Model Identification for Optimal Diesel Emissions Control

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Abstract

In this paper we develop a model based controller for diesel emission reduction using system identification methods. Specifically, our method minimizes the downstream readings from a production NO_x sensor while injecting a minimal amount of urea upstream. Based on the linear quadratic estimator, we derive the closed form solution to a cost function that accounts for the case that some of the system inputs are not controllable. Our cost function can be tuned to emphasize optimization of either the use of inputs or the output. Our approach performs better than a production controller in simulation. Our NO_x conversion efficiency was 92.7% and the production controller achieved 92.4%. For NH_3 conversion, our efficiency was 98.7% compared to 88.5% for the production controller.

1. Introduction

One solution for meeting future NO and NO_2 (collectively NO_x) emission regulations in vehicles running on diesel engines is to use a selective catalytic reduction (SCR) catalyst and inject a urea solution. Precise control of the aftertreatment system is essential because recent progress in advanced combustion technologies has reduced exhaust temperatures demanding improved catalyst performance at lower exhaust temperatures. Urea decomposes to NH_3 upstream of the SCR and aids in the reduction of NO_x on active catalyst sites through a variety of reactions. Numerous SCR models exist and have been postulated for use in control design and on-board diagnostics (Chi & DaCosta, 2005; Upadhyay & Van Nieuwstadt, 2006; Devarakonda et al., 2009; Schar et al., 2006). The tradeoff for most urea injection schemes is between urea usage and NO_x reduction. In addition to the added expense of over-injecting urea to achieve required NO_x reduction levels, the resulting ammonia slip out of the tailpipe is undesirable.

Several previous studies have addressed optimal SCR systems. The effect of the urea injector configuration on NO_x reduction and NH_3 slip for a variety of exhaust gas temperatures and space velocities has been investigated (Jeong et al., 2008; Lee et al., 2008). This is important design information but it did not focus on controlling the urea injection rate to achieve maximum NO_x reduction and minimum NH_3 slip.

Closed-loop and open-loop urea injection strategies have also been examined (Willems et al., 2007). The open loop method was based on steady-state stoichiometry and modest NO_x reduction requirements. Because their focus was closed loop control system comparisons, there was no attempt to optimize the open loop urea dosing profile. An optimal urea injection approach based on stoichiometry of the main SCR NO_x reduction reactions has also been proposed (Nakayama et al., 2006). Since the open loop injection was based on a steady state solution, it was not considered optimal for transient operation. A recent study regarding the effect of biodiesel blend on SCR performance describes using an ultra-low-sulfur diesel (ULSD)-optimal urea injection for subsequent 20% biodiesel fuel (B20) tests (Williams et al., 2008). The optimal trajectory design was not described.

This paper describes a system identification based methodology for determining the optimal urea injection rate in SCR. System identification is used to find a state-space model for SCR based on data from a pro-

Proceedings of the 30th International Conference on Machine Learning, Atlanta, Georgia, USA, 2013. JMLR: W&CP volume 28.

duction engine and aftertreatment system. We also derived a closed form solution to a control function based on the state-space model. The resulting model based controller was compared in simulation to the production control system. Other details about this approach can be found in (Stevens et al., 2013). System identification circumvents some of the uncertainties found in a physical model, such as sensor error or material degradation, by learning these from the data. In SCR the catalyst suffers degradation over time; our approach is a preliminary step toward addressing the degradation issue.

2. Model identification

A depiction of the portion of the diesel aftertreatment system discussed in this paper is shown in Figure 1. The inputs to the model based controller are the sensed NO_x concentrations upstream and downstream of the SCR. The controller computes the dose command for the next update to minimize the expected downstream NO_x sensor reading. The controller also uses the actual dose applied by the doser.

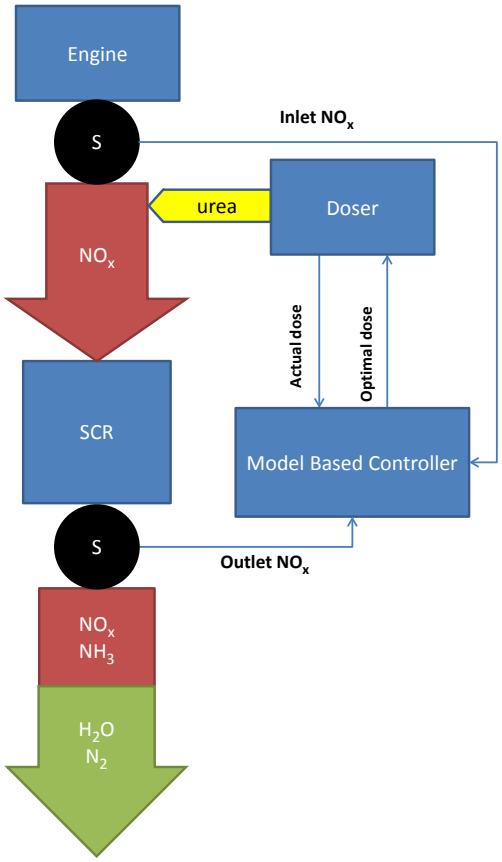

Figure 1. SCR exhaust & data flow. 'S' is a NO_x sensor.

A calibrated Cu-zeolite SCR model is used to simulate aftertreatment dynamics to evaluate the performance of the proposed controller. Details on the model, parameter settings, and calibration can be found in (Song et al., 2013). The physics-based SCR model accurately represents the nonlinear physics but is not tractable for determining an optimal urea injection rate. Thus, a data-driven model that can be used to obtain an optimal dosing strategy was developed.

We assume that the input-output relationships of the SCR system can be represented by a linear time-invariant state-space-innovations model given by

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

where x_t is the system state, y_t is the output, e_t is assumed to be Gaussian noise, and K is the Kalman gain matrix (Anderson & Moore, 1979). When this type of model is identified, the state has no physical meaning. The linear quadratic estimator is a convenient equivalent:

$$\begin{aligned} y_t &= y_{t|t-1} + e_t, \\ y_{t|t-1} &= Cx_t, \\ x_{t+1} &= (A - KC)x_t + Bu_t + Ky_t, \end{aligned} \tag{2}$$

where $y_{t|t-1} \triangleq \mathbb{E}\{y_t | y_{t-1}, y_{t-2}, \ldots\}$ is the mean-square optimal one-step-ahead predictor of y_t and u_t is the input. The parameters A, B, C, K, and x_0 are unknown and must be identified from data. In this form, the state is a deterministic function of the output, the input, and the previous state. We used the University of Newcastle Identification Toolbox (UNIT) to identify the model parameters (Ninness & Wills, 2006). Details about the identification algorithm can be found in (Wills & Ninness, 2008).

2.1. State-space SCR

For simplicity of presentation, we chose a first order model with 2 inputs (NO_x, NH_3) and 1 output (NO_x). We also conducted experiments with higher order models and with multiple inputs and outputs; for example, including NH_3 in the output and using a higher order model allows for control of both NO_x and NH_3 emissions. The first-order model, however, yielded a good fit to the data used in this study.

We employ the linear quadratic estimator to predict the one-step-ahead NO_x output $y_{t+1|t}$ for SCR using upstream NH_3 and NO_x as inputs $u_{t,1}$ and $u_{t,2}$, respectively, and downstream NO_x as the output y_t. Upstream NH_3 was used instead of urea for compatibility with the physical model implementation, but because

the relationship between NH_3 and urea can be calibrated, the choice to use NH_3 is not restrictive.

In order to identify the model parameters, A, B, C, K, and x_0, a surrogate heavy-duty diesel (HD)-FTP data set, shown in Figure 2, was used. From 600 to 900 seconds, the temperature increases substantially causing NH_3 to desorb from the catalyst and showing the cross-sensitivity of the NO_x sensor to NH_3 (the actual NO_x concentration is near zero after 600 seconds). The NH_3 concentration data was derived from the doser's urea injection rate. Details about the experimental setup and data collection process can be found in (Song et al., 2013). The identified parameters are given in Table 1. The identified model has a one second time step inherited from the data; the estimator can thus predict the downstream NO_x concentration one second in the future given the current upstream and downstream conditions and any NH_3 input.

Table 1. Model parameters

Parameter	Value
A	0.964
B	$[0.013, -0.025]$
C	-0.971
K	-1.752

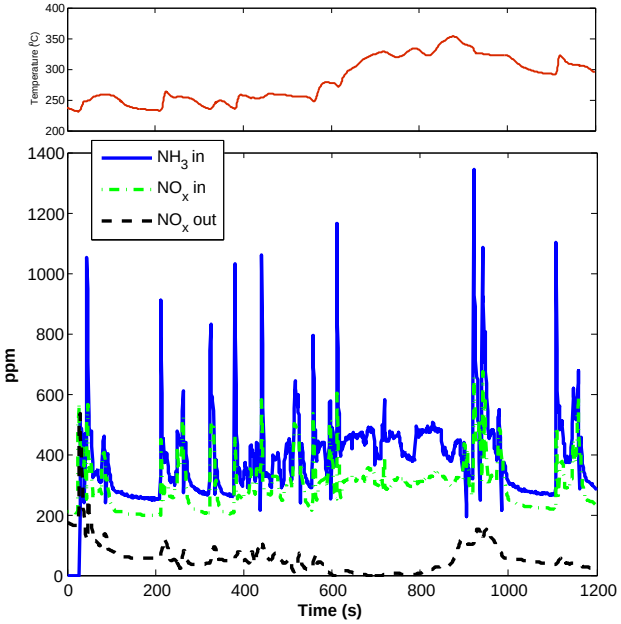

Figure 2. Surrogate HD-FTP data for model identification. Temeperature is given as a reference and was not used in training. The NO_x sensor's cross sensitivity to NH_3 can be seen around 900 s— the actual NO_x values after 600 s are close to zero.

2.2. Validation

The state-space SCR model was validated against several data sets where the inlet NO_x was the same as in Figure 2, but the inlet urea dosing was scaled to: 30%, 50%, 80%, and 120% from the injection levels used in the calibration data set. The goodness-of-fit of the identified model was evaluated using a prediction-error metric. Prediction-error is the difference between the model output prediction (downstream NO_x) for the next time step and the actual value for the next time step. The root mean squared error (RMSE) over all predictions for the 120% case was 5 ppm. The RMSEs for the 80%, 50%, and 30% data were 5, 7, and 9 ppm respectively. The reason for the slight decrease in accuracy for the 50% and 30% data was that the urea input was occasionally below the dosers minimum input threshold, in which case it defaulted to zero, causing a thresholding effect. The goodness-of-fit plot for the 80% data is shown in Figure 3.

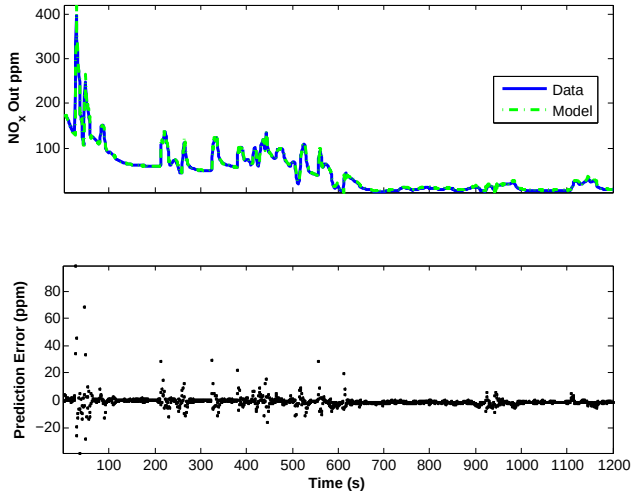

Figure 3. Model performance for predicting downstream NO_x at 0.8 times normal injection.

Another study in model identification for SCR proposed using the Hammerstein-Weiner (HW) model, a generalization of the state-space model (Zambrano et al., 2011). The HW model does not use a feedback mechanism. On a different drive cycle they reported FIT values of 78.64% and 68.05% for training and validation, respectively. Our training results gave 89.60% for training and 89.09% for validation on the 80% data. FIT is defined as

$$\text{FIT} := 1 - \frac{||y - y_p||}{||y - \bar{y}||},$$

where y is the vector of true values, y_p is the predicted model output, and $\bar{y}$ is the mean of y.

3. Model based control

Using (2), we formulated the cost function (3), a combination of the predicted outputs and the controllable inputs. Here we derive the analytic solution to (3). This formulation explicitly invokes the one-step-ahead linear quadratic estimator to find the set of inputs that minimize the output during the next time step while also penalizing the usage of inputs based on a weighting matrix.

From (2), let $Q = C(A-KC), R = CB, S = CK$, and arrange model so that the k controllable elements of u are in the top of the vector (i.e. $u_{1:k}$). The dimension of u is n. The objective function to be minimized is:

$$\begin{aligned} F\left(u_{1:k}\right) &= \left|\left|\hat{y}_{t+1|t}\right|\right|^2 + \left|\left|\Lambda u_{1:k}\right|\right|^2, \\ &= \left|\left|Qx + Ru + Sy\right|\right|^2 + \left|\left|\Lambda u_{1:k}\right|\right|^2, \end{aligned} \tag{3}$$

where $u_{1:k} = [u_1, , u_k]^T$, and $\Lambda \in \mathbb{R}^{k\times k}$ is a weighting matrix for the k controllable inputs. The choice of the tuning parameter Λ determines the priority for minimizing either the controllable inputs $u_{1:k}$ or the system output $y_{t+1|t}$. By the chain rule, since

$$\begin{aligned} \frac{\partial F}{\partial u} &= 2u^{\mathrm{T}}R^{\mathrm{T}}R + 2x^{\mathrm{T}}Q^{\mathrm{T}}R + 2y^{\mathrm{T}}S^{\mathrm{T}}R \\ &\quad + \frac{\partial {u_{1:k}}^{\mathrm{T}}\Lambda^{\mathrm{T}}\Lambda u_{1:k}}{\partial u}, \end{aligned} \tag{4}$$

and

$$\frac{\partial u}{\partial u_{1:k}} = \begin{bmatrix} I_k \\ 0_{(n-k)\times k} \end{bmatrix}, \tag{5}$$

where I_k is an identity matrix, then

$$\frac{\partial F}{\partial u_{1:k}} = \frac{\partial F}{\partial u} \cdot \frac{\partial u}{\partial u_{1:k}}$$

$$\begin{aligned} &= 2u^{\mathrm{T}}R^{\mathrm{T}}R_{(:,1:k)} \\ &\quad + 2x^{\mathrm{T}}Q^{\mathrm{T}}R_{(:,1:k)} + 2y^{\mathrm{T}}S^{\mathrm{T}}R_{(:,1:k)} + 2{u_{1:k}}^{\mathrm{T}}\Lambda^{\mathrm{T}}\Lambda u_{1:k}, \end{aligned}$$

$$\begin{aligned} &= 2{u_{1:k}}^{\mathrm{T}}\left(R^{\mathrm{T}}R_{(:,1:k)}\right)_{(1:k,:)} \\ &\quad + 2{u_{k+1:n}}^{\mathrm{T}}\left(R^{\mathrm{T}}R_{(:,1:k)}\right)_{(:,k+1:n)} \\ &\quad + 2x^{\mathrm{T}}Q^{\mathrm{T}}R_{(:,1:k)} + 2y^{\mathrm{T}}S^{\mathrm{T}}R_{(:,1:k)} + 2{u_{1:k}}^{\mathrm{T}}\Lambda^{\mathrm{T}}\Lambda u_{1:k}, \end{aligned} \tag{6}$$

where $R_{(1:k,:)}$ and $R_{(:,1:k)}$ are the first k rows and k columns of R, respectively. Let $\frac{\partial F}{\partial u_{1:k}} = 0$, then $\mathrm{argmin}_{u_{1:k}} F$ is the solution of

$$\begin{aligned} &\left[\left(R^{\mathrm{T}}R_{(:,1:k)}\right)_{(1:k,:)} + \Lambda^{\mathrm{T}}\Lambda\right]^{\mathrm{T}} u_{1:k} \\ &\quad = -\left[\left(R^{\mathrm{T}}R_{(:,1:k)}\right)_{(:,k+1:n)}\right]^{\mathrm{T}} u_{k+1:n} \\ &\qquad - \left[R_{(:,1:k)}\right]^{\mathrm{T}} Qx - \left[R_{(:,1:k)}\right]^{\mathrm{T}} Sy. \end{aligned} \tag{7}$$

4. Simulated comparison

In this section we show the performance of the identified state-space SCR model (2) and derived control procedure (7) in simulation. The simulation results of the proposed optimal controller are compared to the simulation of the data from Figure 2 where the NH_3 input is from a nominal production controller. We are working to apply the controller on the same experimental setup used to acquire the calibration data.

The proposed controller was inserted into the SCR model described in (Song et al., 2013). We assumed that the doser was capable of applying any nonnegative control signal. Also, we did not simulate NO_x sensor cross-sensitivity, so the controller received the actual, simulated, NO_x value. Also, during data collection, urea dosing was started 30 seconds after the engine, so this same constraint was applied to the simulation study.

In order to determine the tuning parameter λ ($\Lambda \in \mathbb{R}$ since there is one controllable input), we examine the SCR inefficiency using the difference in the upstream and downstream concentrations of NO_x and NH_3 for different values of λ. The inneficiency metric is normalized by the input and accumulated over all time points. Figure 4 shows the response of the SCR simulator in terms of cumulative relative NO_x and NH_3 inefficiency as the tuning parameter varies between 1 and 50. The response of the controller to the tuning parameter is shown in Figure 4. The choice of λ is a trade-off between NO_x conversion and NH_3 slip. Based on Figure 4, we chose $\lambda = 40$ where NH_3 slip was 1.1% and NO_x inefficiency was 7.7%.

Figure 5 shows the upstream NH_3 profiles for both controllers. Throughout the simulation, the proposed optimal controller used less NH_3; however, the usage spikes are mostly larger than the production profile. This is probably because there was less adsorbed NH_3 in the catalyst— a result of having less NH_3 upstream. Another explanation for the larger spikes is that the proposed controller is more aggressive when the NO_x concentration is high and less aggressive when it is low (dependent on λ), resulting in a volatile profile. In contrast, the production controller keeps a relatively constant profile.

The downstream concentrations are presented in Figures 6 and 7. There was a temperature increase near 700 seconds that had a noticeable effect on both controllers. In Figure 6, the optimal controller managed the NH_3 slip caused by the large temperature increase more effectively. The optimal controller was able to use significantly less NH_3 during and prior to the tem-

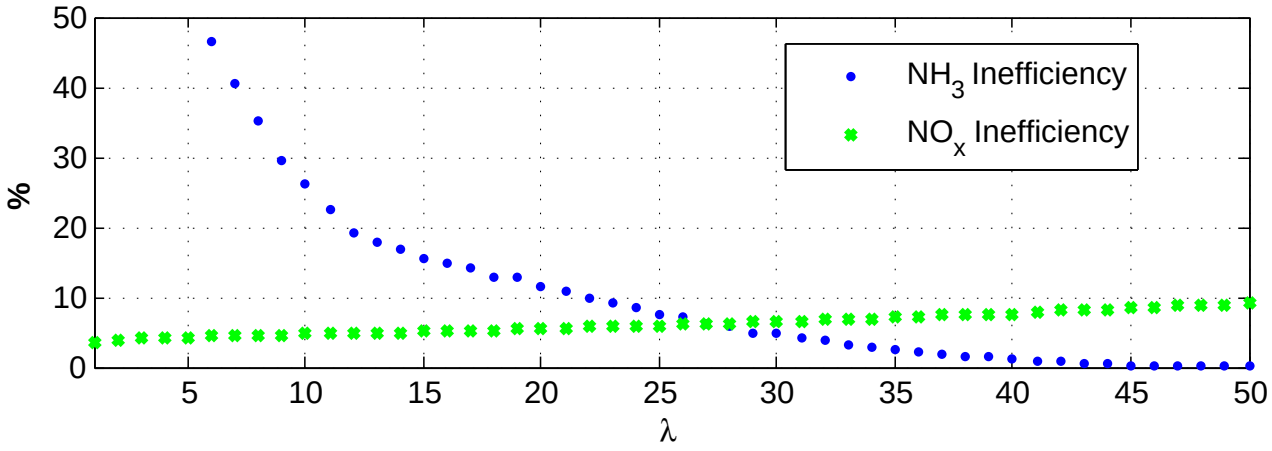

Figure 4. Cumulative NH_3 and NO_x inefficiency as a function of the tuning parameter λ.

perature increase. However, in Figure 7, the NO_x conversion of the proposed controller is deficient just after 700 seconds. A second order model may remedy this effect by allowing for a greater degree of nonlinearity. The deficiency could also be an artifact of NH_3 cross-sensitivity, which is not included in the simulation. As seen in Figure 7, at the beginning of the simulation, when the catalyst had not yet adsorbed much NH_3 the optimal controller reduced more NO_x than the production controller. Throughout the rest of the simulation, the proposed controller has similar NO_x conversion results using less upstream NH_3.

Table 2 gives a synopsis of the relevant performance metrics for the comparison between the nominal production controller and proposed optimal controller. The optimal controller performs better than the production controller for every metric in Table 2. The optimal controller converts a larger mass of NO_x while using and expelling a smaller mass of NH_3.

Table 2. Synopsis of controller comparison

	Nominal	Optimal
Upstream NO_x Mass	63.09 g	63.09 g
Downstream NO_x Mass	4.78 g	4.60 g
NO_x Conversion Efficiency	92.43%	92.71%
Upstream NH_3 Mass	18.67 g	16.33 g
Downstream NH_3 Mass	2.15 g	0.22 g
NH_3 Conversion Efficiency	88.49%	98.67%
Urea Mass	32.92 g	28.79 g

5. Conclusion

We presented a data-driven modeling and optimal control strategy for SCR aftertreatments systems on diesel engines. Our approach used a state-space estimator to predict the optimal urea injection rate for the next timestep. We derived the closed form solution to a cost function that is tunable and separates the controllable and uncontrollable system inputs. The proposed methodology resulted in a model based controller that performed better in simulation than a production aftertreatment system.

One of the next research steps in this application will be to examine models identified from different types of sensor data (e.g. temperature and exhaust flow rate). Moreover, the models should be validated on different engines, aftertreatment systems, and drive cycles.

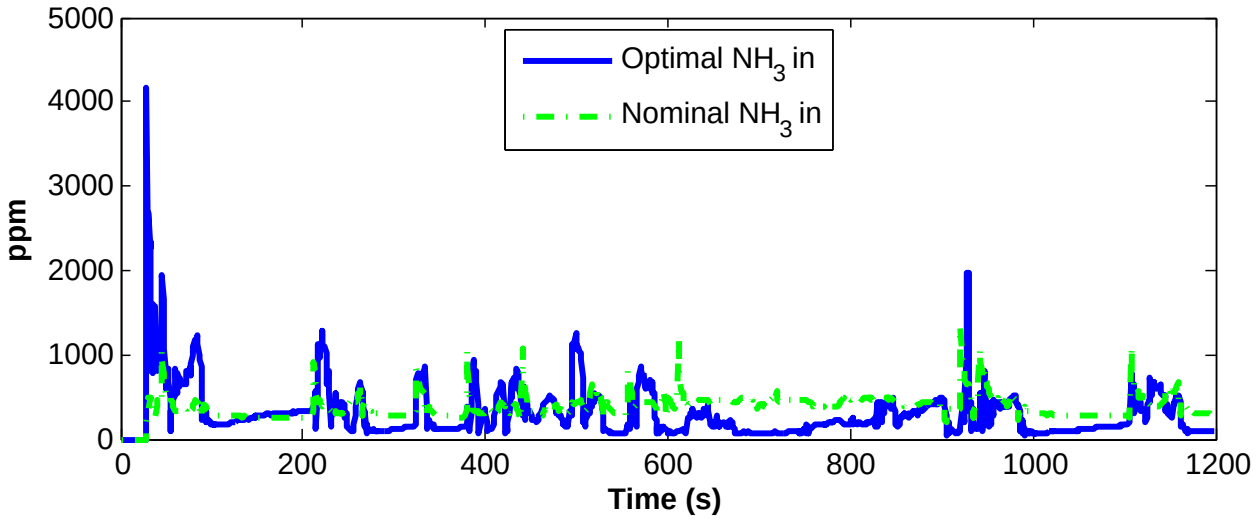

Figure 5. Upstream NH_3 profiles for the optimal and nominal urea dosing.

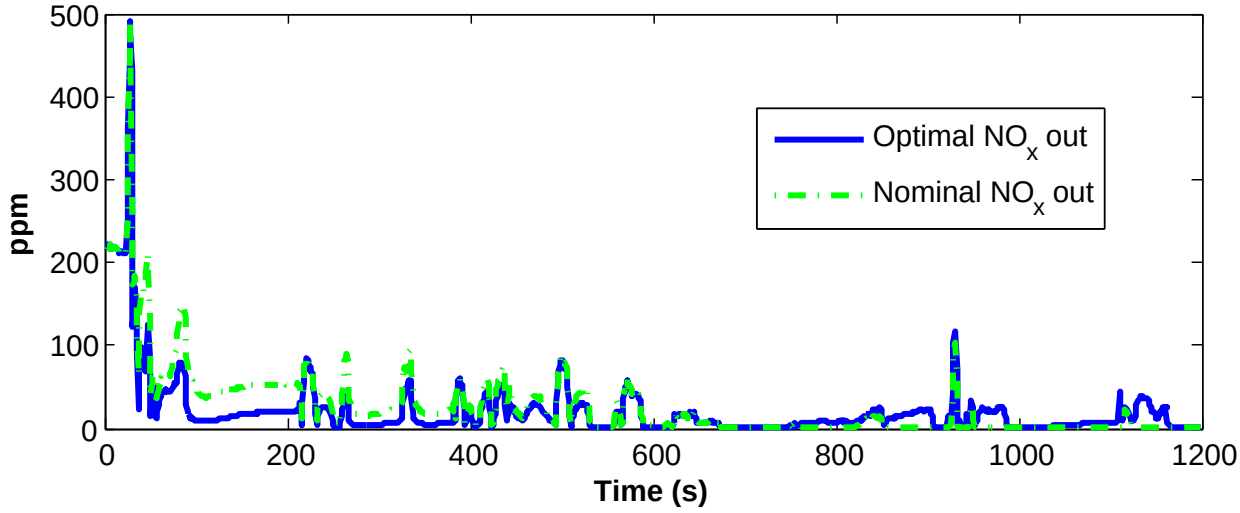

Figure 6. Downstream NO_x concentrations for the optimal and nominal urea dosing.

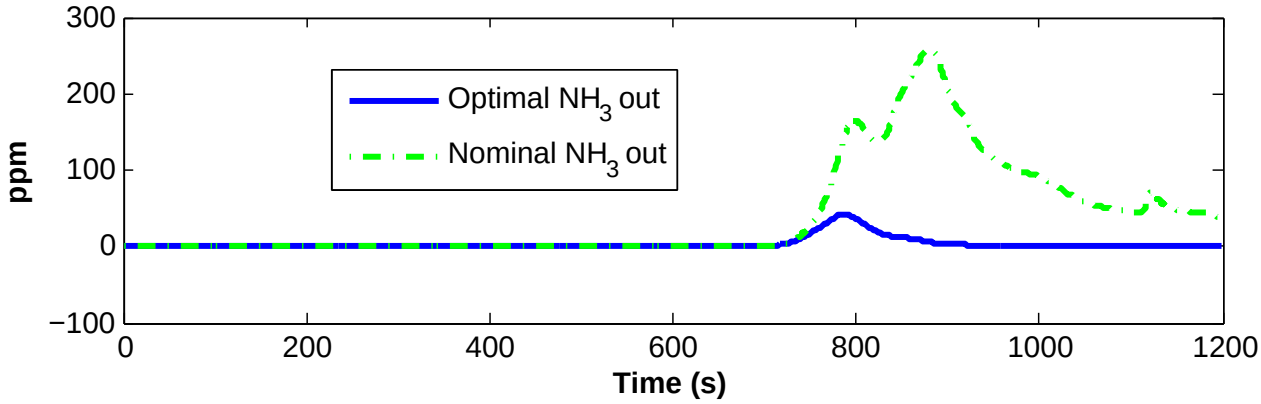

Figure 7. Downstream NH_3 concentration comparison of the optimal and nominal urea dosing.

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