

An Adaptive Proportional Integral Control of a Urea Selective Catalytic Reduction System based on System Identification Models

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ABSTRACT

For urea Selective Catalytic Reduction (SCR) systems, adaptive control is of interest to provide a capability of maintaining high NO_x conversion efficiency and low ammonia slip in the presence of uncertainties in the system. In this paper, the dynamics of the urea SCR system are represented by a control-oriented model which is based on a linear transfer function, with parameters dependent on engine operating conditions. The parameters are identified from input-output data generated by a high fidelity full chemistry model of the urea SCR system. The use of the full chemistry model facilitated the representation of the dynamics of stored ammonia (not a directly measurable parameter) as well as post SCR NO_x and ammonia slip.

A closed-loop Proportional-plus-Integral (PI) controller was first designed using the estimate of stored ammonia as a feedback signal. The performance was evaluated using the full chemistry model, and was shown to result in a NO_x conversion efficiency of over 95%, with a maximum NH_3 slip of less than 5 ppm. An adaptive PI controller was then designed and tested, and was shown to lead to comparable performance. By incorporating nonlinear components and projection maps which accounted for the nonlinear relationship between stored ammonia and post SCR sensor measurement, the adaptive controller was extended to a variant that directly uses the sensor measurements (responsive to both NO_x -slip and ammonia slip). This novel adaptive PI-controller was simulated on the full chemistry

model, and shown to be capable of delivering over 90% of NO_x conversion efficiency at a peak ammonia slip of less than 2 ppm. Experimental results from a test vehicle demonstrated that as adaptation proceeds, efficiency of SCR increases to levels of 90%, when driven in city traffic, with a mean ammonia slip of about 10 ppm.

INTRODUCTION

Urea SCR is one of the most attractive technologies for achieving a high NO_x conversion of over 90% in a diesel aftertreatment system. Urea SCR is preferred due to its high selectivity and reactivity with NO_x in high O_2 environments [1, 2, 3, 4] combined with minimal fuel economy penalty and lower cost implications [5]. Other aftertreatment system components 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. The urea SCR system works by injecting urea (which decomposes to form NH_3) upstream of a specially formulated catalyst monolith that promotes the reduction of NO_x even in the presence of oxygen. Chemical reactions take place on the surface of the catalyst resulting in the conversion of NO_x to harmless constituents such as nitrogen (N_2) and water (H_2O) [6]. While there are many different types of SCR catalysts ranging from base-metal zeolites to vanadium, the work in

this paper is based on the performance of a Cu-zeolite formulation.

There are several challenges in the design of the urea SCR system. The first challenge is a need to maximize NO_x reduction while minimizing NH_3 -slip. It is important that only the correct amount of urea is injected into the exhaust as any excess ammonia may slip into the tailpipe. The second challenge is that the overall efficiency of the catalyst is affected by the operating conditions such as the exhaust temperature and space velocity. In particular, several of the underlying chemical mechanisms such as adsorption, desorption, and oxidation vary with operating conditions.

Adaptive control of urea injection and NO_x reduction, which is the focus of this paper, can lead to better efficiency by compensating for variability due to changes in operating conditions, part-to-part differences and aging.

Several approaches were reported in the published literature to tackle the challenges of the urea SCR system [6, 7, 8, 9]. In the SAE article authored by Jeong Kim et. al. [6], a full chemistry model of the system was presented where the behavior of the catalyst was modeled as a one dimensional single monolith channel. 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 NH_3 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 of NH_3 along the x-axis. 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. In their SAE article, John Chi and Herbert DaCosta [7] presented their work on modeling and control of a urea SCR system. While their starting point was similar to that of [6] and [8], they proposed a different method of controlling the urea injection rate. Using their catalyst test bed, they determined

the Normalized Stoichiometric Ratio (NSR) $\left(\frac{\text{NH}_{3,\text{in}}}{\text{NO}_{\text{in}}} \right)$ required for different levels of NH_3 -slip at different test conditions. 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 achievable NO_x

reduction efficiency, and the corresponding NSR were determined. The authors proposed that the response of the NO_x out of SCR to change in urea can be modeled as a first-order system where the transfer function parameters a_p and b_p are functions of the system operating conditions, namely inlet NO_x concentration, inlet NH_3 concentration, amount of NH_3 stored 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 a composite adaptive control which consisted of both direct and indirect adaptive control components.

In this paper, system-identification based, linear and nonlinear models of the urea SCR dynamics are derived. A linear first-order model was used to relate the excess $\text{NH}_{3,\text{in}}$ to the $\text{NH}_{3,\text{stored}}$, while a linear model together with nonlinear gains was used to relate the same input to the NO_x -slip and NH_3 -slip. In order to account for variations in the model parameters due to changes in operating conditions as well as aging of the catalyst, an adaptive controller is proposed to achieve a high NO_x conversion efficiency. An adaptive PI controller was shown to lead to satisfactory performance in simulations when $\text{NH}_{3,\text{stored}}$ is assumed to be measurable. Then, assuming a single sensor reflective of combined NO_x -slip and NH_3 -slip, a novel nonlinear adaptive PI controller is developed and demonstrated through simulations and experiments to lead to high NO_x conversion efficiency at acceptable levels of NH_3 -slip.

SYSTEM-ID MODEL OF THE DIESEL SCR

In [6], a full chemistry model of the SCR catalyst is presented where it is modeled as a one-dimensional single monolith channel. Eqs. (1) and (2) denote the energy equation of bulk phase in a channel and surface, respectively.

$$\varepsilon \rho_g C_{p,g} V \left(\frac{\partial T_g}{\partial t} + u \frac{\partial T_g}{\partial x} \right) = -h_{in} A_{in} (T_g - T_s) \quad (1)$$

$$(1-\varepsilon)V\rho_s C_{p,s} \frac{\partial T_s}{\partial t} = k_{cond}(1-\varepsilon)V \frac{\partial^2 T_s}{\partial x^2} + h_{in}A_{in}(T_g - T_s) - h_{out}A_{out}(T_s - T_{amb}) - W \sum (R_j \Delta H_j) \quad (2)$$

Equation (3) is conservation equation of species j in the bulk gas phase, and Eq. (4) is the conservation equation of the j 'th species which is in a porous void of washcoat:

$$\varepsilon V \left(\frac{\partial C_{g,i}}{\partial t} + u \frac{\partial C_{g,i}}{\partial t} \right) = -k_m A_{in} (C_{g,i} - C_{s,i}) \quad (3)$$

$$\frac{\partial C_{s,i}}{\partial t} = k_m A_m (C_{g,i} - C_{s,i}) \pm W \sum R_{i,j}$$

$$\frac{\partial C_{s,i}}{\partial t} = k_m A_m (C_{g,i} - C_{s,i}) \pm W \sum R_{i,j} \quad (4)$$

The gaseous phase of NH_3 is adsorbed into the surface of catalyst, and the time derivative of the solid phase NH_3 concentration is given by

$$\frac{\partial C_{NH_3}}{\partial t} = k_m A_m (C_{g,NH_3} - C_{NH_3}) - W \Omega_{total} (k_{abs} C_{NH_3} (1-\theta) - k_{des} \theta) \quad (5)$$

where, θ is the fraction of adsorbed NH_3 and expressed as

$$\theta = \frac{C_{NH_3}|_{adsorbed}}{\Omega_{total}} \quad (6)$$

where, Ω_{total} is total NH_3 adsorption capacity, and NH_3 loading in the catalyst is expressed like:

$$\Omega_{total} \frac{\partial \theta_{NH_3}}{\partial t} = R_{ad} C_{s,NH_3} (1-\theta) - R_{des} \theta_{NH_3} - \frac{W \cdot GSA}{(\varepsilon - \varepsilon_w)} \left(\sum R_i (C_{s,NH_3}, C_{s,i}, T_s) \right) \quad (7)$$

The reaction rates were modeled in the standard Arrhenius form with coefficients that were determined empirically from experimental data. A laboratory-scale flow reactor system was used to run the scale experiments. The forms used for the reaction rates of adsorption and desorption are given by

$$R_{ad} = k_{ad} \exp \left(-\frac{E_{ad}}{R_u T_s} \right) \quad (8)$$

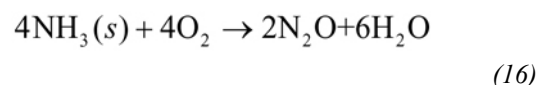
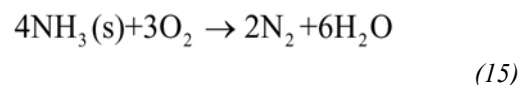
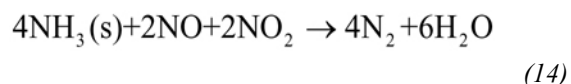
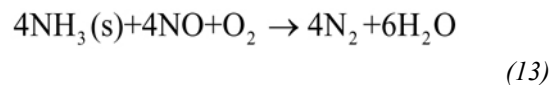
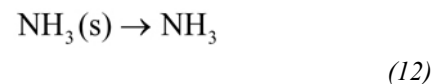
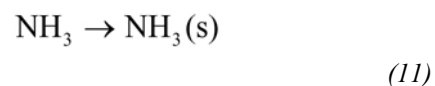
$$R_{des} = k_{des} \exp \left(-\frac{E_{des} (1-\gamma\theta)}{R_u T_s} \right) \quad (9)$$

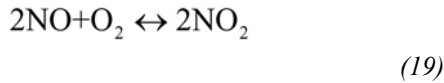
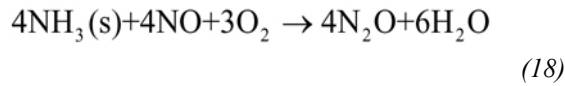
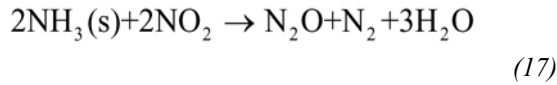
while the reaction rates for other remaining pathways in which adsorbed ammonia reacted with other two species were primarily determined using the form

$$R_j = k_j \exp \left(-\frac{E_j}{R_u T_s} \right) \theta C_a C_b \quad (10)$$

where, R_u is universal gas constant, θ is fractional ammonia loading, C_a and C_b are concentration of gas phase species which are involved in the reaction.

In [6], several reaction pathways were used to simulate the physical phenomena in urea-SCR system including adsorption of NH_3 onto the surface, and desorption of the adsorbed NH_3 , and are listed in Eqs. (11) and (12), respectively. The other pathways included in [6] are standard SCR and fast SCR reactions, oxidation process, and production of N_2O which are listed in Eqs. (13), (14), (15), (16), (17), (18), (19), respectively. In following equations, $NH_3(s)$ means adsorbed NH_3 molecules onto the catalyst surface.





Further details of the rate equations can be found in [reference \[6\]](#). Eqs. (1), 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, (19) completely describe the full chemistry model in [6] and determine $\text{NO}_{x,\text{slip}}$ and $\text{NH}_{3,\text{slip}}$ for different $T_{g,\text{in}}$, $\text{NO}_{x,\text{in}}$ and $\text{NH}_{3,\text{in}}$. As the above equations show, the resulting dynamics is complex, requires the solution of nonlinear partial differential equations, and is not easily amenable to feedback control design. It should also be noted that the full chemistry model does not explicitly account for urea decomposition into ammonia, which can be an important reaction under certain low temperature conditions. However, this model has been shown to correlate well with actual vehicle experiments based on the assumption that the urea undergoes a fast and complete decomposition to ammonia.

A DATA-DRIVEN SYSTEM-IDENTIFICATION BASED MODEL

In order to model the dominant dynamics of the urea SCR, we use a system-identification based approach. The model is derived using input-output data, where the inputs are $\text{NO}_{x,\text{in}}$, $\text{NH}_{3,\text{in}}$, $T_{g,\text{in}}$, and $u_{g,\text{in}}$, and the outputs are $\text{NH}_{3,\text{slip}}$ and $\text{NO}_{x,\text{slip}}$ are determined from the full-chemistry model described above.

The starting point for the derivation of the model was the selection of trim points for $\text{NO}_{x,\text{in}}$, Space Velocity, and $T_{g,\text{in}}$. The trim points for mapping the first order transfer function were selected to be as follows:

$\text{NO}_{x,\text{in}}$ (ppm) : 0, 87.5, 175, 262.5, 350

$\text{NH}_{3,\text{in}}$ (ppm) : 0, 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 chosen based on a trial and error basis, resulting in a total of 225 trim points.

The total $\text{NH}_{3,\text{stored}}$ was denoted as X , the total $\text{NH}_{3,\text{in}}$ as U . Further a trim point $\text{NH}_{3,\text{stored-nominal}}$ is denoted as X_{nominal} , with the nominal value, $\text{NH}_{3,\text{in-nominal}}$ as U_{nominal} . Since the system-identification model presented in this paper is a linear model, our focus is on the deviation of these quantities from their nominal values. That is, denoting $U - U_{\text{nominal}}$ as u , and $X - X_{\text{nominal}}$ as x , our goal is to derive a lumped-parameter dynamic model that captures the relation between u and x at different operating conditions using input-output data. For this purpose, 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.

Using input-output data from the full chemistry model in [6], a first order dynamic model was chosen to represent the relation between u and x , of the form

$$\dot{x} = -\frac{1}{\tau}x + \frac{k}{\tau}u \quad (20)$$

whose transfer function form is shown in [Figure 1](#). Given that the underlying system dynamics is significantly complex and that the model above is first-order, with two fixed parameters, it is easy to see that a family of parameter values (k, τ) needs to be chosen in order to obtain an accurate-enough model. To obtain the maps of k and τ , a basic system-identification based procedure was used. This consists of delivering different kinds of inputs u into the system, and recording the corresponding response x , using which the parameters (k, τ) are then determined. It was also observed that responses to sinusoidal inputs did not yield accurate estimates of the $\text{NH}_{3,\text{stored}}$, and hence a step-response based procedure was adopted. It was also observed that in addition to the dependence on the trim values, k and τ depended on X_{nominal} as well. Using the full chemistry model in [6], a step input was applied to the system to trigger a response in NH_3 storage. Using the full chemistry model to map the values of X_{nominal} , k and τ with small step perturbations in, and the corresponding response in x , the values of k and τ were estimated using the final steady-state value and the rise time to 63% of the final steady state value, respectively, and are shown in [Table A](#) and [B](#) in [Appendix I](#), respectively. [Figure 2](#) shows a simulation run where the system was allowed to reach equilibrium, and small step perturbations of ± 5 ppm of $\text{NH}_{3,\text{in}}$ were introduced. The response in

figure 2 clearly demonstrates that the response of $\text{NH}_{3,\text{stored}}$ can be accurately described using a first-order dynamics as in Eq. (20).

The maps obtained were imported into a Simulink model. Model verification and subsequent control algorithm implementation were developed using this Simulink model as a base.

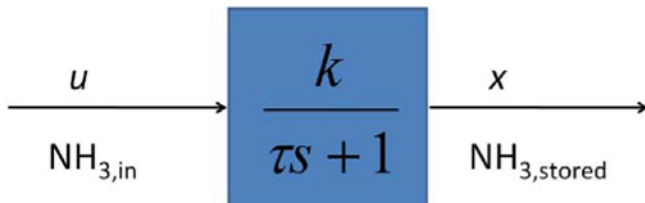


Figure 1. Block diagram for transfer function model from deviation of $\text{NH}_{3,\text{in}}$ to deviation of $\text{NH}_{3,\text{stored}}$.

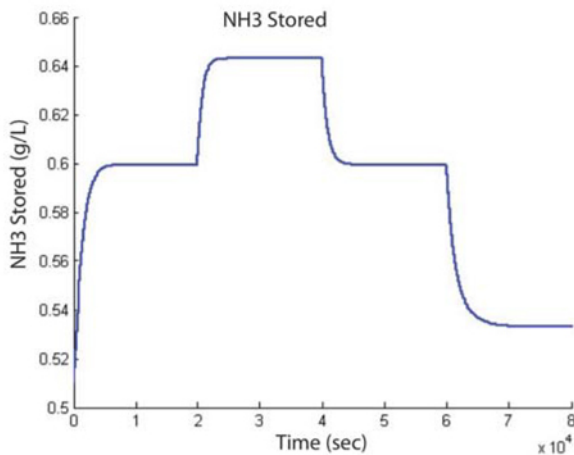


Figure 2. Response of $\text{NH}_{3,\text{stored}}$ for small step perturbations in $\text{NH}_{3,\text{in}}$.

NH3 SLIP AS A FUNCTION OF NH3 STORAGE

In order to complete the transfer function model for the urea SCR system, two more variables need to be estimated, which include the $\text{NH}_{3,\text{slip}}$ and the $\text{NO}_{x,\text{slip}}$ of the system. Based on information obtained from the literature search, it was known that the adsorption of $\text{NH}_{3,\text{in}}$ by the catalyst surface coating was highly efficient. As such, it was logical to assume that in the desirable operating region any of the $\text{NH}_{3,\text{in}}$ injected will be adsorbed by the catalyst surface

coating, and that the NH_3 -slip was only due to desorption. As shown by Eq. (21), this depends on the surface coverage fraction, θ , which depends on X , i.e., the $\text{NH}_{3,\text{stored}}$:

$$Y_1 = f(X) \quad (21)$$

where Y_1 denotes $\text{NH}_{3,\text{slip}}$, and $f(\cdot)$ denotes a nonlinear function. In order to determine the functional form of $f(\cdot)$, simulation studies were carried out using the full chemistry SCR model described above in Eqs. (1), (2), (3), (4), (5), (6), (7), (8), (9), (10), (11), (12), (13), (14), (15), (16), (17), (18), (19). The data collected consisted of pairs (X, Y_1) gathered such that Y_1 was dominantly due to desorption. A simple curve fit procedure was then used to determine f .

NOX-SLIP AS A FUNCTION OF NH3 STORAGE

Similar to the mapping of the $\text{NH}_{3,\text{slip}}$, the $\text{NO}_{x,\text{slip}}$ can be derived from the efficiency level of the urea SCR system, as a function of the level of $\text{NH}_{3,\text{stored}}$. Denoting Y_2 as $\text{NO}_{x,\text{slip}}$, we express this relation as

$$Y_2 = g(X) \cdot \text{NO}_{x,\text{in}} \quad (22)$$

where $g(\cdot)$, the $\text{NH}_{3,\text{slip}}$ fraction, is to be determined. Using the data pairs (X, Y_2) , the amount of Y_2 at each X could be matched and plotted. Expressed as a percentage of $\text{NO}_{x,\text{in}}$, the $\text{NO}_{x,\text{slip}}$ fraction was calculated. Figure 3 shows the plot for one of the operating conditions; $T = 600$ (K), $u_{\text{in}} = 45,000$ (1/hr). It was found that the functional relationship $g(\cdot)$ was sensitive to the amount of $\text{NH}_{3,\text{in}}$ injected. In particular, it was found that the function $g(\cdot)$ was quite distinct when excess $\text{NH}_{3,\text{in}}$ was injected compared to the cases when $\text{NH}_{3,\text{in}}$ was insufficient, for a given $\text{NO}_{x,\text{in}}$. This is shown in Figure 3, where the curves in blue and purple corresponds to the former and latter cases, respectively. The resulting curve-fits of $f(\cdot)$ and $g(\cdot)$ are shown in Figures 4 and 5, respectively. The dependency of $g(\cdot)$ on X_{nominal} was found to be not significant.

FEEDBACK CONTROL DESIGN

CONTROL USING NH₃, STORED

With the transfer function model fully determined, the next step was to start developing and implementing control algorithms for this system. This took place in several steps. Control algorithms were first tested on the linear transfer function model to ensure that minimal performance requirements were satisfied. 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 Y_1 and Y_2 were functions of X , the total $\text{NH}_{3,\text{stored}}$, setting a reference value for $\text{NH}_{3,\text{stored}}$ and having the system track the reference would give the best chance of minimizing both Y_1 and Y_2 . Starting with a Proportional- Integral (PI) Controller on the NH_3 Storage, the closed loop system was first tested on a $\text{NO}_{x,\text{in}}$ profile of random steps and length, and subsequently proceeded onto more complicated profiles with variations in Temperature and Space Velocity. A PI Controller was first developed and tested, followed by an Adaptive PI Controller, both of which are described below.

PI CONTROL

We begin with the linear model in Eq. (20). Figure 6 illustrates the Block Diagram of the transfer function model with a PI Controller added. Setting the command signal that X needs to follow to be X_{nominal} , it follows that the controller needs to maintain the value of x at zero. This can be achieved with a PI controller with the proportional gain (K_p) and integral gain (K_i) values enabling the desired transient response. The control input is therefore chosen as

$$u = -\left(K_p + \frac{K_i}{s}\right)x \quad (23)$$

where u denotes the Excess $\text{NH}_{3,\text{in}}$. By fixing the damping ratio desired for the closed loop system, we can express K_i in terms of k , τ , and K_p as

$$K_i = \frac{(1 + kK_p)^2}{4k\tau} \quad (24)$$

The controller designed above was tested using the full chemistry model for various $\text{NO}_{x,\text{in}}$ profiles at a

Temperature of 500 K and Space Velocity of 30,000 /hr (see Figure 7 for a schematic.) Using a random $\text{NO}_{x,\text{in}}$ profile, the closed loop performance of the system with PI control was plotted for a range of values of K_p , and compared to the open loop performance where only a 1:1 injection of ($\text{NH}_{3,\text{in}}; \text{NO}_{x,\text{in}}$) was supplied. The resulting system performance is summarized in Table 1, which lists the total amount of $\text{NH}_{3,\text{slip}}$ and $\text{NO}_{x,\text{slip}}$ for different choices of K_p and compares it with the open-loop performance. The improvement of the closed-loop PI controller over an open-loop one is apparent from Table 1. The same PI controller was tested over a range of operating conditions listed in Table 2, and was found to lead to a similar improved performance.

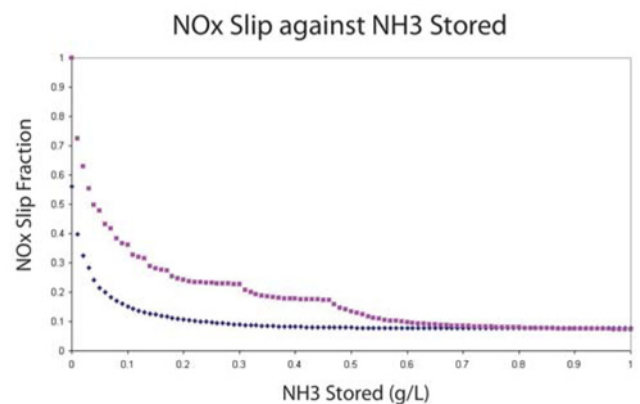


Figure 3. Plot of NO_x Slip Fraction against $\text{NH}_{3,\text{stored}}$. The blue and purple lines correspond to the case when excess $\text{NH}_{3,\text{in}}$ and insufficient $\text{NH}_{3,\text{in}}$ were injected, respectively, for a given $\text{NO}_{x,\text{in}}$.

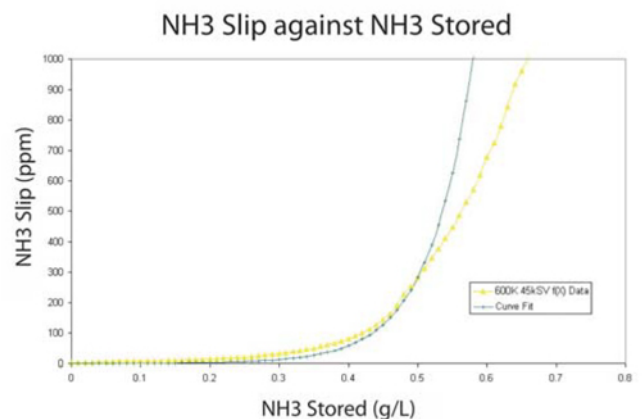


Figure 4. Curve fit for $f(x)$