frac{K_i}{s}\right)x & (3.8)\\
\tau \ddot{x} + \dot{x} &= -kK_p\dot{x} - kK_i x & (3.9)\\
\tau \ddot{x} + (1 + kK_p)\,\dot{x} + kK_i x &= 0 & (3.10)\\
\ddot{x} + \frac{1 + kK_p}{\tau}\dot{x} + \frac{kK_i}{\tau}x &= 0 & (3.11)
\end{aligned}$$

For a second order system, the differential equation can be expressed in the form

$$\ddot{x} + 2\zeta\omega_0\dot{x} + \omega_0^2 x = 0 \tag{3.12}$$

where ζ and ω_0 are the damping ratio and natural frequency respectively. By fixing the damping ratio desired for the closed loop system, we can express K_i in terms of k, τ, and K_p.

$$\begin{aligned}
\zeta &= \frac{\frac{1+kK_p}{\tau}}{2\sqrt{\frac{kK_i}{\tau}}} = 1 & (3.13)\\
2\sqrt{\frac{kK_i}{\tau}} &= \frac{1 + kK_p}{\tau} & (3.14)\\
4\frac{kK_i}{\tau} &= \frac{(1 + kK_p)^2}{\tau^2} & (3.15)\\
K_i &= \frac{(1 + kK_p)^2}{4k\tau} & (3.16)
\end{aligned}$$

With K_i expressed as a function K_p, and k and τ being model parameters, we can adjust the performace of the system through the selection of proportional gain (K_p). Using a random $NO_{x,in}$ profile as shown in Figure 3-2, the closed loop performance of the system with PI control was plotted for a range of values of K_p values, and compared to the open loop performance where only a 1:1 ($NH_{3,in}$:$NO_{x,in}$) injection was supplied.

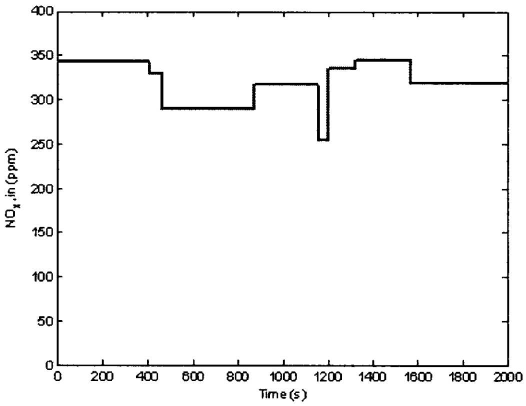


Figure 3-2: Random $NO_{x,in}$ Profile for PI Control

The following plots in Figure 3-3 show the results for a single set: Temperature: 500 (K), Space Velocity: 30k (1/hr), $NO_{x,in}$ Bound: 250 - 350 (ppm). The top left plot shows the amount of Stored NH_3, the top right plot shows the amount of NO_x Slip, the bottom left plot shows the $NH_{3,in}$ and the bottom right plot shows the NH_3 Slip. To translate the system performance into numbers, the total amount of NH_3 Slip and NO_x Slip are summarized into a table format below.

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop, (1:1)	30.94	0.90
Closed Loop, K_p = 50,000	14.44	3.99
Closed Loop, K_p = 100,000	14.11	3.80
Closed Loop, K_p = 200,000	14.05	3.62
Closed Loop, K_p = 300,000	14.11	3.50
Closed Loop, K_p = 400,000	14.18	3.41

Table 3.1: Set 1 Performance Summary

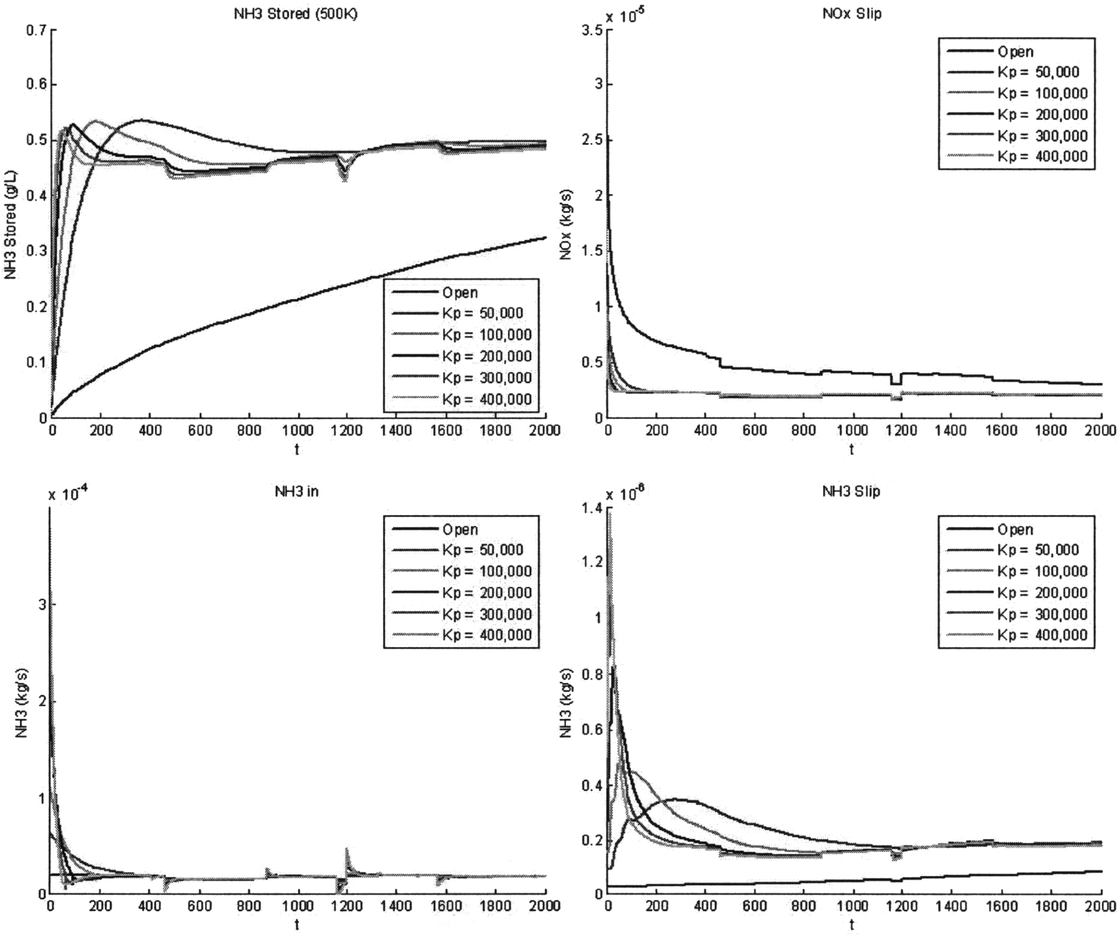


Figure 3-3: Comparison Plots of Closed Loop PI and Open Loop Control (Set 1)

For the range of operating conditions, the testing conditions were varied as follows:

Set	Temperature (K)	Space Velocity (1/hr)	$NO_{x,in}$ Bound (ppm)
1	500	30k	250 - 350
2	500	30k	200 - 300
3	500	30k	150 - 250
4	550	30k	250 - 350
5	550	30k	200 - 300
6	550	30k	150 - 250
7	500	15k	250 - 350
8	500	15k	200 - 300
9	500	15k	150 - 250

Table 3.2: Input Conditions for Sets 1 - 9

The tabular summary for performance of PI Control for Sets 1 - 9 are included in Appendix F.

3.2 Adaptive PI Control

With a working PI Controller, an Adaptive PI Controller algorithm could then be the next step in the testing sequence. Figure 3-4 shows the block diagram for the design adopted for Adaptive PI.

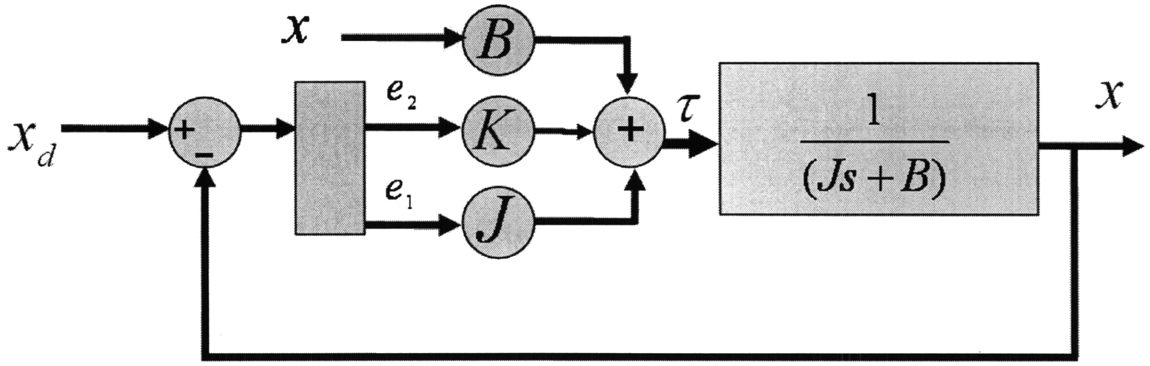


Figure 3-4: Block Diagram for Adaptive PI Control Design

Expressing the transfer function model in a slightly different format, the nominal form of the Adaptive PI Controller can be expressed as follows:

$$\tau_{nominal} = Je_1(t) + Bx + Ke_2(t) \tag{3.17}$$

where

$$\begin{aligned} e &= x_d - x = -x && (3.18) \\ e_1 &= \lambda e && (3.19) \\ e_2 &= e + \lambda \int e \, dt && (3.20) \end{aligned}$$

where the parameters of the Adaptive PI Controller (J, B, K, λ) are to be determined. In the adaptive form of the control input, we apply the following adaptive laws:

$$\begin{aligned} \tau &= \hat{J}e_1(t) + \hat{B}x + Ke_2(t) && (3.21) \\ \dot{\hat{J}} &= \gamma_1 e_2 e_1 && (3.22) \\ \dot{\hat{B}} &= \gamma_1 e_2 x && (3.23) \end{aligned}$$

where γ_1 and γ_2 are the adaptive gains to be selected. The overall differential equation for the plant and adaptive controller becomes:

$$\dot{x} = \frac{1}{J}\left(\hat{B}x - Bx + \hat{J}e_1(t) + Ke_2(t)\right) \tag{3.24}$$

and the error equation becomes:

$$\dot{e_2} = -\frac{K}{J}e_2(t) + \frac{1}{J}\left(-\hat{J}e_1 - \hat{B}\dot{x}\right) \tag{3.25}$$

Selecting the adaptive controller parameters such that the initial values matches of the PI controller, the performance of the adaptive controller can be evaluated against that of the PI controller. Table 3.3 list the initial values chosen for the adaptive parameters, and Figure 3-5 shows the comparison plot between the adaptive controller and a PI controller for the same input conditions. A summary of the average NH_3 Slip and NO_x Slip is included in Table 3.4.

Adaptive Controller Parameter	Value
$J_{initial}$	10,000
$B_{initial}$	500
K	200
λ	1
γ_1	1000
γ_2	1000

Table 3.3: Adaptive PI Controller Parameters

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop, (1:1)	30.94	0.90
Closed Loop, K_p = 50,000	14.44	3.99
Closed Loop, K_p = 100,000	14.11	3.80
Closed Loop, K_p = 200,000	14.05	3.62
Closed Loop, K_p = 300,000	14.11	3.50
Closed Loop, K_p = 400,000	14.18	3.41
Adaptive PI	14.18	3.39

Table 3.4: Set 1 Performance Summary including Adaptive PI Control

While the PI controller relied on the transfer function mapping of k and τ values to determine the optimal gain for K_i, as observed by Eq. (3.16), it can be observed that the Adaptive PI controller relied only on feedback information and was able to achieve a comparable, if not better performance for the same input conditions. Further comparison of the performance between the Adaptive PI controller and the PI controller under different input conditions can be found in Appendix G.

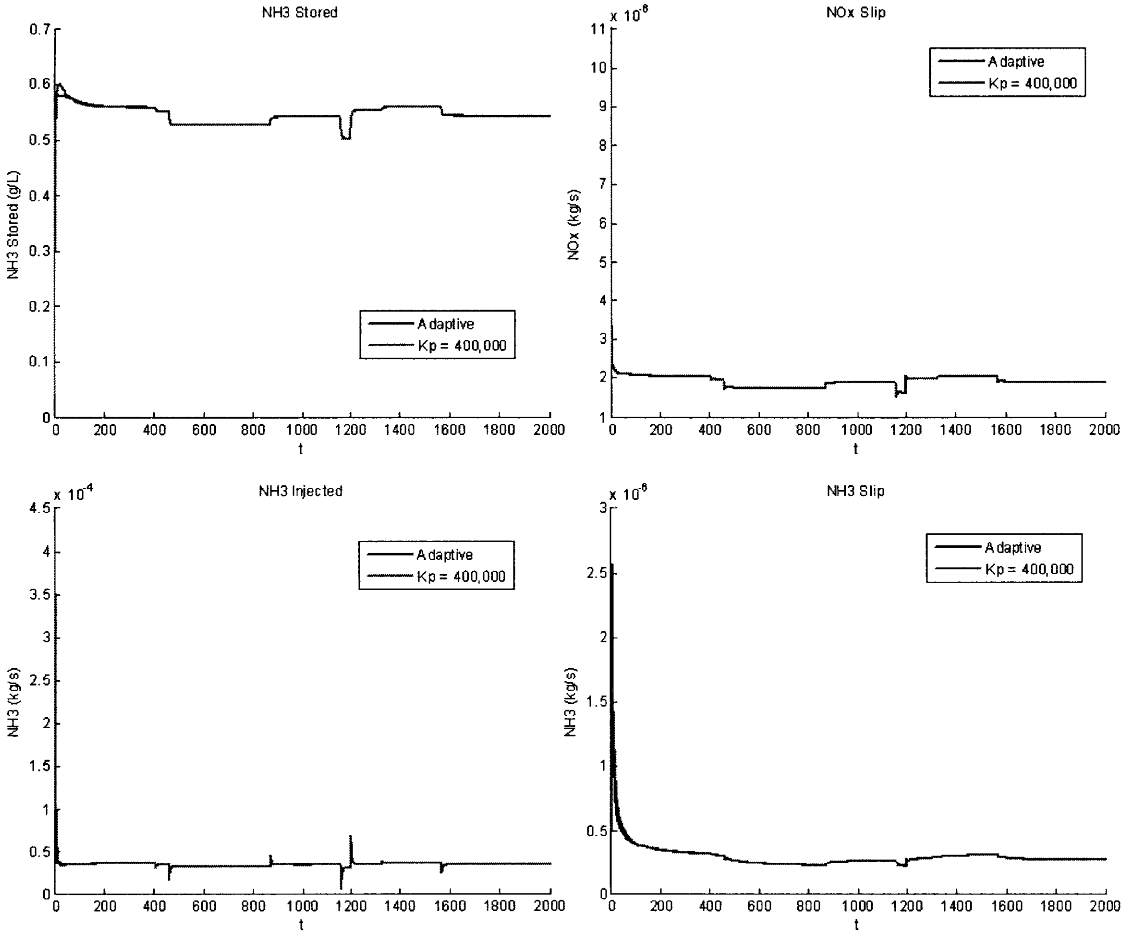


Figure 3-5: Comparison Plots between Adaptive PI Control and PI Control

Chapter 4

Control Using NH_3 and NO_x Slip Feedback

Implementing feedback control using the state of Stored NH_3 was applicable to the transfer function model as the NH_3 Storage was one of the states of the model. On a actual vehicular Urea SCR System, the amount of Stored NH_3 on the catalyst at any point of time will be unmeasurable, and thus will not availble for negative feedback. As such, a new feedback control algorithm that used the states that are available was required. Through the discussions with the research team at Ford Motor Company, it was understood that the current gas sensor that installed on the vehicular system gave a combined measurement of NH_3 Slip and NO_x Slip. The subsequent step was to implement PI and Adaptive PI Control using the combined state of NH_3 Slip and NO_x Slip.

4.1 PI Control

From the maps of NH_3 Slip and NO_x Slip presented in Eq. (2.7) and Eq. (2.8), we can present the combined state (z) as follows:

$$Z = z_{nominal} + z \tag{4.1}$$

$$z = k_1 f(x) + k_2 g(x) \tag{4.2}$$

where k_1 and k_2 were constant gains dependent on sensor behavior. The differential equations for z could be expressed as:

$$\dot{z}(t) = a_p^{''} z(t) + b_p^{''} u(t) \tag{4.3}$$

$$a_p^{''} = \left(k_1 \frac{\delta f}{\delta x} + k_2 \frac{\delta g}{\delta x} \right) a_p \tag{4.4}$$

$$b_p^{''} = \left(k_1 \frac{\delta f}{\delta x} + k_2 \frac{\delta g}{\delta x} \right) b_p \tag{4.5}$$

With the differential equation shown in the form as presented in Eq. (4.3), a fixed PI controller of the following form was proposed:

$$u = -\left(\frac{a_p^{''}}{b_p^{''}} \right) z + \left(\frac{1}{b_p} \right) z_0 \tag{4.6}$$

$$z_0 = -(K + \lambda) z - K\lambda \int z \, dt \tag{4.7}$$

The plant, together with the proposed PI controller, will have the form:

$$\dot{z}_1 = -k z_1 \tag{4.8}$$

$$z_1 = z + \lambda \int z \, dt \tag{4.9}$$

which predicts that the controller should drive to state z to zero, even if a_p and b_p are time varying. Using the mean values of k and τ and the maps of $f(x)$ and $g(x)$ to obtain an estimate for $a_p^{''}$ and $b_p^{''}$, the fixed PI controller was implemented on a full chemistry system to evaluate its performance and its ability to minimize both NH_3 Slip and NO_x Slip. Setting the $z_{nominal}$ at 90%, the following plots in Figure 4-1 present the results for the operating conditions of Set 1. Table 4.1 summarizes the average NH_3 Slip and NO_x Slip.

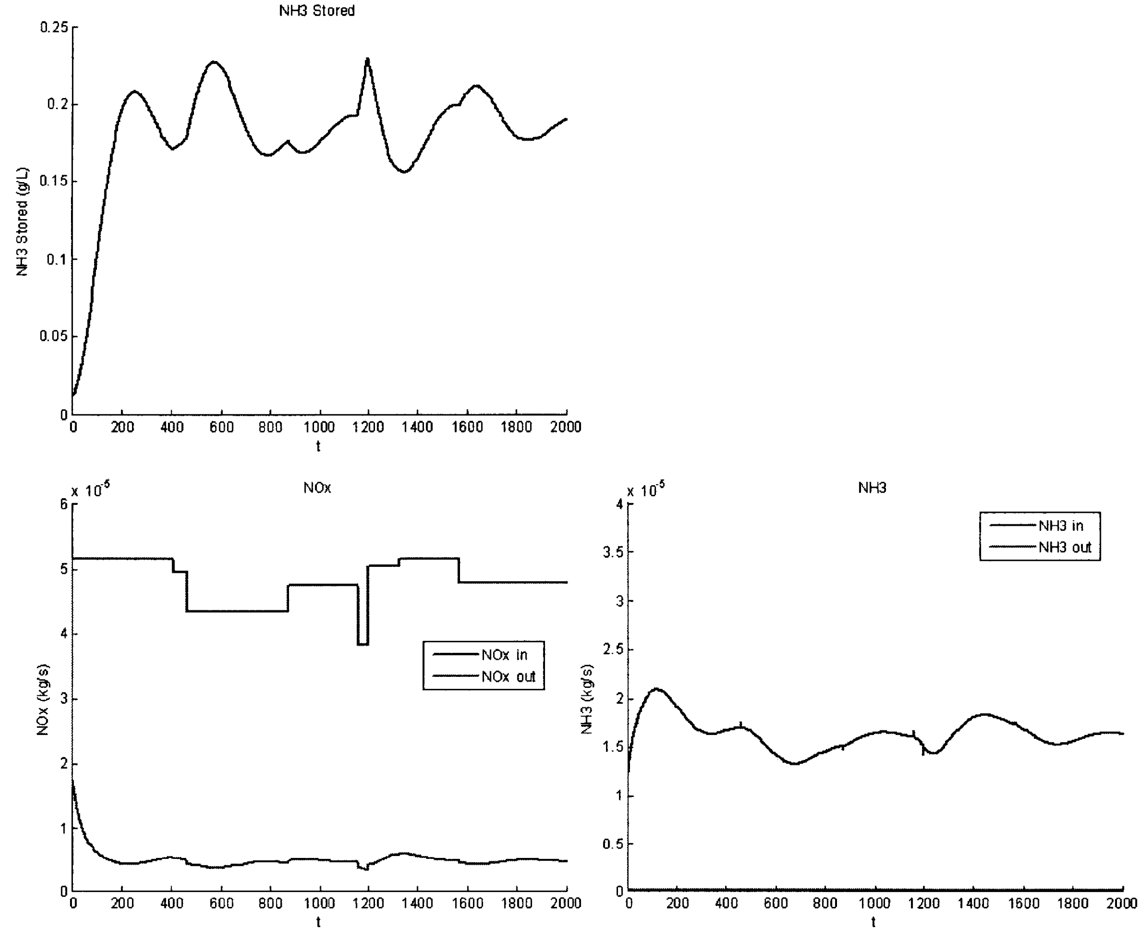


Figure 4-1: Performace Plots for PI Control using z, $z_{nominal} = 0.90$

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	33.2	0.65

Table 4.1: Performance Summary for PI Control using z, $z_{nominal} = 0.90$

From the numbers in Table 4.1, the controller seems to be able to track the efficiency set ($z_{nominal}$) of 90% pretty well. A repeat set with $z_{nominal}$ set at 95% was ran with the following results. Figure 4-2 presents the plots for Stored NH_3, NH_3 Slip and NO_x Slip. Table 4.2 summarizes the average NH_3 Slip and NO_x Slip.

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	14.5	1321

Table 4.2: Performance Summary for PI Control using z, $z_{nominal} = 0.95$

From the plots and the table summary, it can be observed that the PI controller was unable to avoid the positive feedback mechanism inherent in the Urea SCR System. With increasing values of z, the controller increased the injections of NH_3, which furhter increased the values of z, thus resulting in a positive feedback. An Adaptive PI Controller was required in order to skirt this critical issue.

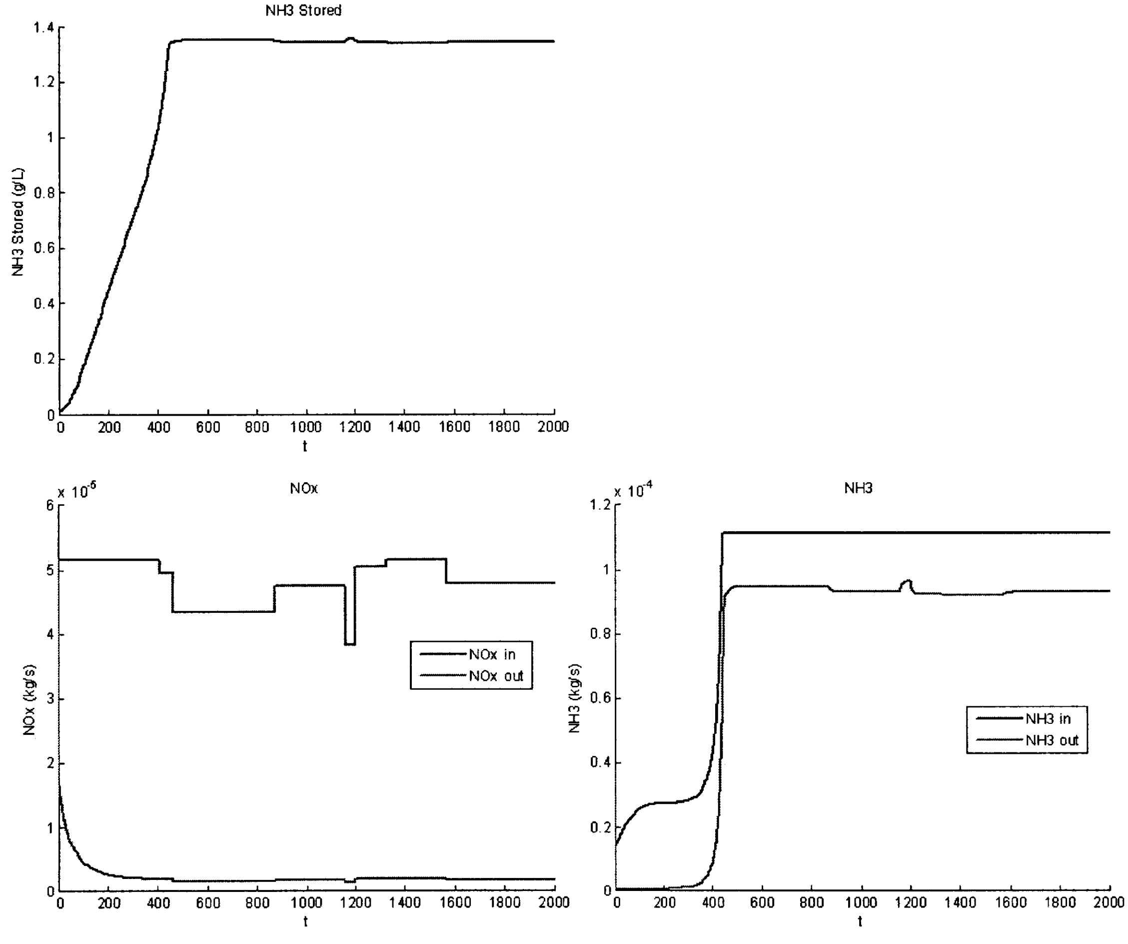


Figure 4-2: Performace Plots for PI Control using z, $z_{nominal} = 0.95$

4.2 Adaptive PI Control

For the differential equation of z in Eq. (4.3), an Adaptive PI Controller of the following format is proposed:

$$\begin{aligned} u &= \theta_z(t)z + \theta_0(t)z_0 && (4.10)\\ z_0 &= -(K+\lambda)z - K\lambda \int z\, dt && (4.11)\\ z_1 &= z + \lambda \int z\, dt && (4.12) \end{aligned}$$

with the adaptive laws as such:

$$\begin{aligned} \dot{\theta}_z &= -b_p(t) z_1 z && (4.13)\\ \dot{\theta}_0 &= -b_p(t) z_1 z_0 && (4.14) \end{aligned}$$

Implementing the Adaptive PI Controller on the same set of operating conditions as before, with $z_{nominal}$ set at 90% and 95%, the plots in Figures 4-3 and 4-4 show the output for NH_3 Slip and NO_x Slip. The numerical results are summarized in Tables 4.3 and 4.4.

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	31.7	0.70

Table 4.3: Performance Summary for Adaptive PI Control using z, $z_{nominal} = 0.90$

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	16.4	8.20

Table 4.4: Performance Summary for PI Control using z, $z_{nominal} = 0.95$

From the plots in Figure 4-4, it can be observed that the Adaptive PI Controller does successfully avoid the positive feedback that occurred in the PI Controller. However,

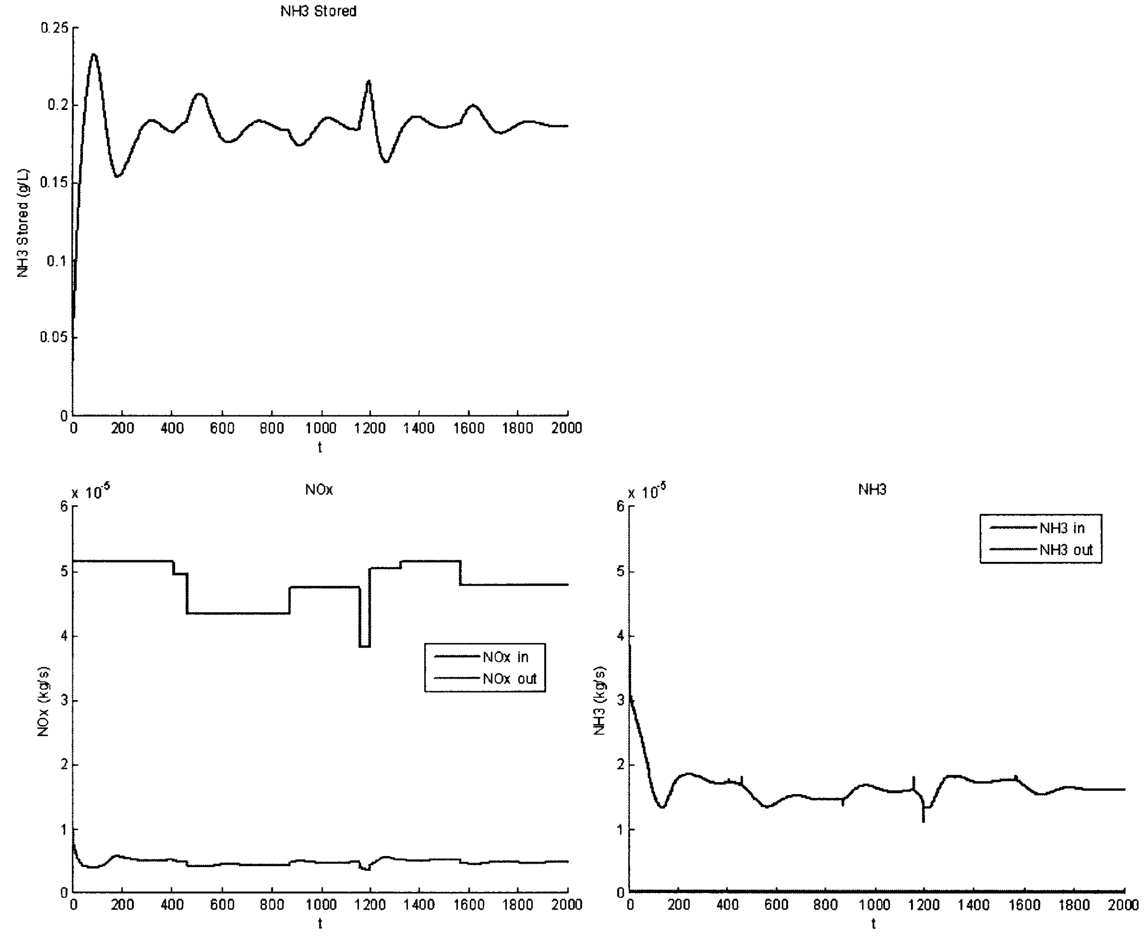


Figure 4-3: Performace Plots for Adaptive PI Control using z, $z_{nominal} = 0.90$

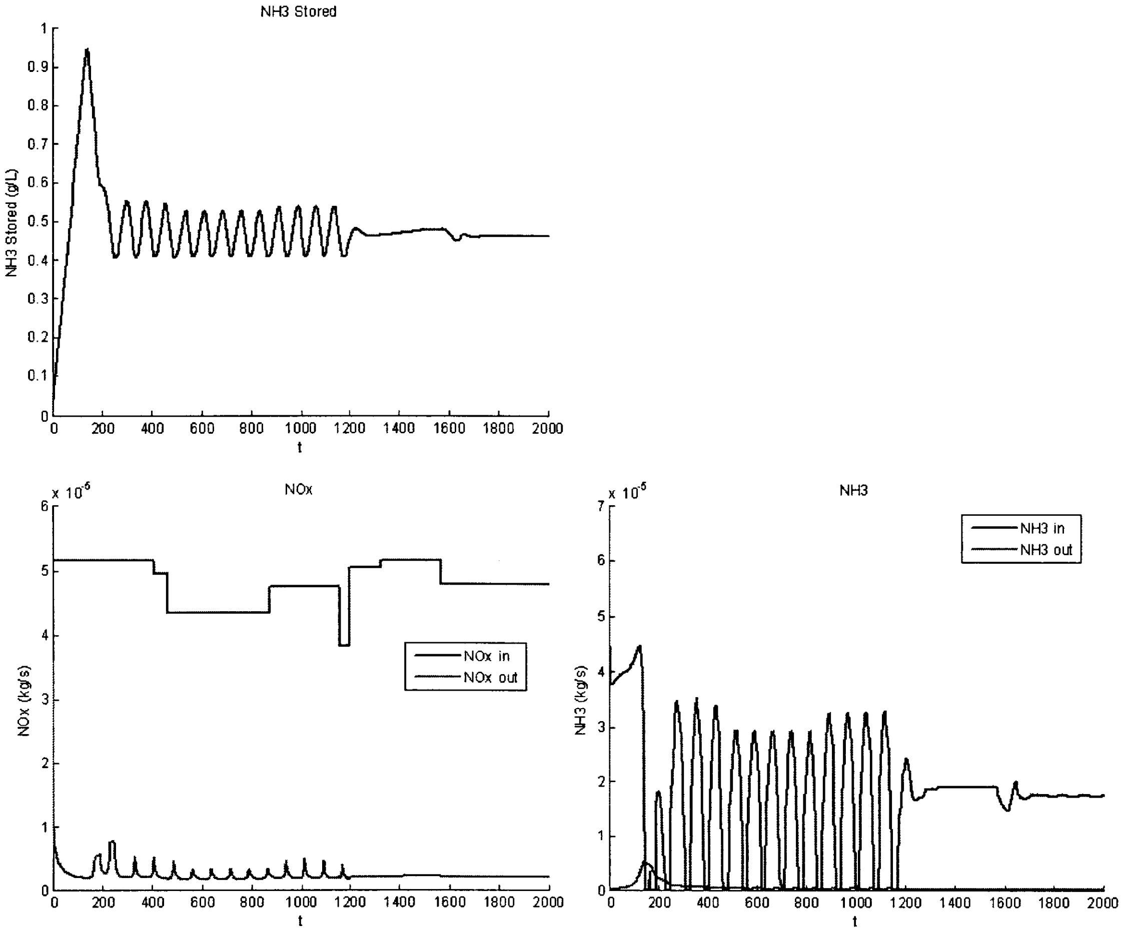


Figure 4-4: Performace Plots for Adaptive PI Control using z, $z_{nominal} = 0.95$

the Controller and Plant does not seem to converge to a steady solution, and instead oscillates between phases of positive and negative feedback. A further investigation in alternate forms of Adaptive Controllers might be required.

4.3 Non-Linear Adaptive PI Control

Revisting the data-driven transfer function model for Stored NH_3, the following block diagram in Figure 4-5 shows the approach for a non-linear Adaptive PI Controller.

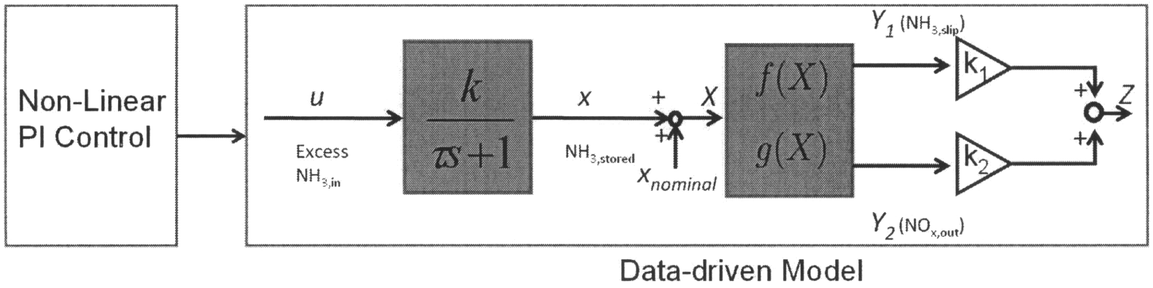


Figure 4-5: Block Diagram for Non-Linear Adaptive PI Control

where the states are as follows

$$x = X - x_{nominal} \tag{4.15}$$

$$z = Z - z_{nominal} \tag{4.16}$$

$$u = ExcessNH_{3,in} \tag{4.17}$$

$$= TotalNH_{3,in} - NH_{3,nominal} \tag{4.18}$$

The combined form for z can be expressed as follows:

$$z = k_1 \frac{\delta f}{\delta X} x + k_2 \frac{\delta g}{\delta X} x \tag{4.19}$$

Defining the variable $h(X)$ and $\gamma(X)$ as follows:

$$
\begin{aligned}
h(X) &= k_1 \frac{\delta f}{\delta X} + k_2 \frac{\delta g}{\delta X} && (4.20)\\
\gamma(X) &= \frac{\frac{\delta h(X)}{\delta X}}{h(X)} && (4.21)
\end{aligned}
$$

We can rewrite Eq. (4.19) and Eq. (4.3) as:

$$
\begin{aligned}
z &= h(X)x && (4.22)\\
\dot{z} &= \frac{\delta h(X)}{\delta X} x\dot{x} + h(X)\dot{x} && (4.23)\\
\dot{z} &= (\gamma(X)x + 1)\left(a_p z + b_p h(X) u\right) && (4.24)
\end{aligned}
$$

For the differential equation for z of the form in Eq. (4.24), the following Adaptive PI Controller was proposed:

$$
u = \frac{1}{h(X)} \theta_z(t) z + \frac{1}{(\gamma(X)x + 1)\, h(X)} \theta_0(t) z_0 \qquad (4.25)
$$

where

$$
\begin{aligned}
z_1 &= z + \lambda \int z dt && (4.26)\\
z_0 &= -(k+\lambda)z - k\lambda \int z \; dt && (4.27)\\
\dot{\theta}_z &= -g_1 \left(1 + x\gamma(X)\right) z_1 z && (4.28)\\
\dot{\theta}_0 &= -g_2 z_1 z_0 && (4.29)\\
g_1, g_2 &= \mathit{constant\ gains} && (4.30)
\end{aligned}
$$

In order to obtain the smooth maps for $h(X)$ and $\gamma(X)$, the maps for $f(X)$ and $g(X)$ were first fitted with exponential curve fits, as shown in Figures 4-6 and 4-7. The smooth curve fit functions were then differentiated with respect to X, to obtain $\frac{\delta}{\delta x}$ and $\frac{\delta^2}{\delta x^2}$, which forms the maps for $h(X)$ and $\gamma(X)$.

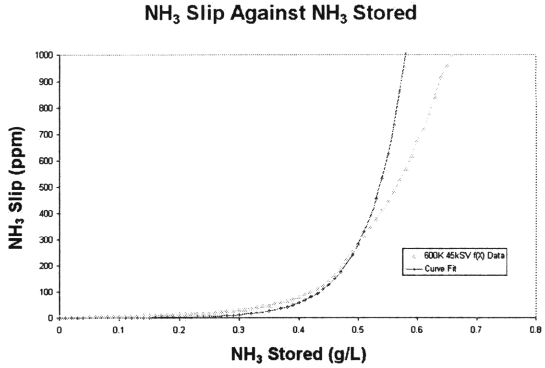


Figure 4-6: Curve Fit for f(X)

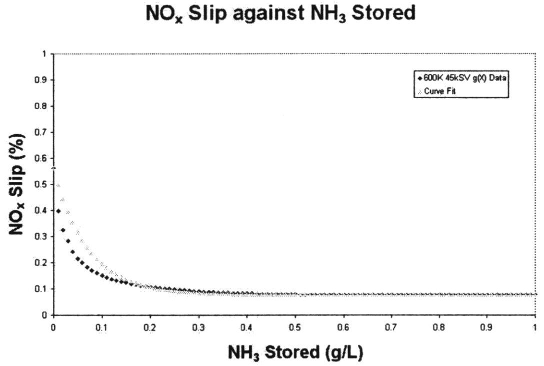


Figure 4-7: Curve Fit for g(X)

Using the maps for $h(X)$ and $\gamma(X)$, the Adaptive Non-Linear PI Controller was tested on the same sets of operating conditions. Figures 4-8 and 4-9 shows the results for $z_{nominal} = 0.90$ and $z_{nominal} = 0.95$. The performance summaries are included in Tables 4.5 and 4.6.

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	21.1	27.09

Table 4.5: Performance Summary for Non-Linear Adaptive PI Control using z, $z_{nominal} = 0.90$

From the plots in Figures 4-8 and 4-9, it can be observed that while positive feedback was achieved, convergence to a steady state value was still lacking. By inspecting the controller output in Eq. (4.25), the values of $h(X)$ and $\gamma(X)$ in the denominator

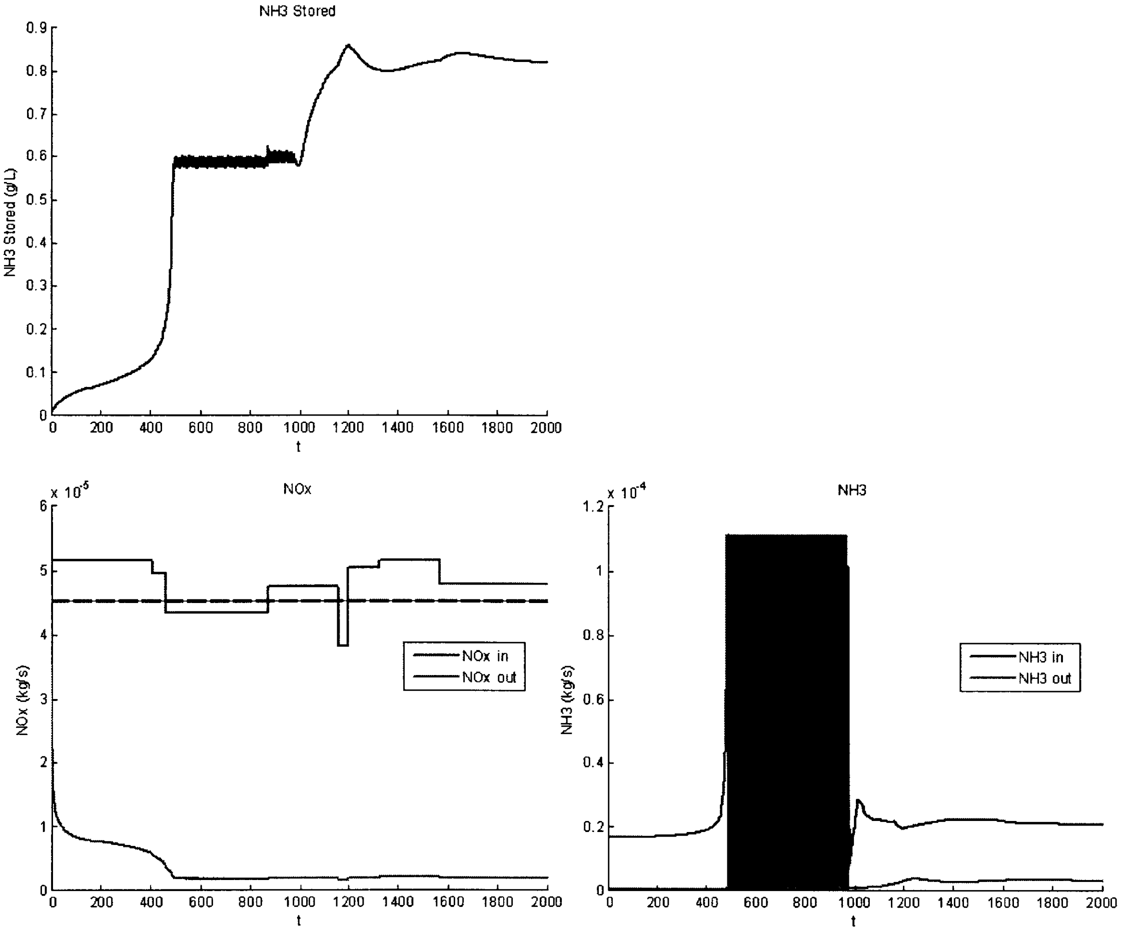


Figure 4-8: Performace Plots for Non-Linear Adaptive PI using z, $z_{nominal} = 0.90$

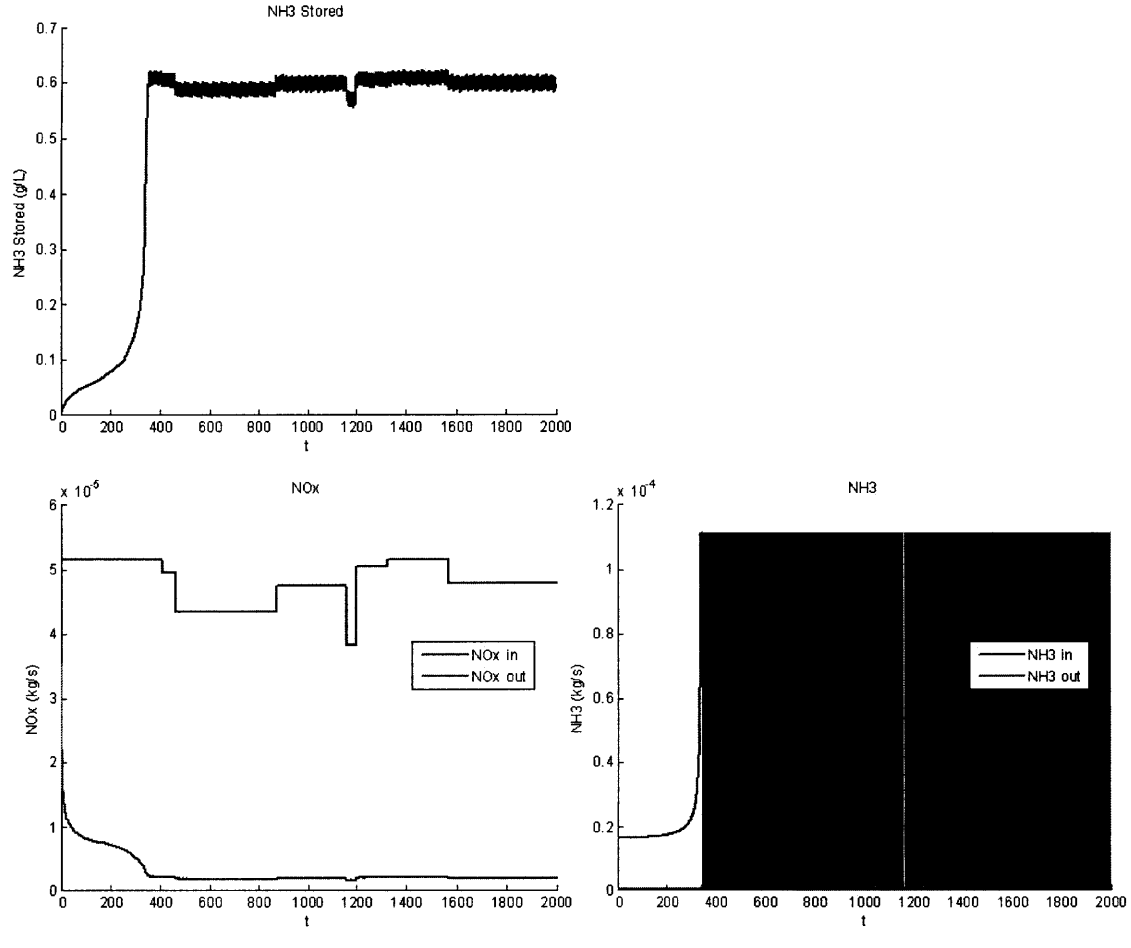


Figure 4-9: Performace Plots for Non-Linear Adaptive PI using z, $z_{nominal} = 0.95$

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	19.2	6.78

Table 4.6: Performance Summary for Non-Linear Adaptive PI Control using z, $z_{nominal} = 0.95$

might be approaching zero, and causing the wild fluctuations in the controller output. As such, a logic gate was proposed to be introduced to the Non-Linear Adaptive Controller.

4.4 Non-Linear Adaptive PI Control with Logic Gate

With the implementation of a logic gate for the Non-Linear Adaptive PI Control, the block diagram for the overall structure becomes as shown in Figure 4-10.

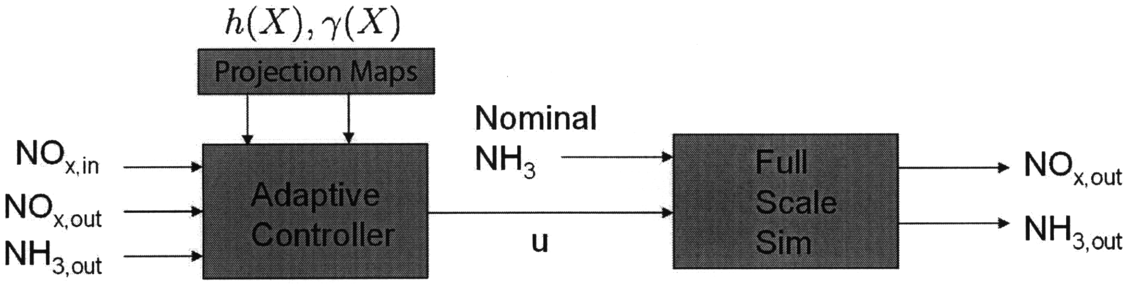


Figure 4-10: Block Diagram of Non-Linear Adaptive PI Control with Logic Gate

As shown in Eq. (4.24), the system response to the controller input decreases dramatically when either $h(X)$ or $\gamma(X)$ approaches zero. As such, the following logic gate criteria could be applied:

If $|h(X)| < h_{limit}$

$$u = 0 \tag{4.31}$$

If $|\gamma(X)| < g_{limit}$

$$u = \frac{1}{h(X)}\theta_z(t)z \tag{4.32}$$

where h_{limit} and g_{limit} are the thresholds to cut off or reduce controller inputs. With the introduction of the logic gates in the Non-Linear Adaptive PI Controller, the same sets were simulated again under the same operating conditions. Figures 4-11 and 4-12 show the plots for $z_{nominal} = 0.90$ and $z_{nominal} = 0.95$. Tables 4.7 and 4.8 summarizes the results in terms of average NH_3 Slip and NO_x Slip.

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	29.0	0.94

Table 4.7: Performance Summary for Non-Linear Adaptive PI using z, $z_{nominal} = 0.90$

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Closed Loop	25.6	1.27

Table 4.8: Performance Summary for Non-Linear Adaptive PI with Logic Gate using z, $z_{nominal} = 0.95$

With the introduction of the logic gates, the Non-Linear Adaptive Pi Controller performed much better without the fluctuations seen before. NH_3 Slip and NO_x Slip numbers were also on par with previous controllers.

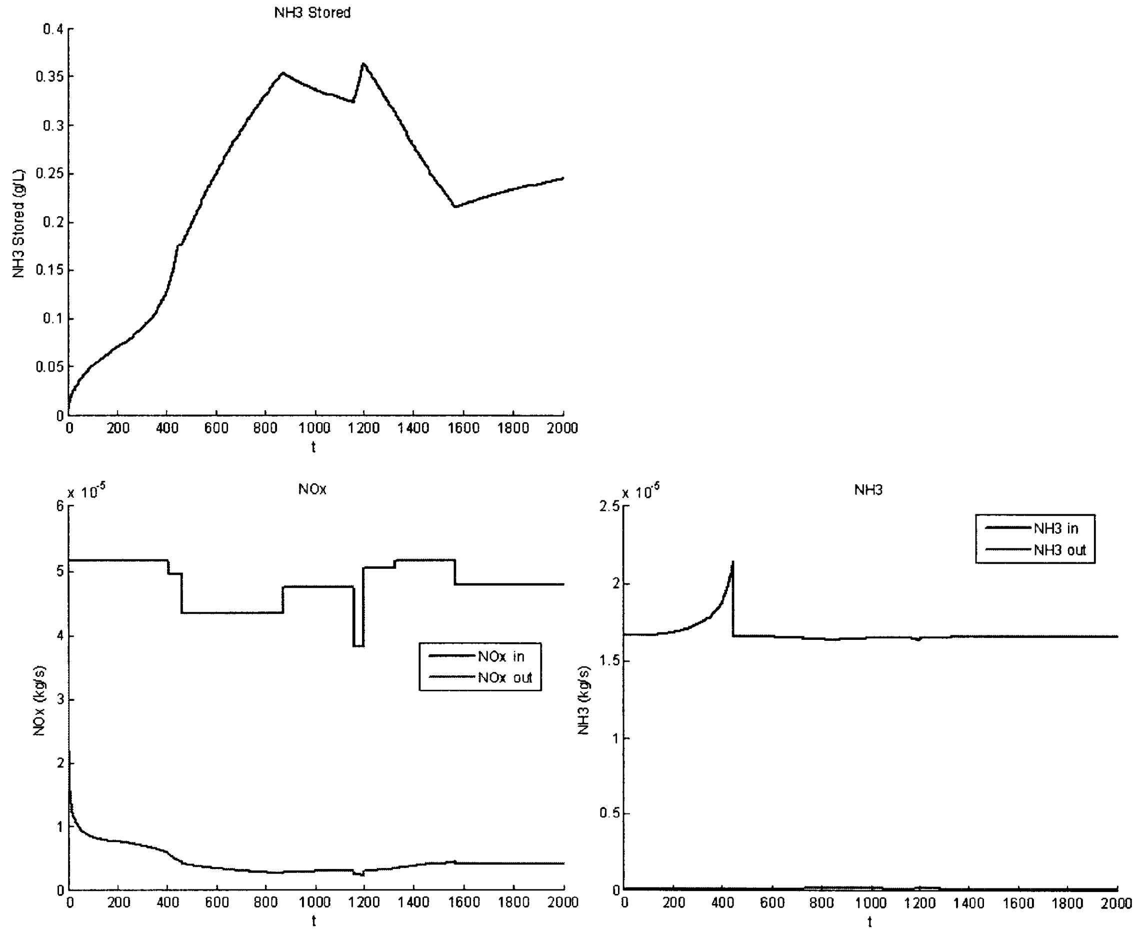


Figure 4-11: Performace Plots for Non-Linear Adaptive PI with Logic Gate using z, $z_{nominal} = 0.90$

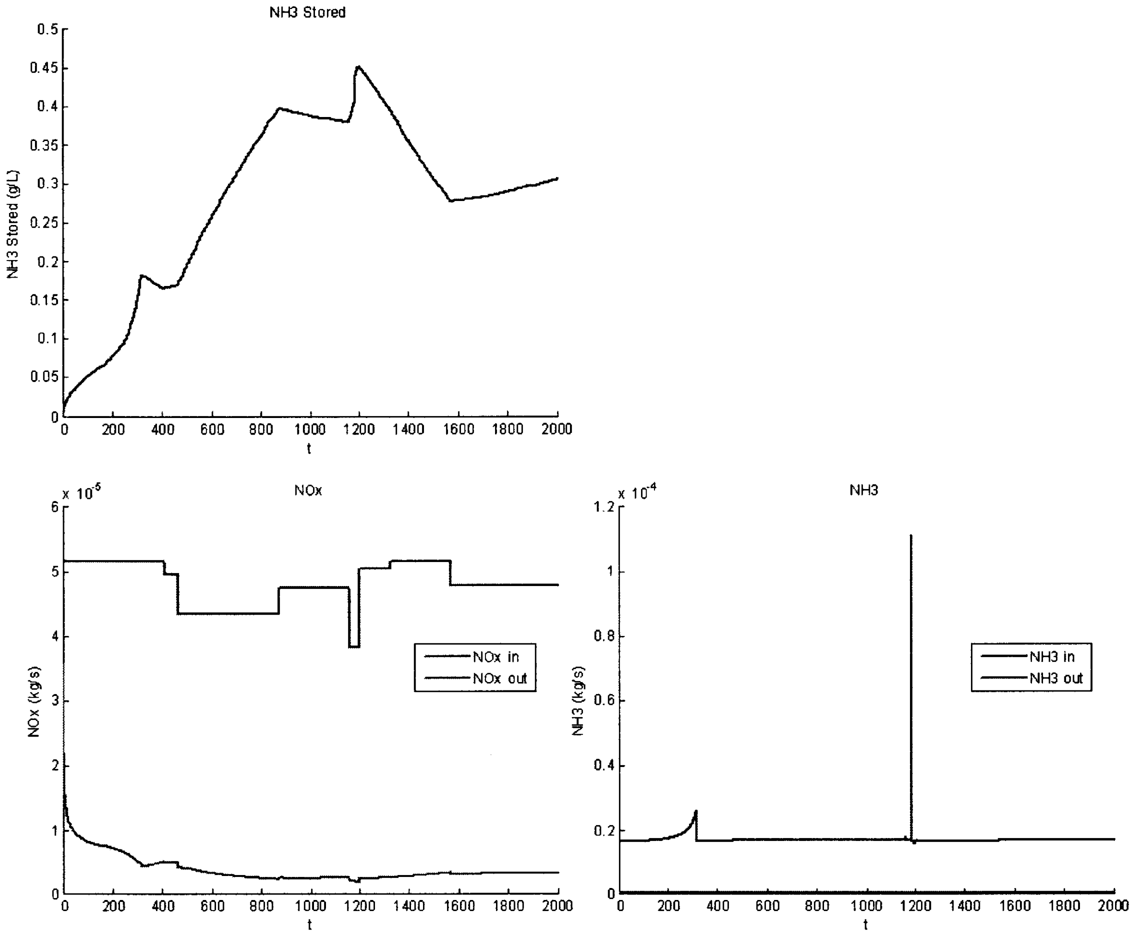


Figure 4-12: Performace Plots for Non-Linear Adaptive PI with Logic Gate using z, $z_{nominal} = 0.95$

4.5 Verification using Random NO_x, Space Velocity and Temperature Profiles

In a transition step-up before applying the Non-Linear Adaptive Controller on the FTP Cycle, a new random NO_x profile, random space velocity profile, and random temperature profile were introduced in three separate stages. The evaluation of the efficiency of the controller was slightly altered with the following new criteria to be met:

Overall NO_x Reduction Efficiency

$$\text{Average}\left(1 - \frac{NO_{x,out}}{NO_{x,in}}\right) > 0.90$$

Overall NH_3 Slip

$$\text{Peak NH}_3\text{ Slip (ppm)} < 20$$

Presented in three separate sets, the first set incorporates only a random NO_x profile, the second set includes the same NO_x profile, with a space velocity profile, and the third set had all three NO_x, space velocity and temperature profiles. Exact descriptions of the profiles are presented below together with the plots.

Figure 4-13 shows the peformance plots for the new random NO_x Profile. Eight separate steps between 250 ppm and 350 ppm were randomly selected and assigned various time lengths within the 2000 seconds NO_x profile. Space Velocity was kept constant at 30k (1/hr) and Temperature was kept constant at 500 (K). The overall mean efficiency was 91.2 % and Peak NH_3 Slip was 14.8 ppm.

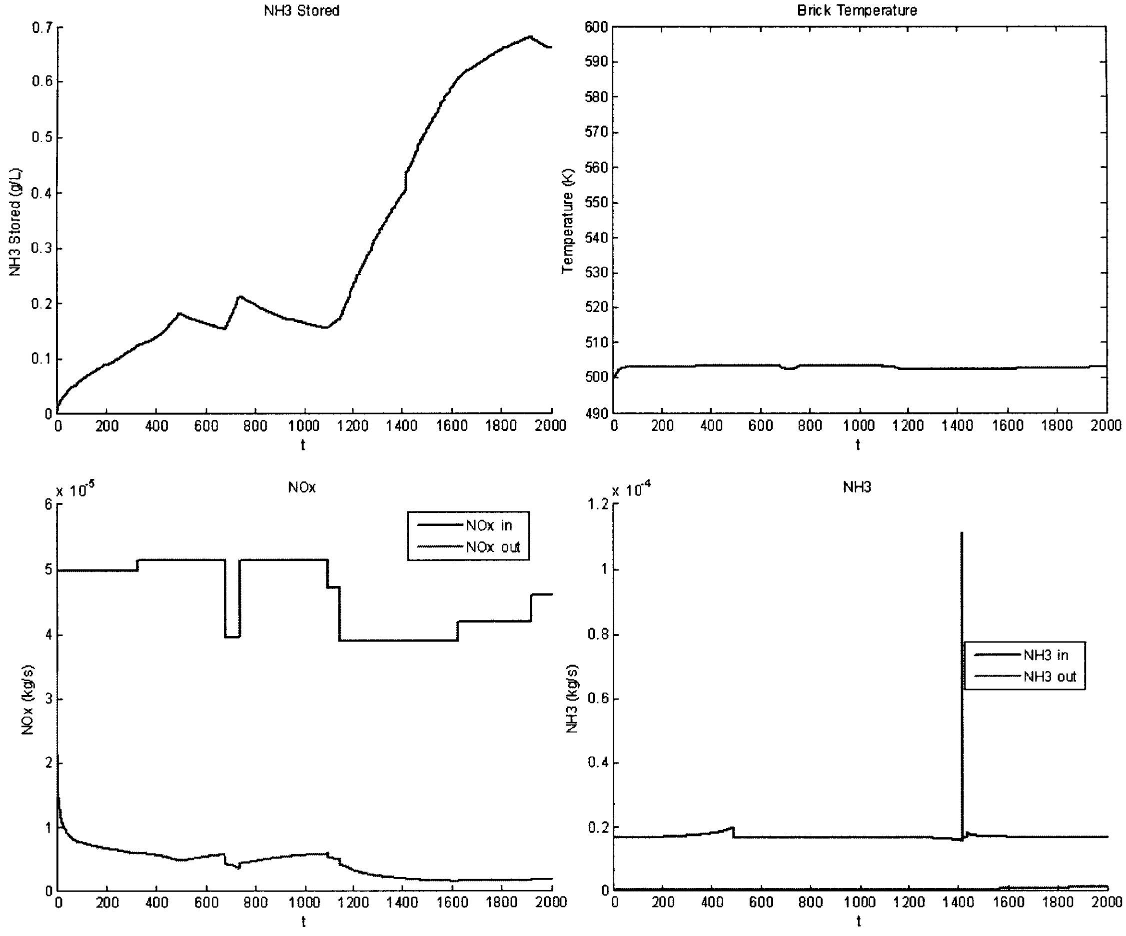


Figure 4-13: Performance Plots for Random NO_x Profile

Figure 4-14 shows the peformance plots for the same random NO_x Profile with a space velocity profile.The space velocity increased from 15k (1/hr) to 30k (1/hr) and dropped back down to 15k (1/hr) over the span of 2000 seconds. Temperature was kept constant at 500 (K). The overall mean efficiency was 91.7 % and Peak NH_3 Slip was 2.2 ppm.

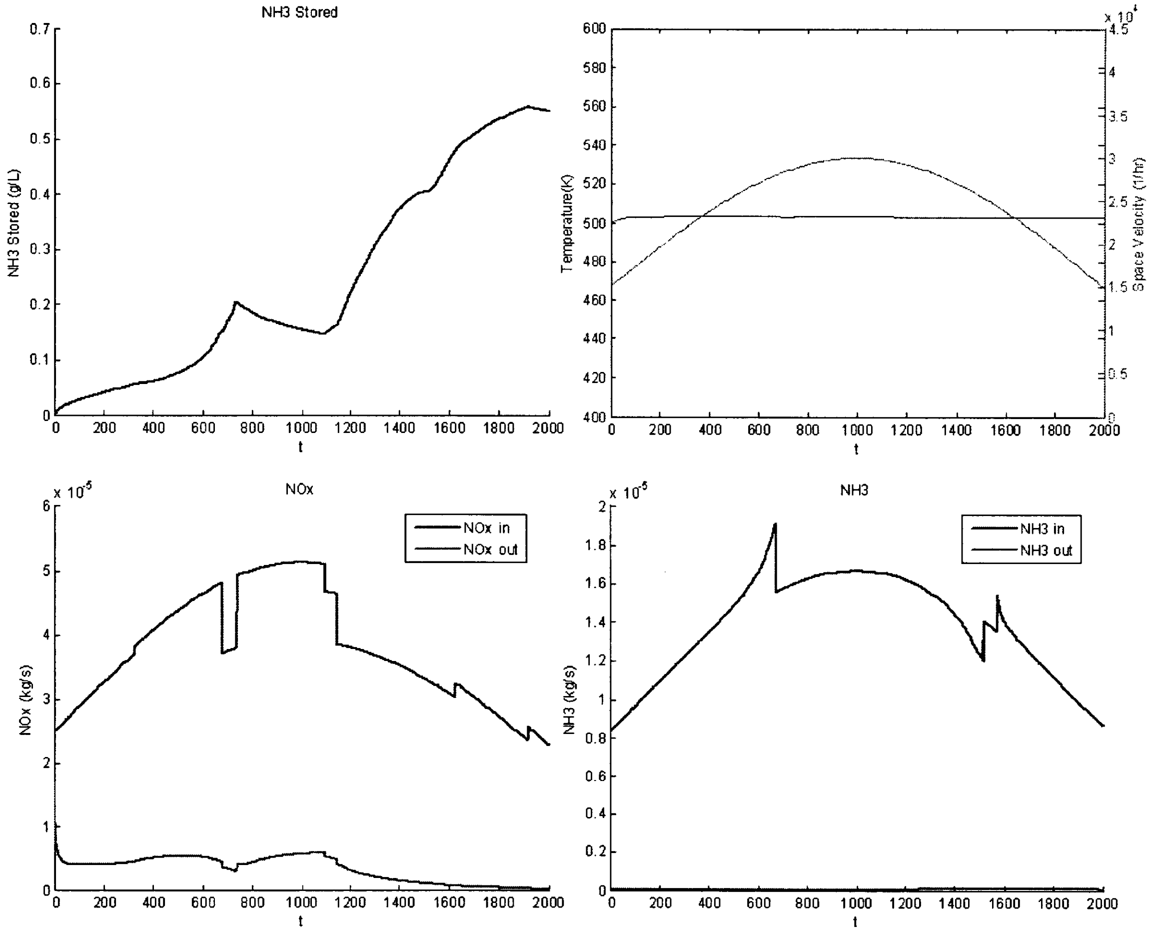


Figure 4-14: Performance Plots for Random NO_x Profile with Space Velocity Profile

Figure 4-15 shows the peformance plots for the same random NO_x and space velocity profiles, with a new temperature profile introduced. The temperature dropped from 600 (K) to 500 (K) and increased back to 600 (K) over 2000 seconds. The overall mean efficiency was 91.0 % and Peak NH_3 Slip was 2.8 ppm.

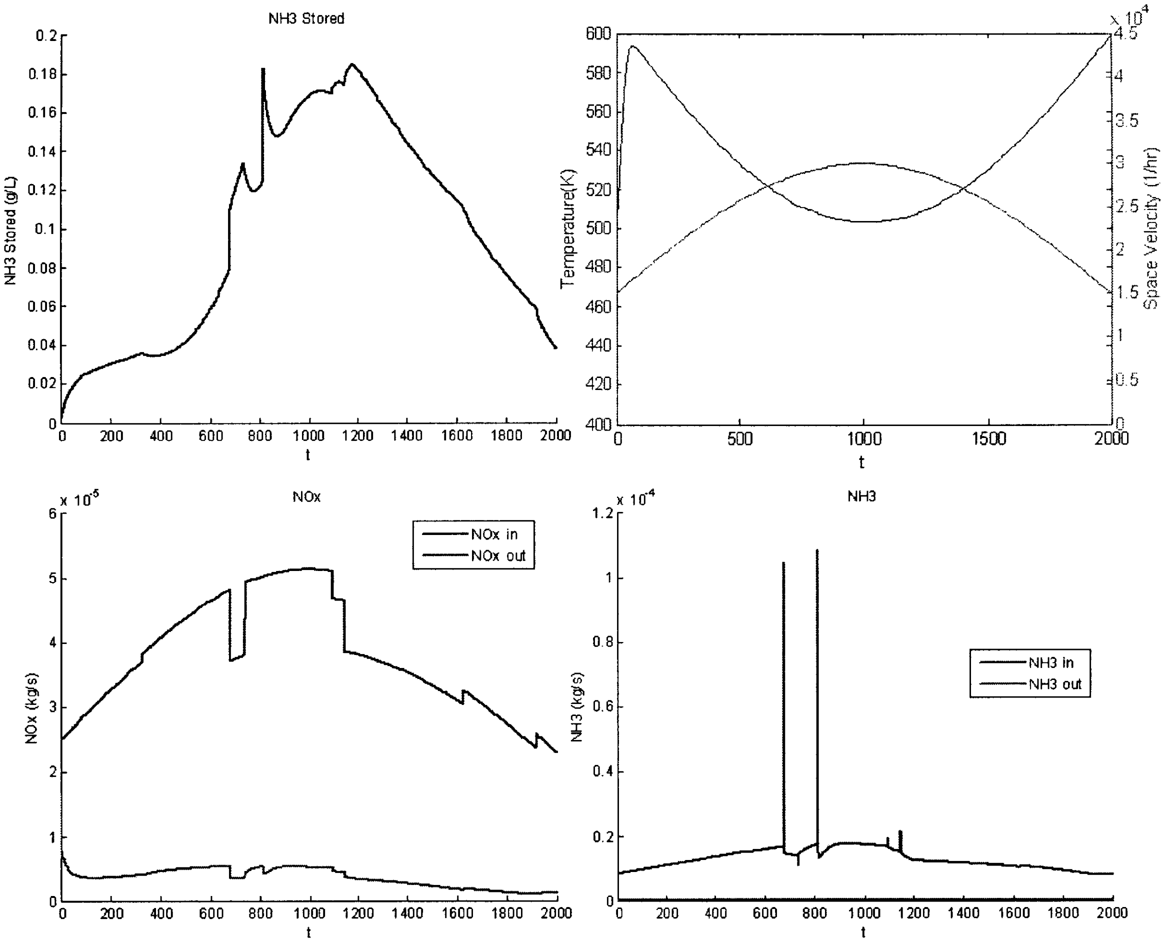


Figure 4-15: Performance Plots for Random NO_x Profile with Space Velocity and Temperature Profiles

4.6 Verification using FTP NO$_x$, Space Velocity and Temperature Profiles

With a similar evaluation critieria as the random NO$_x$, space velocity and temperature profiles presented above, the Non-Linear Adaptive PI Controller was then implemented on the FTP Cycle profiles that had been presented back in Section 2.1. Introducing the FTP profiles presented in Figure 2-2 in three successive simulation sets, the following plots present the performance of the Non-Linear Adaptive PI Controller for each.

Figure 4-16 shows the system peformance plots for the FTP NO_x Profile. Using the mean values for space velocity and temperature, the space velocty was kept constant at about 10k (1/hr) and temperature was kept constant at about 540 (K). The overall mean efficiency was 91.4 % and Peak NH_3 Slip was 0.0002 ppm.

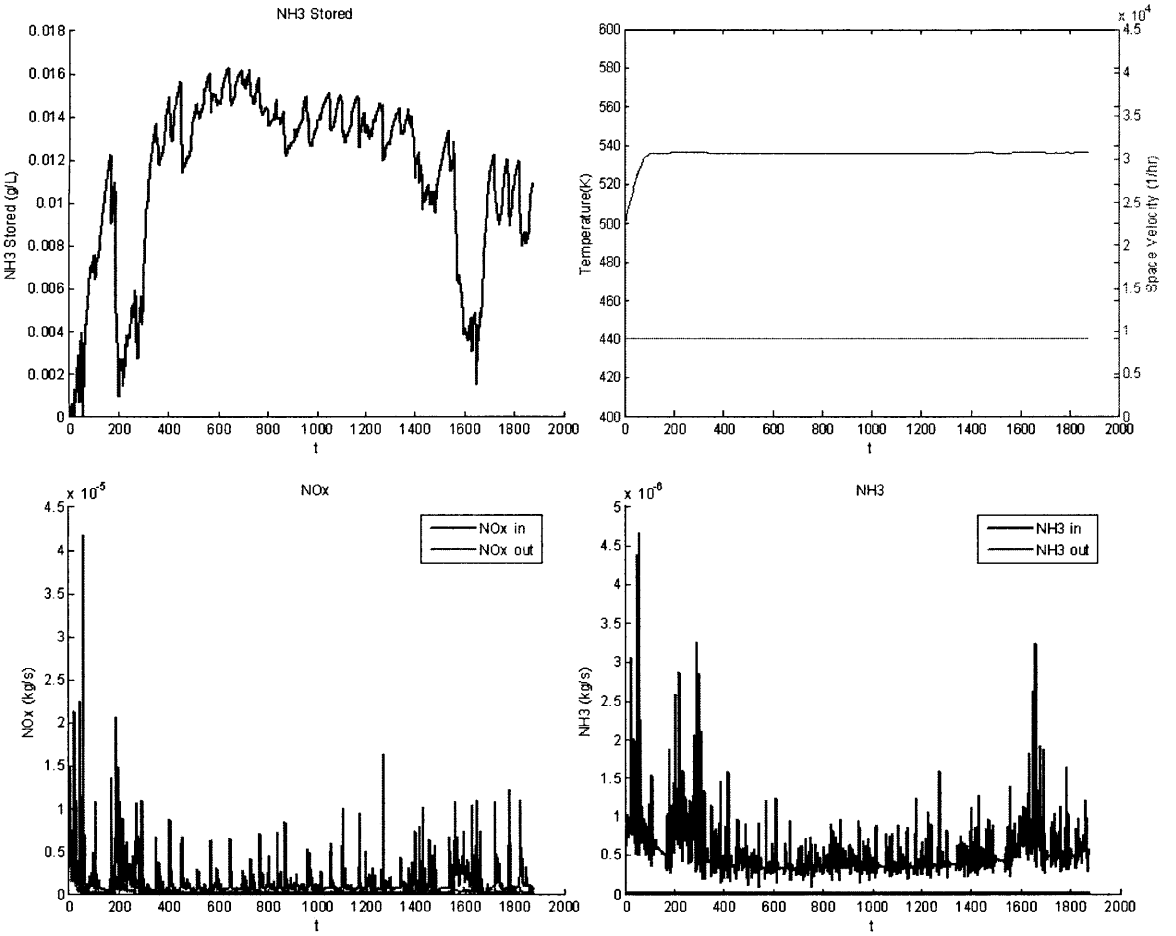


Figure 4-16: Performance Plots for FTP NO_x Profile

Figure 4-17 shows the system peformance plots for the FTP NO_x and space velocity profiles.The Temperature was kept constant at about 540 (K). The overall mean efficiency was 94.4 % and Peak NH_3 Slip was 0.81 ppm.

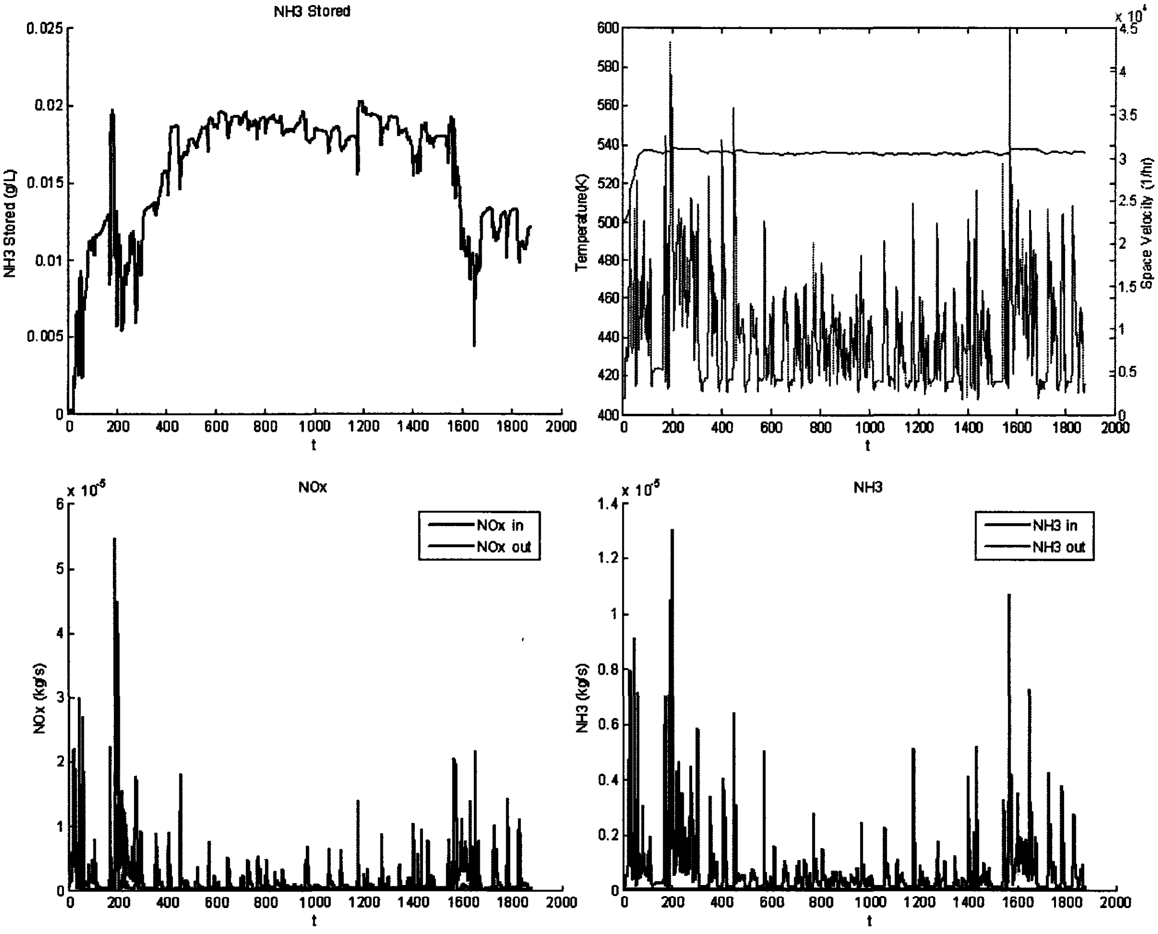


Figure 4-17: Performance Plots for FTP NO_x Profile with Space Velocity Profile

Figure 4-18 shows the system peformance plots for the FTP NO_x, space velocity and temperature profiles. The overall mean efficiency was 96.4 % and Peak NH_3 Slip was 9.3 ppm.

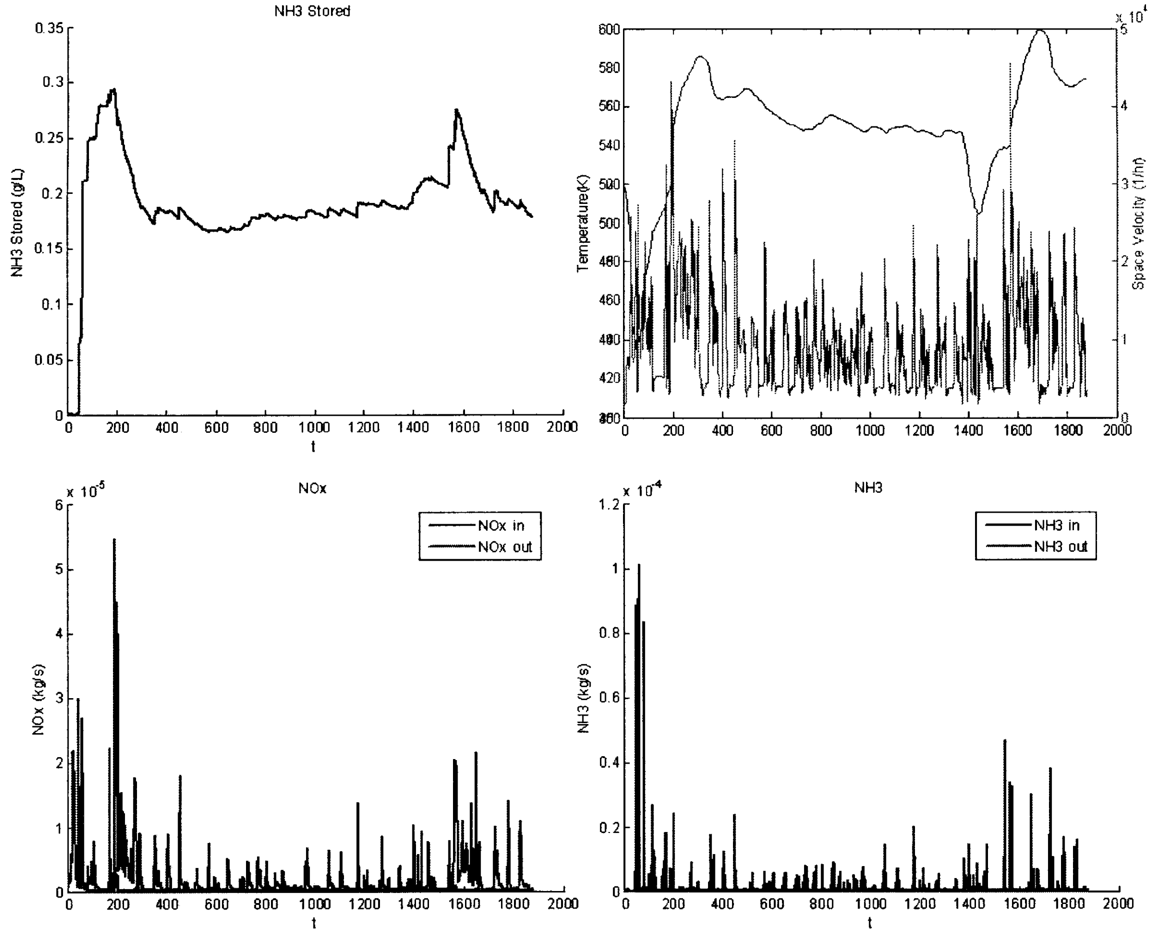


Figure 4-18: Performance Plots for FTP NO_x Profile with Space Velocity and Temperature Profiles

Overall, it can be observed that the Non-Linear Adaptive PI Controller was able to successfully meet the established criteria for all sets of the FTP Cycle.

Chapter 5

Conclusion

The Urea SCR System has shown great potential for implementation on diesel vehicles wanting to meet the upcoming emission regulations by the EPA. The chemical nature of the system had been widely investigated and full chemistry models capturing multiple states of the system had already been developed and verified. Based on a literature search through available published material, proposed methods of developing control algorithms include multiple brick modeling, state-space lumped parameter modeling, and system identification modeling.

This thesis set out to capture the behavior of the Urea SCR System with a first order transfer function model. Focusing on the state of Stored NH_3 as output, and the Excess $NH_{3,in}$ as input, a systems identification approach was adopted to capture the maps for the values of k and τ, the parameters for the transfer function. Using the small step disturbance approach, the maps of k and τ were developed as a function of multiple factors, including $NO_{x,in}$, Space Velocity, Temperature, Excess $NH_{3,in}$ and NH_3 Storage Level. To fully capture the remaining states of the Urea SCR System, namely NH_3 Slip and NO_x Slip, these states were mapped as functions of the state of Stored NH_3, $f(X)$ and $g(X)$. Using a full chemistry model develooped in the literature, the model was tested and verified to ensure that an acceptable level of accuracy was being achieved.

With a step by step approach to implementing a control algorithm on the Urea SCR System, the state of Stored NH_3 was first selected for negative feedback in a PI Controller. Testing the PI Controller through a range of operating conditions, the performance of the system was denoted by the average NH_3 Slip and NO_x Slip and was tabulated for comparison. An Adaptive PI Controller was subsequently developed and tested over a similar range of conditions. The performance was compared to that of the PI Controller, and results showed that the Adaptive PI Controller was able to perform as well as, if not better than the PI Controller, even as the operating conditions varied.

Since the state of Stored NH_3 is not measurable in an actual physical system, the combined state of NH_3 Slip and NO_x Slip was used as system output. Similar to the feedback controllers for Stored NH_3, the same operating conditions and performance evaluators were used to develop a PI Controller and a Adaptive PI Controller. With a final design of a Non-Linear Adaptive PI Controller, the plant and controller system was evaluated over a new range of operating conditions, using new target criteria of average system efficiency and peak NH_3 Slip. Implementing the Non-Linear Adaptive PI Controller on the FTP Cycle, the system was able to meet the requirements of at least 90% reduction efficieny and a peak NH_3 Slip of less than 2 ppm.

In conclusion, the Non-Linear Adaptive PI Controller had successfuly met the target requirements in the scope of a full chemistry simulations, and is ready for testing and development on a actual vehicular emissions set up.

Appendix A

EPA Regulations

United States
Environmental Protection
Agency

Air and Radiation

EPA420-F-00-057
December 2000

Office of Transportation and Air Quality

Regulatory Announcement

Heavy-Duty Engine and Vehicle Standards and Highway Diesel Fuel Sulfur Control Requirements

The U.S. Environmental Protection Agency (EPA) is establishing a comprehensive national control program that will regulate the heavy-duty vehicle and its fuel as a single system. As part of this program, new emission standards will begin to take effect in model year 2007 and will apply to heavy-duty highway engines and vehicles. These standards are based on the use of high-efficiency catalytic exhaust emission control devices or comparably effective advanced technologies.

Because these devices are damaged by sulfur, we are also reducing the level of sulfur in highway diesel fuel by 97 percent by mid-2006. The program provides substantial flexibility for refiners, especially small refiners, and for manufacturers of engines and vehicles, to aid them in implementing the new requirements in the most cost-efficient manner.

Background

The pollution emitted by diesel engines contributes greatly to our nation's continuing air quality problems. Even with more stringent heavy-duty highway engine standards set to take effect in 2004, these engines will continue to emit large amounts of oxides of nitrogen (NOx) and particulate matter (PM), both of which contribute to serious public health problems in the United States. Exposure is widespread, particularly in urban areas.

Diesel exhaust or diesel particulate matter (soot) is likely to cause lung cancer in humans. Other health effects include aggravation of respiratory and cardiovascular disease, aggravation of existing asthma, acute respiratory symptoms, chronic bronchitis and decreased lung function.

Heavy-duty trucks and buses today account for about one-third of NOx emissions and one-quarter of PM emissions from mobile sources. In some urban areas, the contribution is even greater. EPA's new program will result in PM and NOx emission levels that are 90 percent and 95 percent below today's levels, respectively.

The results of this historic program are comparable to the advent of the catalytic converter on cars, as the standards will for the first time result in the widespread introduction of exhaust emission control devices on diesel engines. And, just as removing lead from gasoline enables the use of catalytic converters, this program removes sulfur from diesel fuel to enable the use of these advanced emission controls on diesel vehicles.

New Standards for Heavy-Duty Highway Engines and Vehicles

We are finalizing a PM emissions standard for new heavy-duty engines of 0.01 grams per brake-horsepower-hour (g/bhp-hr), to take full effect for diesels in the 2007 model year. We are also finalizing standards for NOx and non-methane hydrocarbons (NMHC) of 0.20 g/bhp-hr and 0.14 g/bhp-hr, respectively. These NOx and NMHC standards will be phased in together between 2007 and 2010, for diesel engines. The phase-in will be on a percent-of-sales basis: 50 percent from 2007 to 2009 and 100 percent in 2010.

Gasoline engines will be subject to these standards based on a phase-in requiring 50 percent compliance in the 2008 model year and 100 percent compliance in the 2009 model year.

The program includes flexibility provisions to facilitate the transition to the new standards and to encourage the early introduction of clean technologies, and adjustments to various testing and compliance requirements to address differences between the new technologies and existing engine-based technologies.

New Standards for Diesel Fuel

Refiners will be required to start producing diesel fuel for use in highway vehicles with a sulfur content of no more than 15 parts per million (ppm), beginning June 1, 2006. At the terminal level, highway diesel fuel sold as low sulfur fuel will be required to meet the 15 ppm sulfur standard as of July 15, 2006. For retail stations and fleets, highway diesel fuel sold as low sulfur fuel must meet the 15 ppm sulfur standard by September 1, 2006.

This program includes a combination of flexibilities available to refiners to ensure a smooth transition to low sulfur highway diesel fuel. Refiners can take advantage of a temporary compliance option, including an averaging, banking and trading component, beginning in June 2006 and lasting through 2009, with credit given for early compliance before June 2006. Under this option, up to 20 percent of highway diesel fuel may continue to be produced at the existing 500 ppm sulfur maximum standard, though it must be segregated from 15 ppm fuel in the distribution system, and may only be used in pre-2007 model year heavy-duty vehicles.

We are providing additional hardship provisions for small refiners to minimize their economic burden in complying with the 15 ppm sulfur standard and giving additional flexibility to refiners subject to the Geographic Phase-in Area (GPA) provisions of the Tier 2 gasoline sulfur program, which will allow them the option of staggering their gasoline and diesel investments. We are also adopting a general hardship provision for which any refiner may apply on a case-by-case basis under certain conditions.

Health and Environmental Benefits

Without significant new controls on motor vehicle emissions, millions of Americans will continue to breathe unhealthy air. The new standards will result in substantial benefits to the public health and welfare through significant annual reductions in emissions of NOx, PM, NMHC, carbon monoxide, sulfur dioxide, and air toxics. The clean air impact of this program will be dramatic when fully implemented. These emission reductions will prevent 8,300 premature deaths, more than 9,500 hospitalizations, and 1.5 million work days lost.

As a result of this program, each new truck and bus will be more than 90 percent cleaner than current models. The clean air impact of this program will be dramatic when fully implemented. This program will provide annual emission reductions equivalent to removing the pollution from more than 90 percent of today's trucks and buses, or about 13 million trucks and buses.

We project a 2.6 million ton reduction of NOx emissions in 2030 when the current heavy-duty vehicle fleet is completely replaced with newer heavy-duty vehicles that comply with these emission standards. By 2030, this program will reduce annual emissions of NMHC by 115,000 tons and

Appendix B

Table of k and τ Values

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.01502	0.03096	0.01674
175	0.01246	0.02218	0.00874
262.5	0.01098	0.01622	0.00596
350	0.0098	0.012	0.00454

Table B.1: k Values for T = 500 (K) Step Up

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.00856	0.02502	0.02968
175	0.00856	0.02154	0.01334
262.5	0.00814	0.01914	0.00768
350	0.00748	0.01696	0.00544

Table B.2: k Values for T = 500 (K) Step Down

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.00386	0.0103	0.01252
175	0.0034	0.00868	0.00916
262.5	0.0031	0.00774	0.00686
350	0.00288	0.00704	0.00536

Table B.3: k Values for T = 550 (K) Step Up

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.0023	0.00796	0.01156
175	0.00252	0.00734	0.00992
262.5	0.0025	0.00674	0.00818
350	0.00244	0.00626	0.00646

Table B.4: k Values for T = 550 (K) Step Down

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.00098	0.00288	0.00366
175	0.00088	0.00258	0.00314
262.5	0.00082	0.00238	0.00278
350	0.0008	0.00222	0.00246

Table B.5: k Values for T = 600 (K) Step Up

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.00074	0.00244	0.00338
175	0.00072	0.00232	0.00308
262.5	0.00072	0.00218	0.00276
350	0.00068	0.00206	0.0025

Table B.6: k Values for T = 600 (K) Step Down

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	7787	4638	1577
175	6325	3347	820
262.5	5494	2389	557
350	4890	1731	423

Table B.7: τ Values for T = 500 (K) Step Up

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	3575	3551	3376
175	3747	3120	1497
262.5	3550	2868	789
350	3273	2705	541

Table B.8: τ Values for T = 500 (K) Step Down

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	1933	1652	1136
175	1659	1356	922
262.5	1492	1189	683
350	1363	1074	528

Table B.9: τ Values for T = 550 (K) Step Up

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	959	1177	1147
175	1092	1075	1014
262.5	1100	983	867
350	1098	910	686

Table B.10: τ Values for T = 550 (K) Step Down

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	475	450	376
175	416	392	317
262.5	385	355	276
350	361	327	244

Table B.11: τ Values for $T = 600$ (K) Step Up

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	324	362	343
175	319	341	308
262.5	311	319	277
350	303	299	249

Table B.12: τ Values for $T = 600$ (K) Step Down

Appendix C

Table of $x_{steadystate}$ Values

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.0763	0.3092	0.4787
175	0.1093	0.4298	0.5995
262.5	0.132	0.5081	0.6627
350	0.1497	0.5634	0.7042

Table C.1: $x_{steadystate}$ Values for T = 500 (K)

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.0236	0.1008	0.1714
175	0.0358	0.155	0.2594
262.5	0.0454	0.1951	0.3201
350	0.0534	0.2271	0.3641

Table C.2: $x_{steadystate}$ Values for T = 550 (K)

$NO_{x,in}$	SV: 10k (1/hr)	SV: 30k (1/hr)	SV: 45k (1/hr)
87.5	0.0152	0.0523	0.082
175	0.0218	0.0782	0.1239
262.5	0.0268	0.0981	0.1555
350	0.0309	0.1146	0.181

Table C.3: $x_{steadystate}$ Values for T = 600 (K)

Appendix D

Table of NH_3 Slip values

	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$
Stored NH_3	87.5 ppm	175 ppm	262.5 ppm	350 ppm
0	0	0	0	0
0.01	0	0	0	0
0.02	0	0	0	0
0.03	0	0	0	0
0.04	0	0	0	0
0.05	0	0	0	0
0.06	0	0	0	0
0.07	0	0	0	0
0.08	0	0	0	0
0.09	0	0	0	0
0.1	0	0	0	0
0.11	0	0	0	0
0.12	0	0	0	0
0.13	0	0	0	0
0.14	0	0	0	0
0.15	0	0	0	0
0.16	0	0	0	0
0.17	0	0	0	0
0.18	0	0	0	0.005393723
0.19	0	0	0.005393723	0.005393723
0.2	0	0.005393723	0.005393723	0.005393723
0.21	0	0.005393723	0.005393723	0.005393723
0.22	0	0.005393723	0.005393723	0.005393723
0.23	0.005393723	0.005393723	0.005393723	0.005393723
0.24	0.005393723	0.005393723	0.005393723	0.005393723
0.25	0.005393723	0.005393723	0.005393723	0.005393723
0.26	0.005393723	0.005393723	0.005393723	0.010787446
0.27	0.005393723	0.005393723	0.005393723	0.010787446
0.28	0.005393723	0.005393723	0.010787446	0.010787446
0.29	0.005393723	0.010787446	0.010787446	0.010787446
0.3	0.005393723	0.010787446	0.010787446	0.010787446
0.31	0.010787446	0.010787446	0.010787446	0.010787446
0.32	0.010787446	0.010787446	0.016181169	0.016181169
0.33	0.010787446	0.010787446	0.016181169	0.016181169
0.34	0.016181169	0.016181169	0.016181169	0.021574892
0.35	0.016181169	0.016181169	0.016181169	0.021574892
0.36	0.016181169	0.021574892	0.021574892	0.021574892
0.37	0.021574892	0.021574892	0.021574892	0.026968615
0.38	0.021574892	0.026968615	0.026968615	0.026968615
0.39	0.026968615	0.026968615	0.032362338	0.032362338
0.4	0.032362338	0.032362338	0.037756061	0.037756061

Table D.1: $f(X)$ Values for T = 500 (K), u_{in} = 10k (1/hr) [1]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.41	0.037756061	0.037756061	0.037756061	0.043149784
0.42	0.043149784	0.043149784	0.043149784	0.048543507
0.43	0.048543507	0.048543507	0.048543507	0.05393723
0.44	0.059330953	0.05393723	0.05393723	0.059330953
0.45	0.064724676	0.059330953	0.059330953	0.064724676
0.46	0.075512122	0.070118399	0.070118399	0.070118399
0.47	0.086299568	0.080905845	0.080905845	0.080905845
0.48	0.102480737	0.091693291	0.091693291	0.091693291
0.49	0.118661906	0.102480737	0.102480737	0.102480737
0.5	0.134843075	0.113268183	0.118661906	0.118661906
0.51	0.156417967	0.129449352	0.129449352	0.134843075
0.52	0.177992858	0.145630521	0.145630521	0.151024244
0.53	0.210355196	0.167205413	0.156417967	0.167205413
0.54	0.242717534	0.194174027	0.177992858	0.183386581
0.55	0.280473595	0.221142642	0.19956775	0.204961473
0.56	0.323623379	0.248111257	0.231930088	0.226536365
0.57	0.372166886	0.275079872	0.264292426	0.248111257
0.58	0.426104116	0.312835933	0.302048487	0.285867318
0.59	0.490828792	0.350591994	0.339804548	0.323623379
0.6	0.571734636	0.404529224	0.377560609	0.372166886
0.61	0.66882165	0.463860177	0.41531667	0.420710393
0.62	0.77669611	0.533978575	0.458466454	0.4692539
0.63	0.889964292	0.609490697	0.517797407	0.512403684
0.64	1.019413644	0.685002819	0.587915805	0.566340913
0.65	1.175831611	0.765908664	0.674215373	0.625671866
0.66	1.370005638	0.857601955	0.771302387	0.695790265
0.67	1.601935726	0.970870137	0.879176846	0.787483556
0.68	1.866228153	1.111106935	0.987051306	0.900751738
0.69	2.16827664	1.28370607	1.094925766	1.024807367
0.7	2.508081188	1.477880098	1.213587671	1.170437888
0.71	2.885641797	1.682841571	1.348430746	1.305280962
0.72	3.354895696	1.898590491	1.515636159	1.44551776
0.73	3.937417779	2.130520579	1.731385078	1.585754557
0.74	4.649389213	2.389419282	1.984890058	1.747566247
0.75	5.469235106	2.707648938	2.270757376	1.941740274
0.76	6.39695546	3.112178162	2.578199587	2.200638978
0.77	7.470306333	3.597613231	2.880248074	2.497293742
0.78	8.797162188	4.153166698	3.187690284	2.869460628
0.79	10.52854727	4.741082503	3.538282278	3.268596129
0.8	12.7885172	5.366754369	3.958992671	3.673125352

Table D.2: $f(X)$ Values for T = 500 (K), u_{in} = 10k (1/hr) [2]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.81	15.56089081	6.030182297	4.466002631	4.045292238
0.82	18.9373614	6.79609096	5.118643112	4.449821462
0.83	23.71619996	7.756173652	5.889945499	4.902894193
0.84	32.03871453	8.958973877	6.769122345	5.45844766
0.85	48.5758692	10.4422477	7.642905469	6.159631648
0.86	60.6146589	12.10351438	8.516688592	7.033414772
0.87	71.33198647	13.93198647	9.471377561	8.063615862
0.88	82.06010148	15.83597068	10.57169705	9.244841195
0.89	93.04172148	17.99345988	11.93091524	10.3721293
0.9	104.4116895	20.74965232	13.6569066	11.54796091
0.91	116.4073294	24.36884044	15.84675813	12.68603646
0.92	128.877617	29.05598572	18.33326442	14.03986093
0.93	141.9412141	34.69781996	20.9330389	15.71191505
0.94	155.8624131	41.03544447	23.64068784	17.8586168
0.95	170.2312911	48.5758692	26.45621124	20.53929712
0.96	185.3067469	59.50355196	29.80571321	23.65686901
0.97	201.7036647	79.02882917	34.22856606	27.15739523
0.98	218.1922759	118.3544634	40.1994174	30.647134
0.99	236.1587671	148.6941552	47.52948694	34.27171584
1	255.6732569	172.9281526	56.38598008	37.97180981

Table D.3: $f(X)$ Values for $T = 500$ (K), $u_{in} = 10$k (1/hr) [3]

	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$
Stored NH_3	87.5 ppm	175 ppm	262.5 ppm	350 ppm
0	0.125853536	2.364248575	2.490102111	2.615955647
0.01	0.127651444	2.364248575	2.490102111	2.615955647
0.02	0.129449352	2.364248575	2.490102111	2.615955647
0.03	0.131247259	2.364248575	2.490102111	2.615955647
0.04	0.136640982	2.364248575	2.490102111	2.615955647
0.05	0.143832613	2.364248575	2.490102111	2.615955647
0.06	0.154620059	2.364248575	2.490102111	2.615955647
0.07	0.174397043	2.364248575	2.490102111	2.615955647
0.08	0.19956775	2.364248575	2.490102111	2.615955647
0.09	0.233727996	2.364248575	2.490102111	2.615955647
0.1	0.275079872	2.364248575	2.490102111	2.615955647
0.11	0.318229656	2.364248575	2.490102111	2.615955647
0.12	0.359581532	2.364248575	2.490102111	2.615955647
0.13	0.395539686	2.364248575	2.490102111	2.615955647
0.14	0.424306208	2.364248575	2.490102111	2.615955647
0.15	0.451274823	2.364248575	2.490102111	2.615955647
0.16	0.478243438	2.364248575	2.490102111	2.615955647
0.17	0.507009961	2.364248575	2.490102111	2.615955647
0.18	0.541170206	2.364248575	2.490102111	2.615955647
0.19	0.58431999	2.364248575	2.490102111	2.615955647
0.2	0.631065589	2.364248575	2.490102111	2.615955647
0.21	0.683204911	2.364248575	2.490102111	2.615955647
0.22	0.737142141	2.364248575	2.490102111	2.615955647
0.23	0.789281463	2.364248575	2.490102111	2.615955647
0.24	0.83782497	2.364248575	2.490102111	2.615955647
0.25	0.884570569	2.364248575	2.490102111	2.615955647
0.26	0.924124538	2.364248575	2.490102111	2.615955647
0.27	0.963678507	2.364248575	2.490102111	2.615955647
0.28	1.005030383	2.364248575	2.490102111	2.615955647
0.29	1.046382259	2.364248575	2.490102111	2.615955647
0.3	1.094925766	2.364248575	2.490102111	2.615955647
0.31	1.14526718	2.364248575	2.490102111	2.615955647
0.32	1.204598133	2.364248575	2.490102111	2.615955647
0.33	1.265726994	2.364248575	2.490102111	2.615955647
0.34	1.3376433	2.364248575	2.490102111	2.615955647
0.35	1.416751237	2.358854852	2.491900019	2.62134937
0.36	1.495859174	2.36065276	2.500889557	2.632136816
0.37	1.587552465	2.373238113	2.515272818	2.651913801
0.38	1.682841571	2.400206728	2.551230972	2.687871954
0.39	1.787120215	2.450548143	2.608764017	2.747202907
0.4	1.898590491	2.522464449	2.682478231	2.835300382

Table D.4: $f(X)$ Values for T = 500 (K), u_{in} = 30k (1/hr) [1]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.41	2.015454489	2.61415774	2.801140137	2.962951826
0.42	2.141308025	2.718436384	2.943174842	3.124763516
0.43	2.276151099	2.824512936	3.076220009	3.308150097
0.44	2.418185805	2.930589488	3.227244252	3.495132494
0.45	2.576401679	3.043857671	3.351299881	3.671327445
0.46	2.738213368	3.151732131	3.489738771	3.833139134
0.47	2.918004135	3.268596129	3.629975569	3.989557101
0.48	3.101390716	3.399843388	3.784595627	4.149570883
0.49	3.306352189	3.543676001	3.932024056	4.325765833
0.5	3.523899016	3.710881413	4.122602268	4.525333584
0.51	3.754031197	3.869097287	4.331159556	4.751869949
0.52	4.000344547	4.029111069	4.518141953	4.998183299
0.53	4.262839065	4.190922759	4.737486688	5.255284094
0.54	4.541514753	4.37430934	4.956831423	5.51238489
0.55	4.838169517	4.546908476	5.172580342	5.76588987
0.56	5.168984527	4.732092965	5.359562739	6.01220322
0.57	5.506991167	4.955033515	5.584301197	6.256718662
0.58	5.880955961	5.17437825	5.823422915	6.503032012
0.59	6.280091462	5.440468584	6.084119526	6.761930715
0.6	6.706195577	5.70476101	6.325039153	7.038808495
0.61	7.161066216	6.022990666	6.632481363	7.339059074
0.62	7.644703377	6.337624507	6.970488004	7.669874084
0.63	8.184075675	6.713387208	7.340856982	8.031253524
0.64	8.761204034	7.083756186	7.74179039	8.424995302
0.65	9.374290547	7.526041471	8.176884044	8.854695233
0.66	10.03052684	7.961135125	8.647935852	9.316757502
0.67	10.76227526	8.480730439	9.083029506	9.816575832
0.68	11.54436509	9.043475537	9.627795527	10.35415022
0.69	12.38219006	9.654764142	10.21571133	11.0517384
0.7	13.31350623	10.25346739	10.84857483	11.68100608
0.71	14.31134499	10.96723673	11.53177974	12.35522145
0.72	15.42065401	11.74033703	12.26892188	13.07798033
0.73	16.6144647	12.578162	13.06000125	13.85287853
0.74	17.94671428	13.48610537	13.91400739	14.68171396
0.75	19.37784878	14.56305206	14.83273821	15.75506484
0.76	21.0265301	15.63460502	15.96901585	16.71874334
0.77	22.80466078	16.79425547	17.04416463	17.74894443
0.78	24.8524776	18.16605901	18.20021926	18.85285974
0.79	27.06749984	19.53246883	19.44437136	20.03228716
0.8	29.69064712	21.14698991	20.78021675	21.55691286

Table D.5: $f(X)$ Values for T = 500 (K), u_{in} = 30k (1/hr) [2]

	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$
Stored NH_3	87.5 ppm	175 ppm	262.5 ppm	350 ppm
0.81	32.69315292	22.9035457	22.43249389	22.92332268
0.82	36.12176283	24.81472154	23.99127983	24.38502161
0.83	40.31807931	26.88770908	25.91683894	26.27282466
0.84	45.46908476	29.13868947	27.73632149	27.96645367
0.85	52.00987283	31.79240118	29.98011025	30.14911358
0.86	61.21156424	34.68703251	32.09804548	32.10703502
0.87	75.9382259	37.83696674	34.7068095	34.63309528
0.88	87.61563616	41.54065652	37.53491825	36.89486312
0.89	98.67456618	45.58415085	40.59495709	39.81286726
0.9	109.9672242	49.99082253	43.906703	42.96639729
0.91	121.3947253	55.49241997	47.48993297	45.78911232
0.92	133.6384765	61.51541064	51.86424231	49.42627952
0.93	146.7991606	68.49309027	56.08393159	53.35470776
0.94	160.4884295	76.99000188	61.2259475	57.59776984
0.95	174.4150222	86.66454301	66.81923824	62.17524275
0.96	189.5623943	99.56812629	72.8871766	67.11229719
0.97	205.6392846	115.4598321	80.22443776	73.3564305
0.98	222.1566623	138.0019984	88.21793523	79.15648061
0.99	240.171697	168.7372298	97.80258097	86.48295433
1	259.6142705	191.592232	109.2228904	94.45128109

Table D.6: $f(X)$ Values for $T = 500$ (K), $u_{in} = 30$k (1/hr) [3]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0	0.716759546	1.426410733	2.139616099	2.852821465
0.01	0.721498452	1.431149639	2.144355005	2.857560372
0.02	0.727422085	1.435888545	2.150278638	2.863484004
0.03	0.736899897	1.446551084	2.158571723	2.87177709
0.04	0.749931889	1.459583075	2.175157895	2.884809082
0.05	0.771256966	1.483277606	2.196482972	2.914427245
0.06	0.804429309	1.515265222	2.229655315	2.94996904
0.07	0.849448916	1.574501548	2.294815273	3.003281734
0.08	0.920532508	1.650324045	2.37774613	3.085027864
0.09	1.020049536	1.781828689	2.497403509	3.257997936
0.1	1.148	1.939397317	2.722501548	3.455847265
0.11	1.297275542	2.18345098	2.973663571	3.731888545
0.12	1.456028896	2.43579773	3.293539732	4.095599587
0.13	1.606489164	2.758043344	3.670282766	4.545795666
0.14	1.74747162	3.030530444	4.180899897	5.241230134
0.15	1.855281734	3.313680083	4.577783282	5.780280702
0.16	1.946505676	3.516268318	5.011393189	6.283789474
0.17	2.027067079	3.707009288	5.293358101	6.719768834
0.18	2.10525903	3.838513932	5.519640867	7.178257998
0.19	2.188189886	3.973572755	5.74355418	7.441267286
0.2	2.287706914	4.102707946	5.895199174	7.653333333
0.21	2.394332301	4.219995872	6.037366357	7.891463364
0.22	2.512804954	4.375195046	6.222183695	8.060879257
0.23	2.65378741	4.529209494	6.388045408	8.239772962
0.24	2.791215686	4.738906089	6.634468524	8.442361197
0.25	2.939306502	4.978220846	6.869044376	8.764606811
0.26	3.073180599	5.203318885	7.139162023	9.057234262
0.27	3.19876161	5.478175439	7.521828689	9.397250774
0.28	3.324342621	5.754216718	7.854736842	9.91971517
0.29	3.439261094	5.981684211	8.287162023	10.35214035
0.3	3.538778122	6.229292054	8.630732714	10.80352116
0.31	3.641849329	6.45202064	9.037093911	11.40654696
0.32	3.737812178	6.651054696	9.334460268	11.83897214
0.33	3.843252838	6.805069143	9.602208462	12.2394097
0.34	3.954617131	6.972115583	9.898390093	12.71448504
0.35	4.075459236	7.130868937	10.10927141	13.02369866
0.36	4.196301342	7.288437564	10.34740144	13.29973994
0.37	4.338468524	7.428235294	10.52511042	13.62317028
0.38	4.493667699	7.60002064	10.7431001	13.84471414
0.39	4.661898865	7.78720743	10.92080908	14.05559546
0.4	4.844346749	7.992165119	11.15420021	14.33519092

Table D.7: $f(X)$ Values for $T = 500$ (K), $u_{in} = 45$k (1/hr) [1]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.41	5.038641899	8.217263158	11.35560372	14.55199587
0.42	5.24596904	8.429329205	11.63282972	14.78183282
0.43	5.466328173	8.697077399	11.87688338	15.1159257
0.44	5.699719298	8.988520124	12.21334572	15.39433643
0.45	5.946142415	9.302472652	12.50952735	15.80662126
0.46	6.224553148	9.638934985	12.91233437	16.14900722
0.47	6.498224974	9.996722394	13.35423736	16.5233808
0.48	6.786113519	10.37583488	13.73334985	17.06953973
0.49	7.10954386	10.77508772	14.23804334	17.5149969
0.5	7.427050568	11.19566563	14.66572962	18.15474923
0.51	7.783653251	11.63756863	15.22965944	18.66655108
0.52	8.158026832	12.1007967	15.70355005	19.20441692
0.53	8.524107327	12.58653457	16.32553148	19.96145717
0.54	8.936392157	13.09359752	16.97950052	20.55855934
0.55	9.367632611	13.62317028	17.52565944	21.39497626
0.56	9.821382869	14.17762229	18.24004954	22.05131476
0.57	10.32844582	14.75458411	18.98761197	22.96710836
0.58	10.82840041	15.4464644	19.6095934	23.68386791
0.59	11.35204954	16.07910836	20.41994634	24.68140764
0.6	11.93730444	16.73900103	21.26584107	25.46095769
0.61	12.55336223	17.42732714	22.15083179	26.542613
0.62	13.20140764	18.24952735	22.88536223	27.38613829
0.63	13.88144066	19.00064396	23.84143653	28.55664809
0.64	14.59583075	19.78374819	24.84016099	29.46888751
0.65	15.34457792	20.71968215	25.8815356	30.73536017
0.66	16.18336429	21.57386997	26.74638596	31.72223736
0.67	17.06480083	22.5939195	27.86950671	33.09059649
0.68	17.99244169	23.66254283	29.04001651	34.15685036
0.69	18.96865635	24.63875748	30.26028483	35.63301961
0.7	20.05623529	25.80334365	31.53386584	37.17434881
0.71	21.20423529	27.02361197	32.86075955	38.37447678
0.72	22.48137049	28.29956244	34.24452012	40.03546336
0.73	23.75850568	29.63474923	35.6863323	41.76990299
0.74	25.256	31.03272652	37.18856553	43.12049123
0.75	26.83997936	32.49586378	38.75358927	44.99117441
0.76	28.51399794	34.02534572	40.38377296	46.94360372
0.77	30.46287307	35.62591125	42.42979567	48.98014861
0.78	32.52785139	37.5131806	44.21399381	50.56531269
0.79	34.81318885	39.27249948	46.07282972	52.75705676
0.8	37.33784107	41.34814035	48.40555624	55.04239422

Table D.8: $f(X)$ Values for T = 500 (K), u_{in} = 45k (1/hr) [2]

	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$
Stored NH_3	87.5 ppm	175 ppm	262.5 ppm	350 ppm
0.81	40.23331269	43.52922188	50.43736223	57.42843344
0.82	43.5304066	45.82048297	52.5532838	59.91754386
0.83	47.50753354	48.22547781	55.20588648	62.5144644
0.84	52.06043756	51.04038803	57.98999381	65.2215645
0.85	57.66063983	53.70483798	60.415129	68.0447678
0.86	64.89694943	56.81829928	63.45750671	70.98644376
0.87	75.05124045	60.09999174	66.64797523	74.052516
0.88	86.8013581	63.91125697	69.9924582	77.24890815
0.89	96.59193808	67.93695769	73.49806398	81.43691641
0.9	106.5779979	72.18775645	77.1707162	84.94726109
0.91	116.8436533	77.08541589	81.01989267	88.60688132
0.92	127.7466914	82.69983488	85.74221259	93.39554592
0.93	139.1082188	89.10091228	90.72398762	97.40347575
0.94	151.761098	96.34551496	95.97469556	102.6470753
0.95	164.2066502	104.4620764	101.5026295	107.0364871
0.96	178.5679051	115.0073271	107.3160826	112.781226
0.97	192.0678638	127.7502456	114.3261094	118.8197771
0.98	208.3969494	145.3458039	121.7318349	125.1639876
0.99	224.1099773	170.3103612	130.5355377	131.8197812
1	240.3537626	189.9602353	139.8273478	140.2360784

Table D.9: $f(X)$ Values for T = 500 (K), u_{in} = 45k (1/hr) [3]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0	0	0	0	0
0.01	0	0	0	0
0.02	0	0	0	0
0.03	0	0	0	0
0.04	0	0	0	0
0.05	0	0	0	0
0.06	0.005393723	0	0	0
0.07	0.005393723	0.005393723	0	0
0.08	0.010787446	0.005393723	0.005393723	0
0.09	0.021574892	0.005393723	0.005393723	0.005393723
0.1	0.037756061	0.010787446	0.005393723	0.005393723
0.11	0.070118399	0.010787446	0.005393723	0.005393723
0.12	0.124055629	0.021574892	0.010787446	0.010787446
0.13	0.226536365	0.026968615	0.016181169	0.010787446
0.14	0.426104116	0.037756061	0.021574892	0.016181169
0.15	0.852208232	0.05393723	0.026968615	0.021574892
0.16	1.95252772	0.075512122	0.037756061	0.026968615
0.17	6.763728622	0.10787446	0.048543507	0.032362338
0.18	7.756173652	0.156417967	0.064724676	0.043149784
0.19	10.93307649	0.221142642	0.086299568	0.05393723
0.2	14.39584665	0.318229656	0.113268183	0.070118399
0.21	18.19302763	0.458466454	0.151024244	0.091693291
0.22	22.31383199	0.652640481	0.19956775	0.113268183
0.23	26.83916557	0.949295245	0.264292426	0.151024244
0.24	31.76363466	1.380793084	0.355985717	0.194174027
0.25	37.11420786	2.017252396	0.4692539	0.248111257
0.26	42.85852283	2.988122533	0.631065589	0.318229656
0.27	49.12602894	4.487577523	0.841420786	0.41531667
0.28	55.77648938	6.85002819	1.127288104	0.533978575
0.29	63.12274009	10.81980831	1.515636159	0.690396542
0.3	70.92206352	19.44437136	2.033433565	0.884570569
0.31	79.22839692	27.70216125	2.756192445	1.148862996
0.32	88.19276452	36.78519075	3.727062582	1.477880098
0.33	97.72886675	46.31050554	5.064705882	1.925559105
0.34	107.7234354	56.51542943	6.914752866	2.491900019
0.35	118.8830483	67.27590678	9.509133621	3.225446345
0.36	130.3393159	78.70520579	13.18225897	4.207103928
0.37	142.3996805	91.12694982	18.56519451	5.485416275
0.38	155.6035144	104.1473971	26.84995302	7.189832738
0.39	170.0802669	118.0685961	40.45292238	9.390471716
0.4	185.0586356	132.8473971	62.32446908	12.37859425

Table D.10: $f(X)$ Values for T = 600 (K), u_{in} = 10k (1/hr) [1]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.41	201.2991355	148.5700996	81.24564931	16.41849276
0.42	218.8664913	165.5279647	100.0535614	21.95245255
0.43	236.4662094	183.5052434	119.1041909	29.71941364
0.44	256.6117647	202.14595	139.4547078	40.85205788
0.45	278.1057508	223.1598948	160.3176283	57.95015974
0.46	300.8402932	245.5762075	182.1999624	86.85512122
0.47	324.6427927	269.0604774	205.943131	123.8722421
0.48	351.8757001	294.944954	231.7520955	153.6671678
0.49	380.2305018	321.1746288	258.8393723	182.7501222
0.5	409.2649126	351.8163691	287.4854351	213.0844202
0.51	442.3122533	382.0050366	318.6072167	244.6538808
0.52	475.7047923	417.0372674	351.6923135	278.472524
0.53	513.6388461	454.0543883	388.7471904	314.6428303
0.54	551.2654576	492.5493892	426.5841571	352.6146401
0.55	593.8489006	531.7779365	467.5063334	395.1387521
0.56	635.0299756	576.7346176	511.2224582	438.2939297
0.57	681.3350874	621.7560233	557.176978	487.0693667
0.58	733.7351062	673.2175343	604.5338658	536.8588235
0.59	782.9258598	723.49782	659.4527532	590.8499906
0.6	838.082071	780.6551024	715.1537305	641.6103176
0.61	900.3094531	834.5761511	769.8406878	700.8010336
0.62	956.1021237	895.3202593	832.3377561	770.558053
0.63	1034.818117	964.2250705	904.3493516	831.5286976
0.64	1106.338884	1042.97882	973.2325879	901.7064274
0.65	1165.880192	1114.531949	1051.97555	983.2325503
0.66	1254.54221	1195.222045	1123.517891	1061.889213
0.67	1329.191336	1262.805394	1204.1972	1133.36683
0.68	1412.076677	1364.142661	1295.825766	1235.76666
0.69	1504.605995	1450.102424	1400.728284	1330.415711
0.7	1608.53225	1546.25093	1489.897313	1410.393836
0.71	1726.039899	1654.470588	1589.837606	1531.536854
0.72	1813.27258	1777.129243	1702.577204	1635.452321
0.73	1959.998027	1868.380248	1830.683518	1752.95997
0.74	2070.261906	2022.263165	1926.21714	1886.837568
0.75	2192.305676	2138.222815	2087.742962	1986.923492
0.76	2328.092652	2266.900864	2209.824488	2156.631592
0.77	2480.044616	2410.460195	2345.643826	2285.29346
0.78	2651.160477	2571.603063	2497.628153	2428.83661
0.79	2845.253599	2753.705939	2668.787164	2589.96869
0.8	2952.389119	2853.915918	2862.918042	2772.060778

Table D.11: $f(X)$ Values for T = 600 (K), u_{in} = 10k (1/hr) [2]

	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$
Stored NH_3	87.5 ppm	175 ppm	262.5 ppm	350 ppm
0.81	3190.516595	3075.889194	2970.075136	2979.406277
0.82	3323.320842	3332.047886	3208.245762	3094.227852
0.83	3622.030615	3475.472374	3484.501466	3350.38115
0.84	3790.757057	3630.795414	3639.835294	3493.805638
0.85	3974.699192	3983.501748	3808.588705	3817.876696
0.86	4175.960571	4184.790096	4193.846157	4001.835012
0.87	4397.070851	4405.916557	4414.988799	4203.117967
0.88	4641.055911	4649.928585	4659.006221	4424.249821
0.89	4911.588874	4920.483123	4929.566153	4938.816388
0.9	5213.151926	5222.073144	5231.166961	5240.401015
0.91	5551.219696	5560.157095	5569.261699	5578.560477
0.92	5932.755478	5941.692877	5950.808269	5960.101654
0.93	6366.464743	6375.423717	6384.544503	5960.101654
0.94	6863.469348	6872.444503	6384.544503	6393.837888
0.95	6863.469348	6872.444503	6881.576076	6890.864067
0.96	7438.186713	7447.178049	7456.315016	7465.597613
0.97	8109.564988	8118.567111	8127.704078	7465.597613
0.98	8109.564988	8118.567111	8127.704078	8136.970494
0.99	8902.862977	8911.870494	8920.996674	8930.246908
1	9852.266097	8911.870494	8920.996674	8930.246908

Table D.12: $f(X)$ Values for $T = 600$ (K), $u_{in} = 10$k (1/hr) [3]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0	0.064724676	0.131247259	0.195971935	0.262494519
0.01	0.102480737	0.165407505	0.231930088	0.293058949
0.02	0.156417967	0.219344735	0.278675688	0.345198271
0.03	0.231930088	0.294856856	0.357783625	0.4225083
0.04	0.329017102	0.39194387	0.467455992	0.528584852
0.05	0.4458811	0.508807868	0.582522082	0.667023742
0.06	0.586117898	0.641853035	0.735344234	0.828835432
0.07	0.749727495	0.801866817	0.904347554	1.00682829
0.08	0.943901522	0.963678507	1.058967613	1.193810687
0.09	1.166842072	1.163246257	1.254939548	1.393378438
0.1	1.432932406	1.366409823	1.470688467	1.609127357
0.11	1.747566247	1.610925265	1.709810186	1.844653261
0.12	2.107147779	1.880611414	1.972304705	2.107147779
0.13	2.551230972	2.17546827	2.256374115	2.389419282
0.14	3.058240932	2.504485372	2.562018418	2.754394537
0.15	3.660539999	2.901822966	2.892833427	3.078017916
0.16	4.368915617	3.311745912	3.306352189	3.423216187
0.17	5.201346865	3.811564242	3.70548769	3.793585166
0.18	6.208175155	4.372511433	4.147772975	4.279020234
0.19	7.419964919	5.001779114	4.710518073	4.726699242
0.2	8.870876402	5.70476101	5.257082002	5.321806678
0.21	10.59327194	6.558767149	5.951074359	5.870168515
0.22	12.7201967	7.51884984	6.724174654	6.59652321
0.23	15.29659838	8.595796529	7.475700056	7.267142768
0.24	18.52923636	9.800394663	8.424995302	8.155309152
0.25	22.59070977	11.25310405	9.480367099	8.969761323
0.26	27.89633528	12.88200839	10.65080499	10.04670801
0.27	35.12392407	14.70328886	11.95249013	11.24231661
0.28	45.30367725	16.88594876	13.39261417	12.33724237
0.29	54.59346614	19.32750736	15.19591555	13.78096223
0.3	63.97315041	22.23292614	16.97764205	15.37930214
0.31	73.72140575	25.68311094	19.20165382	17.14484746
0.32	83.99285222	29.76256343	21.67917058	19.09557727
0.33	94.8072668	34.28969492	24.43536303	21.24947065
0.34	106.1754369	40.12570319	27.49180605	23.62270876
0.35	118.2933346	46.83010086	31.26921005	26.69713087
0.36	131.232876	55.3827476	35.47990979	29.615135
0.37	144.4205287	66.05332957	40.15806553	33.38354946
0.38	159.3359707	80.05723235	45.87541189	36.95239617
0.39	174.7260603	99.19595941	52.22022803	41.54245443
0.4	191.5724551	122.3422226	59.88291048	46.63053311

Table D.13: $f(X)$ Values for $T = 600$ (K), $u_{in} = 30\text{k}$ (1/hr) [1]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.41	207.8453173	142.1803358	69.05403746	52.25438827
0.42	226.9678632	161.7649439	79.89002694	59.38668797
0.43	246.9929587	182.5127983	93.31140763	67.32265238
0.44	267.4693291	203.7838439	109.2588486	76.1036334
0.45	287.758717	226.0311533	131.3155798	85.76558917
0.46	311.183656	250.9034079	160.653837	99.08988285
0.47	338.519044	274.9540187	198.4386644	113.7554156
0.48	365.0291925	301.582829	228.8053248	131.2562488
0.49	389.2434129	330.5615047	259.8372111	153.2590428
0.5	416.6992608	361.3632588	290.543676	182.4570632
0.51	448.0763453	393.0711583	324.5816638	221.2181545
0.52	484.2502474	424.3116018	357.172336	273.6667168
0.53	526.375224	461.1327507	395.1117835	315.9373238
0.54	562.7864499	495.6417904	432.5010712	358.127025
0.55	604.2551901	535.7872706	472.0550398	398.6626511
0.56	635.2439266	583.0039216	520.9545324	444.6872894
0.57	687.7500219	624.2101673	560.3808495	490.217503
0.58	727.5179415	671.5796404	606.8927207	542.3118775
0.59	795.9624883	726.5488693	662.4444716	589.2858109
0.6	848.7059074	768.337637	711.6550022	647.3887928
0.61	908.4341978	840.5667794	769.0496085	704.5262983
0.62	941.3574829	896.4835056	836.7516194	774.3264675
0.63	1014.415461	960.068308	889.0078056	837.5426987
0.64	1098.949483	1032.971666	980.9420159	912.9145837
0.65	1146.381883	1117.352866	1053.53074	971.6648124
0.66	1253.828441	1164.709754	1093.972875	1038.868803
0.67	1314.986068	1272.008883	1184.808564	1116.405369
0.68	1382.044428	1333.094594	1291.805644	1206.764612
0.69	1455.889889	1400.082835	1352.743927	1313.294237
0.7	1628.444077	1555.486782	1493.214452	1374.000589
0.71	1730.06901	1646.273927	1574.699223	1514.014446
0.72	1844.442905	1747.830539	1665.346132	1595.274478
0.73	1974.127783	1862.163083	1766.762507	1685.700244
0.74	1974.127783	1991.777843	1880.956612	1900.875631
0.75	2122.363472	2139.952402	2010.43473	2030.139798
0.76	2293.382246	2310.911846	2158.476245	2177.970958
0.77	2492.795377	2310.911846	2329.304442	2177.970958
0.78	2492.795377	2510.267443	2528.530589	2348.592395
0.79	2728.206214	2745.622546	2528.530589	2547.615379
0.8	3010.175669	2745.622546	2763.761636	2782.64506

Table D.14: $f(X)$ Values for T = 600 (K), u_{in} = 30k (1/hr) [2]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.81	3010.175669	3027.541659	3045.556694	2782.64506
0.82	3353.802568	3371.118217	3045.556694	3064.245944
0.83	3353.802568	3371.118217	3389.016388	3407.513262
0.84	3781.416927	3798.687628	3389.016388	3407.513262
0.85	3781.416927	3798.687628	3816.470732	3834.782422
0.86	4327.457665	4344.685216	3816.470732	3834.782422
0.87	4327.457665	4344.685216	4362.35685	4380.486951
0.88	5047.800157	4344.685216	4362.35685	4380.486951
0.89	5047.800157	5064.984558	5082.54652	5100.500426
0.9	5047.800157	5064.984558	5082.54652	5100.500426
0.91	6039.076546	6056.205212	5082.54652	5100.500426
0.92	6039.076546	6056.205212	6073.653906	6091.424425
0.93	6039.076546	6056.205212	6073.653906	6091.424425
0.94	7481.86688	6056.205212	6073.653906	6091.424425
0.95	7481.86688	7498.920034	7516.224895	7533.788655
0.96	7481.86688	7498.920034	7516.224895	7533.788655
0.97	7481.86688	7498.920034	7516.224895	7533.788655
0.98	9753.525008	7498.920034	7516.224895	7533.788655
0.99	9753.525008	9770.387584	9787.440738	9804.682672
1	9753.525008	9770.387584	9787.440738	9804.682672

Table D.15: $f(X)$ Values for T = 600 (K), u_{in} = 30k (1/hr) [3]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0	0.723867905	1.448920537	2.172788442	2.897841073
0.01	0.983323013	1.632553148	2.335095975	3.047116615
0.02	1.28424355	2.061424149	2.639570691	3.312495356
0.03	1.426410733	2.543607843	3.285246646	3.762691434
0.04	1.543698658	3.093320949	3.985420021	4.725874097
0.05	1.7510258	3.523376677	4.952156863	5.696165119
0.06	2.051946336	3.820743034	5.670101135	6.776635707
0.07	2.419211558	4.015038184	6.377382869	8.155657379
0.08	2.835050568	4.246059856	6.783744066	9.01695356
0.09	3.323157895	4.53750258	7.155748194	9.891281734
0.1	3.851545924	4.914245614	7.40927967	10.39123633
0.11	4.422584107	5.373919505	7.743372549	10.81299897
0.12	5.08247678	5.908231166	8.054955624	11.32598555
0.13	5.800421053	6.50296388	8.516998968	11.70272859
0.14	6.583525284	7.250526316	9.063157895	12.2216388
0.15	7.493395253	7.960177503	9.559558308	12.63273891
0.16	8.486196078	8.725510836	10.2561775	13.22273271
0.17	9.635380805	9.673292054	11.03928173	13.70965531
0.18	10.96108978	10.57368421	11.91597936	14.43826213
0.19	12.40645614	11.68969659	12.88863983	15.05668937
0.2	14.1468194	12.90641073	13.74164293	15.9961775
0.21	16.03764293	14.22975026	14.90267492	16.79349845
0.22	18.27559133	15.66800826	16.17388648	17.98888751
0.23	20.79076574	17.22592363	17.56120124	19.34302993
0.24	23.70045408	18.9129742	19.06580392	20.46615067
0.25	27.24989474	20.9720289	20.69717234	22.1069969
0.26	31.30521362	22.95289164	22.8261259	23.9160743
0.27	36.24789267	25.36144066	24.7513065	25.38750464
0.28	42.40965531	28.271129	26.82339319	27.50579567
0.29	50.23595872	31.10854902	29.51272239	29.81008875
0.3	61.66501548	34.51463777	31.93311868	32.30867699
0.31	71.01132301	38.19321362	35.06672033	35.01103818
0.32	80.64196491	42.55893086	37.87689164	37.92783488
0.33	90.74531269	47.25400206	41.50452425	41.07091434
0.34	101.2905635	52.74165531	45.42123013	44.45330857
0.35	112.6224727	59.58108153	49.64359546	48.08804954
0.36	124.3702208	66.81383695	54.97249536	51.98698452
0.37	136.3572838	75.40665841	59.89503406	56.16669969
0.38	150.0657544	86.27297007	66.06745924	61.80481321
0.39	164.0751455	99.21136842	72.70429721	66.66337668
0.4	179.3427162	115.5688875	80.85521569	73.19240454

Table D.16: $f(X)$ Values for $T = 600$ (K), $u_{in} = 45\text{k}$ (1/hr) [1]

Stored NH_3	Excess $NH_{3,in}$ 87.5 ppm	Excess $NH_{3,in}$ 175 ppm	Excess $NH_{3,in}$ 262.5 ppm	Excess $NH_{3,in}$ 350 ppm
0.41	195.6765408	139.0631992	89.58783488	80.24982043
0.42	212.7283096	157.6349721	100.0454159	87.85576471
0.43	229.9672652	176.6356161	112.3156285	96.02208462
0.44	250.290064	197.2249783	126.3238349	104.758258
0.45	270.2029474	218.0086357	142.9810898	115.9847265
0.46	288.5685779	240.0042683	163.5112157	127.995484
0.47	315.336289	263.3907699	190.5099484	140.7241858
0.48	340.5674097	286.2642848	225.8633725	158.6265882
0.49	362.2668607	310.2869845	254.7244954	177.2315335
0.5	386.8641527	339.7641651	283.4162023	200.6346213
0.51	414.9670506	369.8739897	311.7311662	229.2208875
0.52	447.3598431	398.7351125	345.3418576	265.9343777
0.53	485.0791662	433.0969205	377.1091146	312.9952693
0.54	513.8514345	463.4448751	412.2173003	351.7630753
0.55	563.7876574	498.7426171	449.2281569	389.1210568
0.56	602.6301011	540.2483261	485.7319505	431.5022786
0.57	646.9945552	589.6810402	530.4565614	474.1524334
0.58	671.6214654	628.1893911	571.0737255	514.5670093
0.59	726.7112487	672.2233065	619.6214489	566.9958968
0.6	791.2113148	723.0208256	678.507096	621.1272363
0.61	827.7613127	782.216871	725.1639959	671.5456429
0.62	867.7019979	815.6226047	779.3462786	733.3184685
0.63	959.7907905	891.7910423	842.9471373	782.6955005
0.64	1013.22788	935.4470299	918.5457214	840.4769825
0.65	1072.686935	1036.838295	961.9185593	908.8665057
0.66	1139.231839	1096.139781	1009.751893	990.9052632
0.67	1214.171715	1162.527117	1121.774894	1038.325127
0.68	1299.201907	1237.32601	1187.887373	1149.525928
0.69	1396.465585	1322.19271	1262.413779	1215.229676
0.7	1508.771736	1419.301189	1347.010361	1289.349721
0.71	1508.771736	1531.449771	1443.851092	1373.562452
0.72	1639.845139	1662.365606	1555.73548	1469.994452
0.73	1794.749317	1662.365606	1686.390675	1581.479587
0.74	1794.749317	1817.112215	1840.880198	1711.736714
0.75	1980.536945	2002.73872	1840.880198	1865.830539
0.76	2207.318481	2002.73872	2026.253172	2050.810184
0.77	2207.318481	2229.356764	2252.622423	2050.810184
0.78	2490.126918	2229.356764	2252.622423	2276.786105
0.79	2490.126918	2511.995785	2535.017391	2276.786105
0.8	2852.284784	2511.995785	2535.017391	2558.785375

Table D.17: $f(X)$ Values for $T = 600$ (K), $u_{in} = 45$k (1/hr) [2]

	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$	Excess $NH_{3,in}$
Stored NH_3	87.5 ppm	175 ppm	262.5 ppm	350 ppm
0.81	2852.284784	2873.975942	2896.760603	2558.785375
0.82	2852.284784	2873.975942	2896.760603	2920.126964
0.83	3331.986477	3353.489263	3376.040533	2920.126964
0.84	3331.986477	3353.489263	3376.040533	3398.991055
0.85	3996.211695	3353.489263	3376.040533	3398.991055
0.86	3996.211695	4017.497676	4039.822663	4062.334836
0.87	3996.211695	4017.497676	4039.822663	4062.334836
0.88	3996.211695	4017.497676	4039.822663	4062.334836
0.89	4973.049515	4994.097366	5016.190147	4062.334836
0.9	4973.049515	4994.097366	5016.190147	5038.715352
0.91	4973.049515	4994.097366	5016.190147	5038.715352
0.92	4973.049515	4994.097366	5016.190147	5038.715352
0.93	6541.905841	6562.710824	6584.529932	6606.670101
0.94	6541.905841	6562.710824	6584.529932	6606.670101
0.95	6541.905841	6562.710824	6584.529932	6606.670101
0.96	6541.905841	6562.710824	6584.529932	6606.670101
0.97	6541.905841	6562.710824	6584.529932	6606.670101
0.98	9428.766869	9449.537494	9470.84954	9492.373651
0.99	9428.766869	9449.537494	9470.84954	9492.373651
1	9428.766869	9449.537494	9470.84954	9492.373651

Table D.18: $f(X)$ Values for $T = 600$ (K), $u_{in} = 45\text{k}$ (1/hr) [3]

Appendix E

Table of NO_x Slip values

	Positive Excess $NH_{3,in}$			Negative Excess $NH_{3,in}$		
	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)
Stored NH_3	10k	30k	45k	10k	30k	45k
0	0.5738	0.565	0.5703	1	1	1
0.01	0.1585	0.3386	0.3974	0.5635	0.797	0.7702
0.02	0.0985	0.2604	0.3229	0.5498	0.6603	0.7392
0.03	0.0756	0.2097	0.2804	0.362	0.6486	0.662
0.04	0.0624	0.1813	0.2418	0.3328	0.5539	0.6455
0.05	0.0541	0.1592	0.2177	0.3249	0.5382	0.6407
0.06	0.0478	0.147	0.2059	0.3237	0.5336	0.5715
0.07	0.043	0.1375	0.1922	0.2235	0.4607	0.5641
0.08	0.0387	0.1298	0.1815	0.2027	0.4488	0.5607
0.09	0.0345	0.1218	0.1729	0.1971	0.4435	0.5054
0.1	0.0308	0.1163	0.168	0.195	0.4417	0.4969
0.11	0.0273	0.1112	0.1614	0.1953	0.3816	0.4936
0.12	0.0243	0.1052	0.1556	0.1346	0.3727	0.459
0.13	0.0221	0.1008	0.1503	0.1236	0.3692	0.4428
0.14	0.0201	0.0956	0.1454	0.1202	0.3673	0.4378
0.15	0.0185	0.0918	0.1409	0.1187	0.3238	0.4347
0.16	0.0172	0.0884	0.1381	0.1183	0.3133	0.433
0.17	0.016	0.0846	0.1342	0.1043	0.3095	0.3943
0.18	0.0149	0.0819	0.1307	0.0788	0.3071	0.3877
0.19	0.0138	0.079	0.1276	0.0746	0.3058	0.3845
0.2	0.0127	0.0764	0.1249	0.0731	0.2725	0.3826
0.21	0.0117	0.0745	0.1224	0.0723	0.262	0.3814
0.22	0.0108	0.0723	0.1202	0.0721	0.2585	0.3498
0.23	0.01	0.0707	0.1183	0.0722	0.2565	0.3427
0.24	0.0092	0.0687	0.1165	0.0495	0.2553	0.3399
0.25	0.0087	0.0672	0.1148	0.046	0.2546	0.3379
0.26	0.0081	0.0654	0.1133	0.0448	0.2246	0.3365
0.27	0.0077	0.0637	0.1118	0.0443	0.2183	0.3358
0.28	0.0072	0.0624	0.1105	0.044	0.2155	0.309
0.29	0.0069	0.0609	0.1092	0.0439	0.2139	0.3032
0.3	0.0065	0.0595	0.108	0.0372	0.2131	0.2998
0.31	0.0061	0.0585	0.1068	0.0294	0.2124	0.2983
0.32	0.0057	0.0573	0.1057	0.0279	0.194	0.2972
0.33	0.0054	0.0562	0.1047	0.0273	0.1851	0.2963
0.34	0.0051	0.0554	0.1038	0.027	0.1812	0.2957
0.35	0.0048	0.0544	0.1029	0.0268	0.1796	0.2767

Table E.1: $g(X)$ Values for $T = 500$ (K) [1]

	Positive Excess $NH_{3,in}$			Negative Excess $NH_{3,in}$		
Stored NH_3	SV (1/hr) 10k	SV (1/hr) 30k	SV (1/hr) 45k	SV (1/hr) 10k	SV (1/hr) 30k	SV (1/hr) 45k
0.36	0.0046	0.0536	0.1018	0.0267	0.1785	0.2688
0.37	0.0043	0.0529	0.1011	0.0267	0.1777	0.2655
0.38	0.0041	0.0522	0.1004	0.0186	0.1772	0.2636
0.39	0.0039	0.0514	0.0998	0.0172	0.1768	0.2624
0.4	0.0037	0.0507	0.0992	0.0168	0.1633	0.2615
0.41	0.0034	0.0502	0.0986	0.0165	0.1539	0.2608
0.42	0.0033	0.0495	0.0981	0.0164	0.1512	0.2602
0.43	0.0031	0.0489	0.0976	0.0163	0.1497	0.2597
0.44	0.0029	0.0483	0.0971	0.0163	0.1487	0.2593
0.45	0.0028	0.0478	0.0967	0.0163	0.148	0.2589
0.46	0.0026	0.0472	0.0961	0.0114	0.1475	0.2585
0.47	0.0025	0.0467	0.0957	0.0105	0.1471	0.2582
0.48	0.0023	0.0462	0.0953	0.0103	0.1467	0.2579
0.49	0.0022	0.0457	0.095	0.0101	0.1464	0.2577
0.5	0.0021	0.0453	0.0946	0.01	0.1461	0.2575
0.51	0.002	0.0448	0.0942	0.0099	0.1459	0.2572
0.52	0.0019	0.0444	0.0938	0.0099	0.1457	0.2571
0.53	0.0018	0.0439	0.0935	0.0099	0.1455	0.257
0.54	0.0017	0.0435	0.0932	0.0098	0.1454	0.2568
0.55	0.0016	0.0431	0.0929	0.007	0.1452	0.2567
0.56	0.0015	0.0428	0.0926	0.0064	0.1452	0.2567
0.57	0.0014	0.0425	0.0922	0.0062	0.1451	0.2364
0.58	0.0014	0.0421	0.092	0.0061	0.145	0.2205
0.59	0.0013	0.0418	0.0917	0.0061	0.1449	0.214
0.6	0.0012	0.0415	0.0915	0.006	0.1313	0.21
0.61	0.0012	0.0412	0.0912	0.006	0.1196	0.2066
0.62	0.0011	0.0409	0.091	0.006	0.1124	0.2049
0.63	0.0011	0.0407	0.0907	0.006	0.1094	0.2036
0.64	0.001	0.0404	0.0905	0.006	0.1076	0.2026
0.65	0.001	0.0402	0.0903	0.0059	0.1063	0.2018
0.66	0.0009	0.04	0.0901	0.0059	0.1054	0.2009
0.67	0.0009	0.0398	0.0899	0.0059	0.1048	0.2004
0.68	0.0008	0.0396	0.0897	0.0059	0.1042	0.2
0.69	0.0008	0.0394	0.0895	0.0059	0.1039	0.1996
0.7	0.0008	0.0392	0.0893	0.004	0.1035	0.1993

Table E.2: $g(X)$ Values for T = 500 (K) [2]

	Positive Excess $NH_{3,in}$			Negative Excess $NH_{3,in}$		
Stored NH_3	SV (1/hr) 10k	SV (1/hr) 30k	SV (1/hr) 45k	SV (1/hr) 10k	SV (1/hr) 30k	SV (1/hr) 45k
0.71	0.0007	0.039	0.0892	0.0032	0.1033	0.199
0.72	0.0007	0.0388	0.089	0.003	0.1031	0.1988
0.73	0.0007	0.0387	0.0888	0.0029	0.103	0.1987
0.74	0.0007	0.0385	0.0887	0.0028	0.103	0.1986
0.75	0.0006	0.0384	0.0886	0.0028	0.1029	0.1986
0.76	0.0006	0.0383	0.0884	0.0028	0.1029	0.1985
0.77	0.0006	0.0381	0.0883	0.0028	0.1029	0.1986
0.78	0.0006	0.038	0.0882	0.0028	0.103	0.1986
0.79	0.0006	0.0379	0.088	0.0028	0.103	0.1986
0.8	0.0006	0.0378	0.0879	0.0028	0.1031	0.1653
0.81	0.0005	0.0377	0.0878	0.0027	0.0889	0.1446
0.82	0.0005	0.0376	0.0877	0.0027	0.0761	0.1334
0.83	0.0005	0.0375	0.0876	0.0027	0.0656	0.1211
0.84	0.0005	0.0374	0.0875	0.0027	0.0563	0.1152
0.85	0.0005	0.0374	0.0874	0.0027	0.0519	0.1106
0.86	0.0005	0.0373	0.0873	0.0014	0.0488	0.1055
0.87	0.0005	0.0372	0.0873	0.0009	0.046	0.1029
0.88	0.0005	0.0372	0.0872	0.0007	0.0445	0.0998
0.89	0.0005	0.0371	0.0871	0.0006	0.0433	0.0982
0.9	0.0005	0.037	0.087	0.0006	0.0423	0.0968
0.91	0.0005	0.037	0.087	0.0005	0.0416	0.0957
0.92	0.0005	0.0369	0.0869	0.0005	0.0407	0.0942
0.93	0.0005	0.0369	0.0869	0.0005	0.0402	0.0934
0.94	0.0004	0.0368	0.0868	0.0005	0.0398	0.0926
0.95	0.0004	0.0368	0.0867	0.0005	0.0394	0.092
0.96	0.0004	0.0368	0.0867	0.0005	0.0391	0.0911
0.97	0.0004	0.0367	0.0866	0.0005	0.0388	0.0906
0.98	0.0004	0.0367	0.0866	0.0005	0.0385	0.0902
0.99	0.0004	0.0367	0.0866	0.0005	0.0383	0.0899
1	0.0004	0.0366	0.0865	0.0004	0.0382	0.0896

Table E.3: $g(X)$ Values for $T = 500$ (K) [3]

	Positive Excess $NH_{3,in}$			Negative Excess $NH_{3,in}$		
	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)
Stored NH_3	10k	30k	45k	10k	30k	45k
0	0.5528	0.5519	0.5619	1	1	1
0.01	0.1619	0.3389	0.3981	0.4173	0.6398	0.7251
0.02	0.0979	0.2461	0.3254	0.3199	0.5287	0.6286
0.03	0.0686	0.2012	0.2826	0.2154	0.455	0.5535
0.04	0.0504	0.173	0.2418	0.1924	0.4228	0.4976
0.05	0.0382	0.1528	0.2147	0.1394	0.3649	0.4776
0.06	0.0301	0.1338	0.2008	0.1194	0.346	0.4306
0.07	0.0245	0.122	0.1841	0.115	0.3027	0.4172
0.08	0.0201	0.1103	0.1708	0.0778	0.2866	0.3822
0.09	0.0167	0.1026	0.1601	0.0717	0.2803	0.3669
0.1	0.014	0.0946	0.1514	0.0697	0.2409	0.3607
0.11	0.0118	0.0879	0.144	0.0476	0.2329	0.3272
0.12	0.01	0.0821	0.1378	0.0441	0.2129	0.3186
0.13	0.0085	0.078	0.1324	0.0426	0.1996	0.3146
0.14	0.0073	0.0735	0.1276	0.0318	0.1917	0.2886
0.15	0.0063	0.0695	0.1234	0.0276	0.1881	0.2809
0.16	0.0054	0.066	0.1196	0.0263	0.1686	0.275
0.17	0.0047	0.0628	0.1162	0.0256	0.1603	0.272
0.18	0.004	0.0594	0.1132	0.0191	0.1558	0.254
0.19	0.0035	0.0569	0.1096	0.017	0.153	0.2455
0.2	0.003	0.0545	0.1072	0.016	0.1515	0.2405
0.21	0.0026	0.0524	0.105	0.0156	0.1365	0.2373
0.22	0.0022	0.0501	0.103	0.0138	0.1299	0.2349
0.23	0.0019	0.0483	0.1005	0.011	0.1271	0.2331
0.24	0.0017	0.0467	0.0989	0.0101	0.1246	0.2321
0.25	0.0015	0.0449	0.0968	0.0097	0.1233	0.2307
0.26	0.0013	0.0436	0.0954	0.0094	0.1223	0.23
0.27	0.0011	0.0421	0.0942	0.0093	0.1215	0.229
0.28	0.001	0.0408	0.0926	0.008	0.1208	0.2284
0.29	0.0008	0.0396	0.0911	0.0067	0.1202	0.2276
0.3	0.0007	0.0387	0.0902	0.0061	0.1197	0.2271
0.31	0.0006	0.0377	0.089	0.0059	0.1193	0.2078
0.32	0.0006	0.0368	0.0879	0.0057	0.1189	0.1997
0.33	0.0005	0.0359	0.0872	0.0056	0.1043	0.1936
0.34	0.0005	0.0352	0.0863	0.0055	0.0995	0.189
0.35	0.0004	0.0346	0.0855	0.0055	0.0943	0.1856

Table E.4: $g(X)$ Values for $T = 600$ (K) [1]

	Positive Excess $NH_{3,in}$			Negative Excess $NH_{3,in}$		
	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)
Stored NH_3	10k	30k	45k	10k	30k	45k
0.36	0.0004	0.034	0.0847	0.0054	0.0918	0.1829
0.37	0.0004	0.0335	0.0841	0.0054	0.0899	0.1808
0.38	0.0003	0.033	0.0835	0.0047	0.0878	0.1792
0.39	0.0003	0.0326	0.0828	0.0038	0.0867	0.1784
0.4	0.0003	0.0322	0.0824	0.0033	0.0858	0.1772
0.41	0.0003	0.0319	0.0819	0.003	0.0851	0.1761
0.42	0.0003	0.0316	0.0814	0.0028	0.0844	0.1756
0.43	0.0003	0.0313	0.0811	0.0027	0.0838	0.1748
0.44	0.0003	0.0311	0.0807	0.0026	0.0833	0.1744
0.45	0.0003	0.0309	0.0805	0.0025	0.0829	0.1737
0.46	0.0003	0.0307	0.0802	0.0025	0.0824	0.1733
0.47	0.0003	0.0306	0.0799	0.0024	0.082	0.1579
0.48	0.0003	0.0305	0.0797	0.0024	0.0727	0.1466
0.49	0.0003	0.0304	0.0795	0.0023	0.0697	0.1408
0.5	0.0003	0.0303	0.0793	0.0023	0.0637	0.1353
0.51	0.0003	0.0303	0.0792	0.0023	0.0608	0.13
0.52	0.0003	0.0303	0.079	0.0019	0.0555	0.125
0.53	0.0003	0.0303	0.079	0.0015	0.0531	0.1161
0.54	0.0003	0.0303	0.079	0.0012	0.0489	0.1122
0.55	0.0003	0.0303	0.079	0.001	0.0472	0.1087
0.56	0.0003	0.0303	0.079	0.0009	0.0455	0.1054
0.57	0.0003	0.0303	0.079	0.0008	0.0427	0.1025
0.58	0.0003	0.0303	0.079	0.0007	0.0415	0.1025
0.59	0.0003	0.0303	0.079	0.0007	0.0404	0.0998
0.6	0.0003	0.0303	0.079	0.0006	0.0394	0.0974
0.61	0.0003	0.0303	0.079	0.0006	0.0384	0.0952
0.62	0.0003	0.0303	0.079	0.0006	0.0376	0.0931
0.63	0.0003	0.0303	0.079	0.0005	0.0368	0.0931
0.64	0.0003	0.0303	0.079	0.0005	0.0361	0.0912
0.65	0.0003	0.0303	0.079	0.0005	0.0354	0.0895
0.66	0.0003	0.0303	0.079	0.0005	0.0347	0.0878
0.67	0.0003	0.0303	0.079	0.0005	0.0341	0.0878
0.68	0.0003	0.0303	0.079	0.0005	0.0336	0.0863
0.69	0.0003	0.0303	0.079	0.0005	0.0331	0.0863
0.7	0.0003	0.0303	0.079	0.0005	0.0326	0.0849

Table E.5: $g(X)$ Values for T = 600 (K) [2]

	Positive Excess $NH_{3,in}$			Negative Excess $NH_{3,in}$		
	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)	SV (1/hr)
Stored NH_3	10k	30k	45k	10k	30k	45k
0.71	0.0003	0.0303	0.079	0.0004	0.0326	0.0849
0.72	0.0003	0.0303	0.079	0.0004	0.0321	0.0835
0.73	0.0003	0.0303	0.079	0.0004	0.0316	0.0822
0.74	0.0003	0.0303	0.079	0.0004	0.0316	0.0822
0.75	0.0003	0.0303	0.079	0.0004	0.0312	0.0822
0.76	0.0003	0.0303	0.079	0.0004	0.0308	0.0809
0.77	0.0003	0.0303	0.079	0.0004	0.0308	0.0809
0.78	0.0003	0.0303	0.079	0.0004	0.0304	0.0797
0.79	0.0003	0.0303	0.079	0.0004	0.0304	0.0797
0.8	0.0003	0.0303	0.079	0.0004	0.03	0.0797
0.81	0.0003	0.0303	0.079	0.0004	0.03	0.0785
0.82	0.0003	0.0303	0.079	0.0004	0.0296	0.0785
0.83	0.0003	0.0303	0.079	0.0004	0.0296	0.0785
0.84	0.0003	0.0303	0.079	0.0004	0.0292	0.0773
0.85	0.0003	0.0303	0.079	0.0004	0.0292	0.0773
0.86	0.0003	0.0303	0.079	0.0004	0.0292	0.0773
0.87	0.0003	0.0303	0.079	0.0004	0.0288	0.076
0.88	0.0003	0.0303	0.079	0.0004	0.0288	0.076
0.89	0.0003	0.0303	0.079	0.0004	0.0288	0.076
0.9	0.0003	0.0303	0.079	0.0004	0.0284	0.076
0.91	0.0003	0.0303	0.079	0.0004	0.0284	0.076
0.92	0.0003	0.0303	0.079	0.0004	0.0284	0.0748
0.93	0.0003	0.0303	0.079	0.0004	0.0284	0.0748
0.94	0.0003	0.0303	0.079	0.0004	0.028	0.0748
0.95	0.0003	0.0303	0.079	0.0004	0.028	0.0748
0.96	0.0003	0.0303	0.079	0.0004	0.028	0.0748
0.97	0.0003	0.0303	0.079	0.0004	0.028	0.0733
0.98	0.0003	0.0303	0.079	0.0004	0.0275	0.0733
0.99	0.0003	0.0303	0.079	0.0003	0.0275	0.0733
1	0.0003	0.0303	0.079	0.0003	0.0275	0.0733

Table E.6: $g(X)$ Values for $T = 600$ (K) [3]

Appendix F

Performance Summary for PI Control Sets 1-9

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop, (1:1)	30.94	0.90
Closed Loop, K_p = 50,000	14.44	3.99
Closed Loop, K_p = 100,000	14.11	3.80
Closed Loop, K_p = 200,000	14.05	3.62
Closed Loop, K_p = 300,000	14.11	3.50
Closed Loop, K_p = 400,000	14.18	3.41

Table F.1: Set 1 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	27.71	0.71
Closed Loop, K_p = 50,000	12.54	3.28
Closed Loop, K_p = 100,000	12.25	3.15
Closed Loop, K_p = 200,000	12.19	3.00
Closed Loop, K_p = 300,000	12.24	2.91
Closed Loop, K_p = 400,000	12.30	2.84

Table F.2: Set 2 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	24.20	0.54
Closed Loop, K_p = 50,000	10.61	2.60
Closed Loop, K_p = 100,000	10.35	2.53
Closed Loop, K_p = 200,000	10.29	2.42
Closed Loop, K_p = 300,000	10.31	2.36
Closed Loop, K_p = 400,000	10.37	2.28

Table F.3: Set 3 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	24.63	0.86
Closed Loop, K_p = 50,000	15.31	1.76
Closed Loop, K_p = 100,000	14.99	1.71
Closed Loop, K_p = 200,000	14.93	1.67
Closed Loop, K_p = 300,000	14.98	1.64
Closed Loop, K_p = 400,000	15.05	1.62

Table F.4: Set 4 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	21.92	0.68
Closed Loop, K_p = 50,000	13.57	1.39
Closed Loop, K_p = 100,000	13.26	1.36
Closed Loop, K_p = 200,000	13.21	1.33
Closed Loop, K_p = 300,000	13.25	1.31
Closed Loop, K_p = 400,000	13.31	1.30

Table F.5: Set 5 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	19.01	0.52
Closed Loop, K_p = 50,000	11.74	1.06
Closed Loop, K_p = 100,000	11.43	1.04
Closed Loop, K_p = 200,000	11.38	1.02
Closed Loop, K_p = 300,000	11.41	1.01
Closed Loop, K_p = 400,000	11.46	1.00

Table F.6: Set 6 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	24.20	0.01
Closed Loop, K_p = 50,000	7.67	0.07
Closed Loop, K_p = 100,000	6.52	0.07
Closed Loop, K_p = 200,000	6.00	0.07
Closed Loop, K_p = 300,000	5.88	0.07
Closed Loop, K_p = 400,000	5.85	0.07

Table F.7: Set 7 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	21.87	0.01
Closed Loop, K_p = 50,000	7.19	0.05
Closed Loop, K_p = 100,000	6.19	0.05
Closed Loop, K_p = 200,000	5.72	0.05
Closed Loop, K_p = 300,000	5.61	0.05
Closed Loop, K_p = 400,000	5.58	0.05

Table F.8: Set 8 Performance Summary

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	19.30	0.01
Closed Loop, K_p = 50,000	6.61	0.04
Closed Loop, K_p = 100,000	5.71	0.04
Closed Loop, K_p = 200,000	5.29	0.04
Closed Loop, K_p = 300,000	5.19	0.04
Closed Loop, K_p = 400,000	5.16	0.04

Table F.9: Set 9 Performance Summary

Appendix G

Performance Summary for Adaptive PI Control Sets 1,4,7

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop, (1:1)	30.94	0.90
Closed Loop, K_p = 50,000	14.44	3.99
Closed Loop, K_p = 100,000	14.11	3.80
Closed Loop, K_p = 200,000	14.05	3.62
Closed Loop, K_p = 300,000	14.11	3.50
Closed Loop, K_p = 400,000	14.18	3.41
Adaptive PI	14.18	3.39

Table G.1: Set 1 Performance Summary including Adaptive PI Control

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	24.63	0.86
Closed Loop, K_p = 50,000	15.31	1.76
Closed Loop, K_p = 100,000	14.99	1.71
Closed Loop, K_p = 200,000	14.93	1.67
Closed Loop, K_p = 300,000	14.98	1.64
Closed Loop, K_p = 400,000	15.05	1.62
Adaptive PI	15.06	1.61

Table G.2: Set 4 Performance Summary including Adaptive PI Control

Controller	Average NO_x Slip (ppm/s)	Average NH_3 Slip (ppm/s)
Open Loop (1:1)	24.20	0.01
Closed Loop, K_p = 50,000	7.67	0.07
Closed Loop, K_p = 100,000	6.52	0.07
Closed Loop, K_p = 200,000	6.00	0.07
Closed Loop, K_p = 300,000	5.88	0.07
Closed Loop, K_p = 400,000	5.85	0.07
Adaptive PI	5.85	0.07

Table G.3: Set 7 Performance Summary including Adaptive PI Control

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