Two-Level Nonlinear Model Predictive Control for Lean NOx Trap Regenerations

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Abstract
This paper describes a two-level nonlinear model predictive control (NMPC) scheme for diesel engine lean NOx trap (LNT) regeneration control. Based on the physical insights into the LNT operational characteristics, a two-level NMPC architecture with the higher-level for the regeneration timing control and the lower-level for the regeneration air to fuel ratio (AFR) profile control is proposed. A physically-based and experimentally-validated nonlinear LNT dynamic model is employed to construct the NMPC control algorithms. The control objective is to minimize the fuel penalty induced by LNT regenerations while keeping the tailpipe NOx emissions below the regulations. Different choices of cost functions were examined in terms of the impacts on fuel penalty and tailpipe NOx slip amount based on physical insights into the LNT system dynamics. The designed control system was evaluated on an experimentally-validated vehicle simulator, cX-Emissions, with a 1.9L diesel engine model through the FTP75 driving cycle. Compared with a conventional LNT control strategy, 31.9% of regeneration fuel penalty reduction was observed during a single regeneration. For the entire cold-start FTP75 test cycle, a 28.1% of tailpipe NOx reduction and 40.9% of fuel penalty reduction were achieved.

1. Introduction
Diezel engines possess noticeable advantages in terms of efficiency, reliability, and power density compared with their gasoline counterparts. However, diesel engine emission control, especially NOx reduction, is much more challenging than that for gasoline engines. The lean burn combustion characteristic of diesel engines is notable of high engine-out NOx emissions. It is very challenging to achieve the tight NOx emission regulations by engine control and combustion

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improvements alone [29]. A catalytic aftertreatment is necessary for diesel engine-powered vehicles to control the NO\textsubscript{x} emission level below the stringent regulations. Among a variety of selections, the most promising NO\textsubscript{x} aftertreatment systems are lean NO\textsubscript{x} traps (LNT) for light-duty diesel vehicles and selective catalytic reduction (SCR) catalysts for medium- and heavy-duty diesel vehicles. This paper deals with the control of LNTs.

The main LNT operation process can be described by two steps [16]. The first step, named NO\textsubscript{x} absorption, is a NO\textsubscript{x} storage process in which the LNT traps the NO\textsubscript{x} from engine exhaust gas and stores them as solid state NO\textsubscript{x} compound. Because the LNT storage capacity is finite, it has to be periodically purged when NO\textsubscript{x} slip reaches to a limited level. The second step is called NO\textsubscript{x} desorption or regeneration. In this step, the solid state NO\textsubscript{x} compound stored in LNT is released as NO\textsubscript{2} in gaseous phase. In the meantime, the released NO\textsubscript{2} is converted to nontoxic gases such as nitrogen by available reductants. To produce the rich gas that can activate NO\textsubscript{x} desorption and produce reductants for NO\textsubscript{x} conversion, extra fuel can be injected by post-injection or in-exhaust injection at the upstream of the LNT catalyst [4][6][24][32]. After regeneration is finished, LNT regains the NO\textsubscript{x} adsorption capacity and returns to the NO\textsubscript{x} adsorption phase. The LNTs have been demonstrated of being able to capture more than 90% of engine-out exhaust NO\textsubscript{x} [6]. However, a common concern about LNTs is the associated regeneration fuel penalty that can lead to higher overall vehicle fuel consumption. Fuel penalty is the extra fuel mass used for LNT regenerations, and can be defined by the following equation,

$$\text{fuel penalty} \equiv \int_{t \in \text{regeneration}} MAF(t) \left( \frac{1}{AFR_{\text{reg}}(t)} - \frac{1}{AFR_{\text{eng}}(t)} \right) dt.$$  \hspace{1cm} (1)

\begin{itemize}
  \item \textit{MAF:} \hspace{1cm} mass air flow rate (g/sec)
  \item \textit{AFR\textsubscript{reg}:} \hspace{1cm} LNT up-stream exhaust gas air to fuel ratio during regeneration
  \item \textit{AFR\textsubscript{eng}:} \hspace{1cm} engine-out (without regeneration) exhaust gas air to fuel ratio
\end{itemize}

Different LNT regeneration control strategies aiming at fuel penalty and emission reductions have been proposed by researchers in industry and academia, e.g. [13][20][26][30][31][33][34]. For instance, in [26], a model-based approach to control the rich pulse timing and its duration for LNT regenerations was proposed. A LNT model adaptation mechanism was used to adjust the rich pulse timings and durations to reduce the tailpipe emissions. In [30], the authors proposed an adaptive LNT purge control strategy, in which on-line adaptations for the LNT capacity and LNT-in NO\textsubscript{x} flow rate were conducted with the assistance provided by an exhaust gas
oxygen sensor. The estimated LNT capacity usage percentage was then employed to trigger the LNT regeneration events. The adaptive regeneration trigger control schemes benefited the reduction of the tailpipe NO\textsubscript{x} slip because the LNT dynamics variations due to temperature and other environmental factors were taken into account. Owing to the highly nonlinear NO\textsubscript{x} desorption efficiency, the actual AFR profile control during regenerations is also of importance for fuel penalty and emission reductions. However, less attention has been devoted to this aspect. In order to systematically handle the LNT system nonlinearities and achieve overall optimal regeneration fuel efficiency and tailpipe NO\textsubscript{x} emissions, LNT regeneration timing control and AFR profile control during regenerations need to be synergistically combined. In this paper, a two-level nonlinear model predictive control approach is thus proposed to control both the regeneration trigger timings and the AFR profiles during regenerations. A higher-level NMPC controller was designed to find the optimal regeneration points for maximizing the regeneration efficiency and also ensuring the tailpipe NO\textsubscript{x} emission below the desired limit. A lower-level NMPC controller minimizes the fuel penalty during LNT regenerations by controlling the AFR profiles based on a physically-based LNT model. Compared with a conventional LNT controller [4][24], the NMPC control approach reduced 27.9% of tailpipe NO\textsubscript{x} emission and 36.4% of fuel penalty during a warmed-up FTP75 cycle simulation, and achieved 28.1% of tailpipe NO\textsubscript{x} reduction and 40.9% fuel penalty reduction during a cold-start FTP75 cycle in simulation.

The rest of this paper is organized as follows. In section 2, a physically-based LNT model and its experimental validation are briefly described. A description of the two-level NMPC LNT control architecture is presented in section 3. Sections 4 and 5 describe the NMPC designs of the two levels, respectively, followed by simulation results and analyses in section 6. Conclusive remarks are summarized in section 7.

2. LNT Model and Experimental Validation

As outlined in the introduction, the LNT operation includes two steps: NO\textsubscript{x} adsorption and NO\textsubscript{x} desorption. The NO\textsubscript{x} in the exhaust gas of diesel engines is primarily NO. During adsorption step, the first reaction is the oxidation of NO to NO\textsubscript{2} over the catalyst. The second reaction is the storage of the NO\textsubscript{2} on BaCO\textsubscript{3} sites on the catalyst surface [33]. The chemical reaction can be explained by the following equations:

\[
2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2
\]
\[ 2\text{NO}_2 + \text{BaCO}_3 + \frac{1}{2}\text{O}_2 \rightarrow \text{Ba(NO}_3)_2 + \text{CO}_2, \]

where the \( \text{Ba(NO}_3)_2 \) is in solid state cohered with the LNT surface. Because oxygen is required in the reaction, the \( \text{NO}_x \) adsorption process is active only in lean environment (excessive oxygen is available). Once most \( \text{BaCO}_3 \) have reacted with \( \text{NO}_x \) and became \( \text{Ba(NO}_3)_2 \), LNT will not be able to trap \( \text{NO}_x \) anymore and regeneration should be triggered to purge the stored \( \text{NO}_x \). The purged LNT can then conduct \( \text{NO}_x \) adsorption again.

The regeneration process occurs only in rich environment where the \( \text{Ba(NO}_3)_2 \) becomes unstable and releases \( \text{NO}_2 \). The surface sites become \( \text{BaO} \), which then react with \( \text{CO}_2 \) and are converted back to \( \text{BaCO}_3 \). At the same time, the released \( \text{NO}_2 \) is converted to \( \text{N}_2 \) by the reductants (CO and HC). The regeneration process can be summarized by the following chemical equations:

\[ \text{Ba(NO}_3)_2 \rightarrow \text{BaO} + 2\text{NO}_2 + \frac{1}{2}\text{O}_2, \]
\[ \text{NO}_2 \rightarrow \text{NO} + \frac{1}{2}\text{O}_2, \]
\[ \text{BaO} + \text{CO}_2 \rightarrow \text{BaCO}_3, \]
\[ \text{NO} + \text{CO} \rightarrow \text{CO}_2 + \frac{1}{2}\text{N}_2, \]
\[ \left(2n + \frac{m}{2}\right)\text{NO} + c_n\text{H}_m \rightarrow n\text{CO}_2 + \frac{m}{2}\text{H}_2\text{O} + \left(n + \frac{m}{4}\right)\text{N}_2. \]

A mathematical model that describes the dynamics of the physical process while maintaining affordable computational burden is essential in order to capture the real LNT behaviors and to construct NMPC. Figure 1 shows the block diagram of the LNT model. The inputs are the exhaust gas mass flow rate and temperature, together with the composition of the feed gas. The outputs are the outlet gas temperature (assumed equal to the catalyst brick temperature) as well as the outlet mixture composition. The input/output characterization of the LNT model results from the interaction of three subsystems: an oxygen storage dynamics model, a \( \text{NO}_x \) storage dynamics model, and a model for the catalyst temperature dynamics. The models of the above subsystems, originally developed in [6][28], will be briefly summarized in this section for the sake of completeness. Interested readers can refer [6][28] for details regarding the LNT model.
2.1 Oxygen Storage/Release Dynamics

The modeling of the oxygen storage and release dynamics was based on application of the continuity equation to the oxygen stored (in solid state) and to the oxygen present in the exhaust stream (gas phase), as the following:

\[ \frac{dM_{O_2}}{dt} = C_{O_2} \frac{dx_{O_2}}{dt} = r_{O_2,stor} - r_{O_2,rel}, \]  
\[ m_{O_2,\text{out}} = m_{O_2,\text{in}} - r_{O_2,stor} + r_{O_2,rel}, \]

where \( M_{O_2} \) is the mass of oxygen (solid state) stored in the LNT catalyst, \( m_{O_2,\text{in}} \) and \( m_{O_2,\text{out}} \) denote the mass of oxygen flow into and out of the LNT, \( C_{O_2} \) is the oxygen storage capacity and \( x_{O_2} \) represents the catalyst oxygen fill ratio.

The oxygen storage and release rate, \( r_{O_2,stor} \) and \( r_{O_2,rel} \), can be described as:

\[ r_{O_2,stor} = k_{st} \left( \frac{1 - e^{\alpha x_{O_2}}}{e^\alpha - 1} + 1 \right) m_{O_2,\text{in}}, \]
\[ r_{O_2,rel} = k_{rel} \left( \frac{1 - e^{\beta x_{O_2}}}{e^\beta - 1} + 1 \right) (m_{CO} + m_{HC})_{in}, \]

where \( k_{st} \) and \( k_{rel} \) are the two empirical constants, and the multipliers \( \alpha \) and \( \beta \) are linear functions of the catalyst temperature.

2.2 NO\textsubscript{x} Storage/Release Dynamics

The dynamics associated with the NO\textsubscript{x} adsorption and release (desorption) are described using a similar approach.

\[ \frac{dM_{NOx}}{dt} = C_{NOx} \frac{dx_{NOx}}{dt} = r_{NOx,stor} - r_{NOx,rel}, \]
\[ \dot{m}_{NOX, \text{out}} = \dot{m}_{NOX, \text{in}} - r_{\text{NOX,stor}} + r_{\text{NOX,rel}}. \]

The \( x_{\text{NOX}} \) is the LNT NO\(_x\) fill ratio and \( C_{NOX} \) is the LNT NO\(_x\) storage capacity. The NO\(_x\) storage and release rates can be expressed by:

\[ r_{\text{NOX,stor}} = k_{\text{st}} \eta_c \left( \frac{1 - e^{\gamma x_{\text{NOX}}}}{e^\gamma} + 1 \right) \dot{m}_{NOX, \text{in}}, \]

\[ r_{\text{NOX,rel}} = k_{\text{rel}} \left( \frac{e^{-\phi x_{\text{NOX}} - 1}}{e^{-\phi - 1}} \right) (\dot{m}_{CO} + \dot{m}_{HC})_{\text{in}}, \]

\[ k_{\text{st}} \eta_c \left( \frac{1 - e^{\gamma x_{\text{NOX}}}}{e^\gamma} + 1 \right): \text{NO}_x \text{ storage efficiency}, \]

\[ k_{\text{rel}} \left( \frac{e^{-\phi x_{\text{NOX}} - 1}}{e^{-\phi - 1}} \right): \text{NO}_x \text{ release efficiency}, \]

\((\dot{m}_{CO} + \dot{m}_{HC})\) denotes the mass flow rate of reductant and the multipliers \( \gamma \) and \( \phi \) depend linearly on the catalyst temperature with a positive first order derivative. The efficiency term \( \eta_c \) accounts for the oxygen available to promote the NO\(_x\) storage reactions.

The trap regeneration was modeled by considering two sequential phases. First, the stored NO\(_x\) are released from the trap in presence of rich exhaust gas. After that, the released NO\(_x\) is converted to N\(_2\) by the reductants. The conversion process depends on the catalyst temperature, fill ratio, and concentration of carbon monoxide and hydrocarbons (reductants) available in the mixture. Therefore, the mass rate of NO\(_x\) conversion to N\(_2\) can be defined as:

\[ r_{\text{NOX,conv}} = k_{\text{conv}} \eta_{\text{conv}} r_{\text{NOX,rel}}, \]

where the conversion efficiency \( \eta_{\text{conv}} \) is a complex function that includes the effects of the aforementioned variables.

\[ \eta_{\text{conv}} = \left( \frac{e^{\lambda x_{\text{conv}} - e^\lambda}}{1 - e^\lambda} \right) \left( \frac{e^{-\sigma u - 1}}{e^{-\sigma - 1}} \right), \]

where \( \lambda \) is a linear function of the catalyst temperature with a positive first order derivative, \( x_{\text{conv}} \) is the mass flow ratio of reductant and NO\(_x\), and \( u \) represents the mass of equivalent reductant \((CO + C_r H_m)\) that is required to convert the released NO\(_x\) normalized to the corresponding stoichiometric value [6][8][28].

2.3 Catalyst Temperature Dynamics

The LNT temperature dynamics can be characterized by applying the energy conservation principle to the catalyst brick, assuming its temperature equal to the one of the gas contained in the system. With this assumption, the energy balance yields:
\[
\frac{dT}{dt} = \frac{1}{M_{\text{cat}} c_{\text{cat}}} \left[ m_{\text{gas}} c_p (T_{\text{in}} - T) - \dot{Q}_{\text{reac}} - \dot{Q}_{\text{ht}} \right],
\]

\[T_{\text{out}} = T(t - t_d),\]

where \(T\) is the LNT temperature, \(T_{\text{in}}\) is the LNT inlet temperature, \(T_{\text{out}}\) is the LNT outlet temperature, \(t_d\) is a delay time, \(M_{\text{cat}} c_{\text{cat}}\) denotes the catalyst thermal capacity, \(c_p\) is the specific heat of the feed gas, and \(\dot{Q}_{\text{ht}}\) is relative to the heat losses, mainly due to convection. The term \(\dot{Q}_{\text{reac}}\) represents the total reaction enthalpy produced by the release and conversion of the stored \(O_2\) and \(NO_x\) approximated from the results of an exothermic analysis of a LNT catalyst [22].

### 2.4 LNT Model Validation

The developed LNT model was validated with experimental data obtained on a laboratory setup consisting of a four-cylinder, 1.9L Diesel engine equipped with an aftertreatment system consisting of dual-LNT and a bypass regeneration system [7][24]. Figure 2 shows a schematic of the experimental setup for model validation, while Table I reports the main system specifications.

#### Table I Testing specifications

<table>
<thead>
<tr>
<th>Engine configuration</th>
<th>Inline, four cylinder DI Diesel, turbocharged, intercooler</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement</td>
<td>1.9 L</td>
</tr>
<tr>
<td>Fuel injection system</td>
<td>Bosch Common Rail Direct Injection</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>17.5:1</td>
</tr>
<tr>
<td>Max Power/Torque</td>
<td>105kW at 4000rpm; 320Nm at 2000rpm</td>
</tr>
</tbody>
</table>

The experimental setup provides the possibility of controlling the engine speed and torque, monitoring the emissions during the LNT storage phase. The gas composition, particularly the
NOx concentration at the catalyst inlet and outlet, was determined by measurements using a NOx analyzer and by elementary mass balances based on equilibrium reactions [15]. The rich conditions for catalyst regeneration were provided by partially diverting the gas flow from the LNT with a bypass valve and by injecting a rich gas through a flame reformer system [4][23]. This methodology allowed for controlling the composition of the feed gas, particularly the concentration of H2 and CO.

The tests were carried out by alternating cycles with fixed storage and regeneration durations (2 minutes and 20 seconds, respectively). The inputs to the model are the engine air mass flow rate, the AFR, the exhaust gas temperature and the inlet NOx concentration. The validation was conducted by comparing the NOx concentration and outlet temperature with the measured data. Figure 3 shows the inlet and outlet NOx concentration and temperature values during the 10 consecutive storage and regeneration cycles, compared to the predictions of the model. The results shown were taken from an experimental test conducted at a steady-state engine operating point (2000r/min, 120Nm).

![Figure 3. Comparison of NOx emissions and catalyst temperatures during a validation test.](image)

The validation results show how the model response agrees with the experimental data, in terms of outlet NOx concentration and temperature. The model is accurate in characterizing the dynamics of the system, during both the storage and regeneration phase. During the storage phase,
the error on the cumulative NO\textsubscript{x} emissions is typically less than 5%, which indicates a good agreement with the experimental data. During the regeneration phase, the simplified approach adopted to characterize the desorption and conversion reactions caused some differences between the model and experimental data, but the error is within the range of 10%.

Figure 4 compares the model behavior with the experimental data during a single storage and regeneration cycle, showing that the NO\textsubscript{x} storage dynamics and temperature dynamics are well tracked by the model. From a dynamic standpoint, the model captures accurately the slow filling dynamics of the catalyst, which results in a progressive increase of the LNT-out NO\textsubscript{x} concentration. Furthermore, the model also captures the characteristic NO\textsubscript{x} spike at the start of regeneration, which is a consequence of the interactions with the oxygen release dynamics that causes a temporary lack of reductants, thereby preventing from a complete conversion of NO\textsubscript{x} into N\textsubscript{2}. The second peak at each cycle is due to the stop of regeneration. At these times, the exhaust gas AFR became lean and reductants for NO\textsubscript{x} conversion were limited. So the rest of the released NO\textsubscript{x} inside the catalyst was directly emitted to the tailpipe.

![Figure 4. Comparison of NO\textsubscript{x} emissions and catalyst temperatures during a single storage and regeneration cycle (2000r/min, 120Nm).](image)

The LNT model was integrated into a full-vehicle experimentally-validated simulator, cX-Emissions. The simulator was used by the Challenge-X team at the Ohio State University for controller design and has demonstrated sufficient model accuracy and resulted in successful vehicle control designs [4]. To this extent, the simulator was extended to include an estimate of
engine-out emissions, with the objective of determining the composition of the gas at the LNT inlet [6]. A simple emission characterization was therefore implemented in the model, as a function of the engine air mass flow rate and air/fuel ratio, based on the engine steady-state emission maps. The composition during rich operations was estimated from experimental data obtained on a diesel fuel reformer for regeneration of LNT systems [4][23]. This allowed one to extend the engine-out emission maps to include rich exhaust mixture conditions (where the air/fuel ratio falls below the stoichiometric value). On a real engine setup, the generation of rich gas can be done by commanding the diesel engine fuel injection system to operate a late post-injection (or in-exhaust injection), during the expansion stroke. This additional injection of fuel leads to the formation of partial combustion products (namely, CO and H₂), without causing any relevant perturbation in the engine torque.

3. NMPC for LNT Control

Model predictive control (MPC) is an optimization-based control strategy that predicts system behavior in a receding horizon and then calculates the optimal control sequence in this future time span [1]. The advantages of MPC lie in that it can systematically handle most kinds of dynamics and constraints and achieve optimal control by predicting the system dynamics. Linear model predictive control methods have been well established for many years. For nonlinear systems, recently, with the improved MPC algorithms in the aspect of computational efficiency [5][9][14][17][18][35], and the increased controller computational capacity, it has become attractive as well [10], and has been successfully demonstrated in several applications [2][3][11][27]. The challenges of LNT control are primarily induced by the highly nonlinear dynamics, e.g. Eqs. (5)(7)(9), and system constraints, e.g. minimum/maximum feasible AFR. Besides, LNT control also needs to minimize the regeneration fuel penalty while satisfying the tailpipe NOₓ emission constraint. Such challenges make MPC an attractive choice for LNT control because it aims at finding an optimal control within the constraints at each receding horizon. In this paper, grounded in the physical insights into the LNT characteristics, a novel two-level NMPC scheme for LNT control was proposed and implemented on an experimentally-validated full-vehicle simulator to demonstrate its effectiveness.

3.1 Two-level NMPC for LNT Control

A two-level NMPC control scheme for LNT regeneration control is shown in Figure 5.
The LNT regeneration control structure is naturally divided into two parts: regeneration trigger control and regeneration AFR profile control. The main objective of the LNT control is to minimize the fuel penalty, as defined in Eq. (1), while keeping the tailpipe NOx emission under the regulation levels. Three LNT system efficiencies should be considered in the regeneration control: NOx release efficiency, NOx conversion efficiency, and NOx storage efficiency, as expressed in Eq. (7) and Eq. (9). Increasing the NOx release efficiency can directly reduce the regeneration fuel penalty. According to Eq. (7), the available control variable for NOx release efficiency is the reductant mass flow rate, which can be controlled by the AFR. Because the LNT release efficiency is highly relevant to the NOx fill ratio, to release a certain amount of NOx with minimum fuel penalty, NOx release rate should be optimally distributed with respect to the fill ratio variation. This requires the prediction of NOx storage dynamics. Furthermore, external factors such as temperature and engine load also affect the LNT NOx release behavior, predictions of these factors are therefore necessary for NOx release efficiency optimization. To accommodate the aforementioned high nonlinearities of the LNT dynamics, a NMPC of the AFR profile is employed. In this paper, this part is referred as a lower-level control (LLC).

According to Eqs. (6), (7), and (8), the tailpipe NOx emissions are relevant to the LNT NOx storage efficiency during NOx adsorption, NOx conversion efficiency during regeneration, and the number of regenerations. In other words, the tailpipe NOx emission amount is dominated by the regeneration trigger (timing) control. To ensure that the NOx emissions are under the regulation while minimizing the fuel penalty, regeneration timings should be carefully selected to avoid unnecessary and inefficient regenerations. To systematically address the LNT nonlinear and
time-varying characteristics and thus achieve better tradeoff between the NOx emissions and fuel penalty, a NMPC higher-level control (HLC) is specifically designed to trigger the regenerations.

The model used in the NMPC is a 3-state LNT model derived from the one described in Section 2. The model utilizes the available measurements from a typical aftertreatment system as the inputs including temperature sensor ($T_{in}$), NOx sensor ($\dot{m}_{N_{Ox, in}}$), oxygen sensor ($\dot{m}_{o_2, in}$), and mass air flow sensor (MAF) at upstream and downstream of the LNT catalyst. Note that a map which considers the engine speed and torque together with a MAF sensor were used to predict the exhaust gas flow rate into the LNT. The three states of the model are the oxygen storage, $x_1$, NOx storage, $x_2$, and LNT temperature, $x_3$. The simplified model is expressed by the following equations:

$$\begin{align*}
\dot{x}_1 &= kst \left( \frac{1 - e^{\alpha x_1}}{e^{\alpha} - 1} + 1 \right) \dot{m}_{o_2, in} - k_{rel} \left( \frac{1 - e^{\beta x_1}}{e^{\beta} - 1} + 1 \right) g_1(AFR, \dot{m}_{o_2, in}, MAF), \\
\dot{x}_2 &= kst \eta_c \left( \frac{1 - e^{\gamma x_2}}{e^{\gamma} + 1} \right) \dot{m}_{N_{Ox, in}} - k_{rel} \left( \frac{e^{-\phi x_2} - 1}{e^{-\phi} - 1} \right) g_2(AFR, \dot{m}_{o_2, in}, MAF), \\
\dot{x}_3 &= \frac{1}{M_{cat} c_{cat}} \left[ \dot{m}_{gas} c_p (T_{in} - x_3) - \dot{Q}_{reac} - \dot{Q}_{in} \right],
\end{align*}$$

where $\alpha$, $\beta$, $\gamma$ and $\phi$ are temperature-dependent variables as in Eqs. (5) and (7) and $g_n(AFR, \dot{m}_{o_2, in}, MAF)$ is a combination of experimental functions and maps to approximate the reductant (CO and HC) mass flow rate by AFR, oxygen concentration, and exhaust gas mass flow rate. In addition, the AFR is the engine-out air to fuel ratio during NOx adsorption period, and is controlled to a desired value, $AFR_{reg}$, dictated by the LLC during regeneration period. A separate exhaust gas AFR controller may be utilized to inject the extra fuel amount based on the measured and estimated engine operating conditions such as mass air flow rate, exhaust gas recirculation, in-cylinder charge, and fueling rate etc. Design and implementation of such an extra fuel injection controller depend on the particular engine-aftertreatment system configuration.

4. Lower-Level AFR Profile Controller

To reduce the computational effort, the LNT model described in (11) was further simplified to a rich condition only model for the LLC NMPC since regeneration is only active in a rich environment.
\[
\begin{align*}
\dot{x}_1 &= -k_{rel} \left( \frac{1 - e^{\beta x_1}}{e^\beta - 1} + 1 \right) g_1(AFR_{reg}, \dot{m}_{O_2,in}, MAF), \\
\dot{x}_2 &= -k_{rel} \left( \frac{e^{-\phi x_2} - 1}{e^{-\phi} - 1} \right) g_2(AFR_{reg}, \dot{m}_{O_2,in}, MAF), \\
\dot{x}_3 &= \frac{1}{M_{cat} c_{cat}} \left[ m_{gas} c_p (T_{in} - x_3) - \dot{Q}_{rea} - \dot{Q}_{ht} \right].
\end{align*}
\] (12)

The inputs and outputs of the simplified model can be described by the following figure.

Figure 6. Input-output diagram of the rich LNT model for state prediction in LLC NMPC

Here, the initial values of the three states are obtained from the model. Several LNT state estimation and adaption methods using sensor information downstream of the LNT have been developed by other researchers in the literature such as [22][26][30]. Two independent external signals are engine speed and engine torque. These signals are linearly predicted based on their current and previously measured values as shown in Eq. (13). According to the predicted engine speed and torque, engine exhaust (LNT inlet) mass flow rate and air to fuel ratio \( AFR_{eng} \) in the receding horizon are obtained from engine maps. The control output is the regeneration air to fuel ratio, \( AFR_{reg} \), which is also the design variable of this NMPC. The model output is the estimated \( NO_x \) release rate \( \dot{x}_2 \).

\[
\begin{align*}
V_{eng}(k + i|k) &= V_{eng}(k|k) + i \cdot \left( V_{eng}(k|k) - V_{eng}(k - \Delta t) \right), \\
T_{eng}(k + i|k) &= T_{eng}(k|k) + i \cdot \left( T_{eng}(k|k) - T_{eng}(k - \Delta t) \right), \\
V_{eng}: & \text{ engine speed (rad/sec)},
\end{align*}
\] (13)
\( T_{\text{eng}} \): engine torque (N·m),
\( \Delta t \): sampling time.

Besides the linear prediction shown in Eq. (13), the states can also be predicted based on engine pedal position by utilizing the engine and exhaust gas transport delays, or combining these two methods. Details of these approaches were explained in [9]. In the rest of this paper, only the linear prediction is utilized.

The objective of the LLC is to minimize the fuel penalty caused by regenerations while removing the stored NO\(_x\) by appropriately controlling the AFR profile. An intuitive cost function that can directly minimize the fuel penalty and ensure NO\(_x\) removal is the ratio of fuel penalty and the released NO\(_x\) mass:

\[
J = \min_{\text{AFR}_{\text{reg}}(k), \text{AFR}_{\text{reg}}(k+1), \ldots, \text{AFR}_{\text{reg}}(k+n-1)} \left\{ \sum_{t=0}^{n-1} \frac{\text{MAF}(k + i | k) - \text{MAF}(k + i | k + 1)}{\text{AFR}_{\text{reg}}(k + i | k) - \text{AFR}_{\text{reg}}(k + i | k + 1)} \right\}
\]

(14)

\( \text{AFR}_{\text{reg}} \): design variables, LNT inlet air to fuel ratio
\( \text{AFR}_{\text{eng}} \): engine output air to fuel ratio
\( \text{MAF} \): mass air flow rate (g/sec)
\( r_{\text{NO}_x,\text{rel}} \): LNT NO\(_x\) release rate (\( \dot{x}_2 \)) (g/sec)

However, a possible defect of the cost function in Eq. (14) is that the NO\(_x\) release rate can be slow. If the release rate decreases to a very small value, excessively long regeneration duration would be required to recover the LNT storage capacity. In general, the exhaust gas AFR in a diesel engine is around 20–50, while the rich AFR during LNT regeneration is 10–13. If the AFR evolving process is divided into lean-to-stoichiometric and stoichiometric-to-rich phases, one can see that 85% of the fuel penalty is dedicated to reduce the AFR from lean to stoichiometric. In other words, because majority of the reductant is generated when the AFR is below the stoichiometric value, the required fuel penalty is mostly spent on reducing the AFR from the regular lean value (e.g. 35) to stoichiometric (14.6), and only a small portion of the fuel penalty (stoichiometric to rich, e.g. 14.6 to 11) is actually used to generate the required reductant for regenerations. This brings out a preliminary assumption that the faster NO\(_x\) release rate is beneficial for fuel penalty reduction. However, the maximum NO\(_x\) release rate is limited by the NO\(_x\) release efficiency and also too fast NO\(_x\) release rate can lead to high NO\(_x\) emission during regeneration due to the limited NO\(_x\) conversion rate. Based on the above insights, an improved
cost function and the overall optimization problem of the LLC NMPC is proposed as follow:

Cost function:

\[
J = \min_{AFC_{reg}(k|k), AFC_{reg}(k+1|k), \ldots, AFC_{reg}(k+n-1|k)} \left\{ \sum_{i=0}^{n-1} \left[ \frac{MAF(k+i|k)}{AFC_{reg}(k+i|k)} - \frac{MAF(k+i|k)}{AFC_{reg}(k+i|k)} \right] + k \right\} + \frac{x_2(k+n-1)}{C_{NOx}} \]

Constraint:

\[AFC_{min} < AFC_{reg}(i) < AFC_{sto},\]

Design variables:

\[AFC_{reg}(k|k), AFC_{reg}(k+1|k), \ldots, AFC_{reg}(k+n-1|k),\]

Subjected to:

\[r_{NOx,rel}(i+1), x(i+1) = Model(x(i), u(i)).\]

\[AFC_{min}: \text{ minimum air to fuel ratio}\]

\[AFC_{sto}: \text{ stoichiometric air to fuel ratio}\]

\[k: \text{ NOx storage weighting factor}\]

\[Model: \text{ the simplified LNT model in Eq. (12)}\]

By adding the NOx fill ratio term \(\frac{x_2(k+n-1)}{C_{NOx}}\) in the cost function, the controller tries to minimize the fill ratio at the end of the horizon such that the NOx release rate can be increased. It is worth to mention that the two terms in the cost function have the same order of magnitude.

Based on the MPC concept, numerical optimization algorithm was implemented to minimize the cost function by specifying the optimal design variables \(AFC_{reg}(k|k), AFC_{reg}(k+1|k), \ldots, AFC_{reg}(k+n-1|k)\) in the horizon. And the first design variable \(AFC_{reg}(k|k)\) is applied to the exhaust gas AFR controller accordingly. At the next time controller was updated, \(t = k + 1\), the initial states \(x(k+1|k+1)\) of the new receding horizon were obtained from the LNT model. At the same time, NMPC started calculating the new optimal control sequence according to these initial states. The overall control scheme of NMPC for LNT regeneration AFR control is shown in the Figure 7, and the receding horizon parameters used in the LLN NMPC is presented in Table II.
Figure 7. Lower-level control (LLC) MPC scheme for regeneration AFR control

Table II: Horizon Parameters used in LLC NMPC

<table>
<thead>
<tr>
<th>Predicted receding horizon</th>
<th>Sampling time</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 (sec)</td>
<td>0.2 (sec)</td>
<td>15</td>
</tr>
</tbody>
</table>

5. NMPC for Higher-Level Controller

The LNT model used in the HLC NMPC is a two-mode model based on (11). The two modes are lean and rich modes, which correspond to NO\textsubscript{x} adsorption and desorption (regeneration), respectively. The state of mode depends on the regeneration trigger control, i.e. when the regeneration is triggered. The mode is in rich until regeneration is finished, and otherwise it is in lean mode. The two-mode model equations are expressed as follows.

Lean mode:

\[
\begin{align*}
\dot{x}_1 &= k_{st} \left( \frac{1 - e^{\alpha x_1}}{e^\alpha - 1} + 1 \right) \dot{m}_{O_2,\text{in}} \\
\dot{x}_2 &= k_{st} \eta_c \left( \frac{1 - e^{\gamma x_2}}{e^\gamma - 1} + 1 \right) \dot{m}_{NOx,\text{in}} \\
\dot{x}_3 &= \frac{1}{M_{cat} c_{cat}} \left[ m_{gas} c_p (T_{in} - x_3) - \dot{Q}_{\text{reac}} - \dot{Q}_{\text{ht}} \right]
\end{align*}
\]

Rich mode:
\[
\begin{align*}
\dot{x}_1 &= -k_{rel} \left( \frac{1-e^\rho \phi x_1}{e^{\rho}-1} + 1 \right) g_1 (AFR_{reg}, \dot{m}_{O_2,in}, MAF) \\
\dot{x}_2 &= -k_{rel} \left( \frac{e^{-\phi x_2}}{e^{-\phi}-1} \right) g_2 (AFR_{reg}, \dot{m}_{O_2,in}, MAF) \\
\dot{x}_3 &= \frac{1}{M_{cat}} \left[ m_{gas} c_p (T_{in} - x_3) - \dot{Q}_{reac} - \dot{Q}_{ht} \right] 
\end{align*}
\]

(17)

The input/output diagram of the two-mode model is shown in Figure 8.

Figure 8. Input/output diagram of the 2-mode LNT model for state prediction in HLC NMPC

The objective of the HLC NMPC is to minimize the fuel penalty and regulate the tailpipe NO\textsubscript{x} emissions under a threshold value by controlling the regeneration timing. LNT efficiencies, which affect the fuel penalty and NO\textsubscript{x} emissions as well as can be improved by regeneration timing control, include: release efficiency, storage efficiency, and NO\textsubscript{x} conversion efficiency. The HLC NMPC was designed with considerations of the mechanisms of these efficiencies.

Based on Eqs. (7) and (9), temperature plays an important role in the NO\textsubscript{x} storage and conversion efficiencies. LNT NO\textsubscript{x} storage capacity can be considerably low at low temperatures. A lower NO\textsubscript{x} capacity means a higher NO\textsubscript{x} fill ratio for the same amount of stored NO\textsubscript{x} mass. In other words, at low temperatures (e.g. cold-start), conversion and storage efficiencies are relatively low but NO\textsubscript{x} release efficiency is relatively high. Intuitively, more regenerations should be conducted at low temperatures. However, even though low temperatures can increase NO\textsubscript{x} release efficiency during regenerations, because the release NO\textsubscript{x} cannot be efficiently converted to molecular nitrogen, LNT is functionally inefficient during regenerations. The regeneration inefficiency may lead to more frequent regenerations but most released NO\textsubscript{x} will be directly emitted without being converted to molecular nitrogen. In this case, the regenerations do not
contribute to adequate NO\textsubscript{x} reductions. Therefore, temperature effect must be considered in regeneration trigger control to prevent inefficient regenerations from both fuel penalty and NO\textsubscript{x} emission reduction points of view. The receding horizon optimization problem is formulated by the following equations.

Cost function:

$$J = \min \sum_{i=0}^{n-1} \left[ \frac{MAF(k+i|k)}{AFR_{reg}(k+i|k)} - \frac{MAF(k+i|k)}{AFR_{eng}(k+i|k)} \right],$$

(18)

Constraint:

$$r_{NOX, out}(k + n - 1) < [r_{NOX, out, max} + p(T(k))],$$

Design variable:

$RegTime$,

Subjected to:

$$[r_{NOX, out}(i + 1), x(i + 1), AFR_{eng}(i)] =
\begin{cases}
    (Model_{rich}(x(i), u(i)), & \text{if } (Reg(i) = 1) \\
    (Model_{lean}(x(i), u(i)), & \text{if } (Reg(i) = 0)
\end{cases}$$

$$Reg(i) = \begin{cases}
    1, & \text{if } (i > RegTime \text{ and } x_2 > x_{2, min}) \\
    0, & \text{else}
\end{cases}$$

$$RegTime \in (k, k+1, ..., k+n)$$

$$p(T) = k_1 \frac{1}{1 - e^{-k_2(T-k_3)}} - k_4$$

$r_{NOX, out}$: cumulated tailpipe NO\textsubscript{x} emission (g/mile)

$r_{NOX, out, max}$: maximum tailpipe NO\textsubscript{x} emission (g/mile)

$p(T)$: constraint weighting function with respect to temperature

$k_1, k_2, k_3, k_4$: constants, $(k_1, k_2, k_3, k_4) \in R^+$

$Model_{rich}$: rich mode LNT model

$Model_{lean}$: lean model LNT model

$x_{2, min}$: minimum NO\textsubscript{x} storage

$RegTime$: regeneration time $(k, k+1, ..., k+n)$

The cost function to be minimized is the fuel penalty in the receding horizon. Assuming, at most, one regeneration in a receding horizon, the control variable is the regeneration trigger time $RegTime$. Regeneration starts from the time of $RegTime$ until the NO\textsubscript{x} storage is reduced to a value which is lower than the minimum NO\textsubscript{x} storage $x_{2, min}$. The AFR during regeneration is set to
a constant in the prediction model in order to increase the computational speed. The constraint restricts the cumulated tailpipe NO_x emissions at the end of the receding horizon \( r_{\text{NO}_x,\text{out}}(k + n - 1) \) to be smaller than the maximum tailpipe NO_x emission level required by regulation plus a constraint weighting function \( p(T) \), which is a function of the horizon initial temperature \( T(k) \). This constraint loosens the tailpipe NO_x emission restriction \( (p(T) \in R^+) \) when the temperature is low to prevent inefficient regenerations. On the other hand, it tightens the NO_x emission restriction \( (p(T) \in R^-) \) when the temperature is advantageous for regeneration. In such a way, the NMPC achieves a better LNT regeneration timing with respect to the temperature variations.

To reduce the computational effort, the NMPC optimization problem is simplified to a minimization problem by discretizing the design variable. As shown in Eq. (18), the design variable was discretized to a finite number \( \text{RegTime} \in (k, k + 1, \ldots, k + n - 1, k + n) \) according to the sampling time of the LNT model. The optimization becomes a problem of finding the regeneration time that minimizes the cost function and satisfies the constraint from the \( n + 1 \) samples, which can be done by a for-loop examining all the \( n + 1 \) values. Note that \( \text{RegTime} = k + n \) means there is no regeneration in the current horizon. Based on our observations, this approach is much faster and always obtains a better cost function comparing to numerical optimization algorithms. The receding horizon parameters are listed in Table III. Note that the horizon length of 10 seconds was chosen as a result of comparison for the particular engine-aftertreatment system configuration in this study. In other applications, the length should be chosen based on the engine-aftertreatment system configurations (e.g. engine displacement, LNT size, and length of the exhaust pipe etc.) and the available state prediction length using the aforementioned prediction methods.

Table III: Horizon Parameters used in HLC NMPC

<table>
<thead>
<tr>
<th>Predicted receding horizon</th>
<th>Sampling time</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 (sec)</td>
<td>0.5 (sec)</td>
<td>20</td>
</tr>
</tbody>
</table>

The following figure shows the scheme of the HLC NMPC.
6. Simulation Results and Analyses

A complete diesel engine NOx aftertreatment simulator named cX-Emissions was built in Matlab/Simulink by OSU Center for Automotive Research (CAR) [4]. The aftertreatment model was coupled with a quasi steady-state vehicle model that includes models for engine, transmission, and powertrain components. Sensor dynamics are included in the simulator models. The simulator is calibrated with data obtained from a 1.9L Diesel engine. In the following sub-sections, comparisons of simulation results and analyses based on the physical insights into the LNT operations are presented. In the first sub-section, improvement of regeneration efficiency using the LLC NMPC is demonstrated. In the second and third sub-sections, the two-level NMPC LNT regeneration control was evaluated for both warmed-up and cold-start cases, respectively. FTP75 test cycle was used in the simulations.

6.1 Lower-Level Controller Case

Four different cases are compared in this section. In Case 1, no regeneration was applied to the LNT. This case was set as a reference to be compared with other cases using different LNT regeneration controllers. In Case 2, a PID controller from a previous work [4] was used to control the LNT regeneration AFR. The PID controller attempts to regulate the NOx slip to zero by adjusting the exhaust gas AFR during regenerations. The NOx slip $S_{NOx}$ is defined by the following equation,
In Case 3, the proposed LLC NMPC control scheme was used. In this case, the weighting factor $k$ was set to zero. In Case 4, besides the fuel cost minimization, the NOx fill ratio at the end of the horizon was taken into account in the cost function. The weighting factor $k$ was set to 0.8.

In last three cases, the regeneration trigger controls were done by a logical approach used in [4][24]. The regenerations were triggered by the following conditions:

$$
\text{Reg}(i) = \begin{cases} 
\text{switch to } 1, & \text{if } \left( \frac{\dot{m}_{\text{NOx,in}} - \dot{m}_{\text{NOx,out}}}{\dot{m}_{\text{NOx,in}}} > \eta_{\text{reg,on}} \right) \\
\text{switch to } 0, & \text{if } \left( \frac{\dot{m}_{\text{NOx,out}} - \dot{m}_{\text{NOx,in}}}{\dot{m}_{\text{NOx,in}}} > \eta_{\text{reg,off}} \right)
\end{cases}
$$

where $\eta_{\text{reg,on}}$, $\text{AFR}_{\text{reg,min}}$, $\text{MAF}_{\text{reg,min}}$, $\eta_{\text{reg,off}}$, and $\text{AFR}_{\text{reg,off}}$ are constant thresholds.

Figure 10 to Figure 12 show the LNT NOx storage, fuel consumption, and AFR during the first regeneration. The first regeneration was compared because all the three regenerations started at the same time and had the same initial conditions. Because different amounts of NOx were removed in the three cases, the reference for fuel penalty comparison was chosen as the fuel penalty per NOx removal, which is named as “unit NOx fuel penalty” and defined by the following equation.

$$\text{unit NOx fuel penalty} = \frac{\text{fuel penalty during regeneration (g)}}{\text{total mass of removed NOx during regeneration (g)}}$$

In Figure 10, all the three regenerations show slow NOx release rates at the beginnings of the regenerations because the generated reductant reacted with the stored oxygen before it contributed to NOx desorption as described before. According to the NOx storage curves, one can see Case 4 has the fastest oxygen and NOx release rates, and then Case 3 and Case 2. Table IV shows the comparisons of the released NOx, fuel penalty, and the unit NOx fuel penalty of the four cases. Among them, Case 4 has the lowest unit NOx fuel penalty, Case 3 is the second, and Case 4 is the third. The results verify that the NMPC approach can reduce the fuel penalty by minimizing the fuel-penalty/NOx-removal. As can be seen in Table IV, the unit NOx fuel penalty was reduced
6.8% in Case 3 comparing to Case 2. In the light of a faster \( \text{NO}_x \) release rate leading to a lower fuel penalty, the \( \text{NO}_x \) fill ratio term was added to the cost function in Case 4. As Figure 12 illustrates, the AFR is brought farther away from the initial value and a faster \( \text{NO}_x \) release rate and lower unit \( \text{NO}_x \) fuel penalty were achieved. From Table IV, one can see the proposed LLC NMPC in Case 4 reduced 26.6% of unit \( \text{NO}_x \) fuel penalty comparing to the conventional controller in Case 2 during this single regeneration.

![Figure 10. Comparison of the \( \text{NO}_x \) storages with different AFR control strategies during the first LNT regeneration, the ‘PID control’ and ‘MPC with k=0.8’ have the same \( \text{NO}_x \) storage level at the end.](image1)

![Figure 11. Comparison of the fuel consumptions, the ‘PID control’ and ‘MPC with k=0.8’ have the same \( \text{NO}_x \) storage level at the end.](image2)
Table IV: Comparison of fuel consumption at the first regeneration

<table>
<thead>
<tr>
<th>Controller</th>
<th>Released NOx (g)</th>
<th>Fuel Penalty (g)</th>
<th>Unit NOx Fuel Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Case 2</td>
<td>1.361</td>
<td>4.7</td>
<td>3.453</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.963</td>
<td>3.1</td>
<td>3.219</td>
</tr>
<tr>
<td>Case 4</td>
<td>1.263</td>
<td>3.2</td>
<td>2.533</td>
</tr>
</tbody>
</table>

6.2 Combined Higher-Level Control and Lower-Level Control Case

In this section, the simulation results using the entire two-level LNT regeneration control scheme are presented. Three cases were compared: Case 1 and Case 2 as mentioned in the foregoing section, and Case 5, which uses LLC NMPC and HLC NMPC for regeneration AFR control and regeneration trigger control, respectively. The tailpipe NOx emission constraint $r_{NOX, out, max}$ was set to 0.07 g/mile according to the US EPA Tier II Bin 5 light-duty vehicle regulation. Notice that the 0.07 g/mile is calculated as the ratio of cumulated tailpipe NOx emission (g) and cumulated distance which has been traveled (instead of the total distance of the FTP75 cycle of 11 miles). Such presentation can make sure that the NMPC constraint can be satisfied throughout the cycle and also the emission regulation can be satisfied at the end of the cycle. Figure 13 shows the comparison of total fuel costs at the end of the FTP75 cycle. The numeric values are presented in Table V. One can see the NMPC LNT control approach reduced 36.4% of fuel penalty compared with the conventional LNT controller. Besides, the NOx emission of Case 5 is 0.061 g/mile, which is 27.9% less than Case 2 and is under the EPA regulation as expected. The tailpipe NOx emission of the y-axis in Figure 14 is the ratio of cumulated tailpipe
NO\textsubscript{x} emissions (g) and cumulated millage which has been traveled (mile). Such a ratio is the constraint of the NMPC LNT control scheme. With such a presentation, the difference between the instantaneous emission level and the target value can be clearly shown. This ratio is used in the rest of the figures in this paper.

![Figure 13. Comparison of the fuel consumptions at the end of the FTP 75 cycle](image13.png)

Figure 13. Comparison of the fuel consumptions at the end of the FTP 75 cycle

![Figure 14. Comparison of the tailpipe NO\textsubscript{x} emissions during the FTP 75 cycle](image14.png)

Figure 14. Comparison of the tailpipe NO\textsubscript{x} emissions during the FTP 75 cycle

Figure 15 shows the comparison of NO\textsubscript{x} storage during the cycle, the fast storage reductions are the points where regenerations were triggered.
Figure 15. Comparison of the NOx storages during the FTP 75 cycle

Figure 16 shows regeneration triggers with a reference to the vehicle speed and Figure 17 is the zoom-in of the first regeneration. Figure 17 also illustrates, as an example, the HLC NMPC can find the best regeneration point in the finite horizon. From Figure 14, one can see that the tailpipe NOx emission ratio (accumulated NOx/accumulated miles) of Case 5 just passed 0.05 g/mile when the first regeneration started. Intuitively, the regeneration should be triggered later because the NOx emission was still 28% below the constraint (0.07 g/mile). However, by observing the speed curve, one can see the vehicle slowed down just after the regeneration, which means the engine load started to decrease after the regeneration and regeneration would be less efficient after that point due to relatively high engine exhaust gas AFR (excessive oxygen) at light loads.
Figure 16. Comparison of the regeneration timings between the conventional regeneration trigger control and the NMPC based regeneration trigger control with reference to the vehicle speed profile during the FTP 75 cycle.

Figure 17. Comparison of the first regeneration timing between the conventional regeneration trigger control and the MPC based regeneration trigger control.

The scenario of the first regeneration can be explained as follows. At a time instance that is close the first regeneration point, a HLC NMPC predicted regeneration was required within the receding horizon, and it found out regeneration efficiency would decrease before the NOx emission reaches the limitation. Therefore, the controller decided to advance the regeneration timing in order to have high regeneration efficiency. This scenario can be more clearly illustrated by Figure 18. As can be seen the regeneration was triggered very close to the peak of the engine power curve, where the engine exhaust gas AFR was the lowest (less excessive oxygen and therefore requires less fuel). This result confirms that the NMPC is capable of triggering regenerations at points where the fuel penalty can be minimized in the nearby time region. On the other hand, the conventional regeneration trigger controller can only trigger regeneration when the considered values exceed the thresholds. As can be seen in Table V, by implementing HLC NMPC as the regeneration trigger controller, with only 1 gram extra fuel penalty, the tailpipe NOx emission was reduced by 24.3% compared with that of Case 4.
Figure 18  Comparison of regeneration timing, engine output power, mass air flow rate (MAF), and air to fuel ration (AFR) in the first regeneration region.

Table V: Comparison of fuel consumption and NOx emission at the end of the FTP 75 cycle

<table>
<thead>
<tr>
<th>Controller</th>
<th>Fuel Consumption (g)</th>
<th>Fuel Penalty (g)</th>
<th>Tailpipe NOx Emission (g/mile)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>1149.35</td>
<td>0</td>
<td>0.3125</td>
</tr>
<tr>
<td>Case 2</td>
<td>1164.71</td>
<td>15.4</td>
<td>0.0847</td>
</tr>
<tr>
<td>Case 3</td>
<td>1162.41</td>
<td>13.0</td>
<td>0.0922</td>
</tr>
<tr>
<td>Case 4</td>
<td>1158.16</td>
<td>8.8</td>
<td>0.0807</td>
</tr>
<tr>
<td>Case 5</td>
<td>1159.16</td>
<td>9.8</td>
<td>0.0611</td>
</tr>
</tbody>
</table>

6.3 Cold-Start Case

Cold-start tailpipe NOx emission control is particularly challenging for LNT control. In this section, simulation results comparing the conventional LNT controller, the NMPC approach without temperature consideration, and the NMPC with temperature consideration for the cold-start FTP75 cycle are presented. The cold-start temperature was set as 25°C and the initial LNT NOx fill ratio was set as 50%. Three different cases to be compared are the conventional LNT control (Case A), the LLC HLC NMPC with $k_1$ and $k_4$ equal to zero (Case B), and the LLC HLC NMPC with temperature consideration ($k_1$ and $k_3$ not equal to zero, Case C). Figure 19 shows the temperature variation during the simulation cycle and Figure 20 shows the regeneration trigger signals of the three cases. The temperature reached the normal LNT operational temperature range after 200 seconds. From Figure 21, Figure 22, and Table VI, one can see the NMPC with temperature consideration reduced 40.9% of fuel penalty compared with the conventional LNT controller, and 20.2% compared to the NMPC approach without considering
temperature effect. At the same time, 28.1% reduction of tailpipe NO\textsubscript{x} emission, compared to Case A, was achieved and the value is below the EPA regulation.

![Figure 19. Comparison of the LNT temperatures with initial temperatures equal to 25 degree C.](image)

From the regeneration triggers shown in Figure 20, one can observe that the controller in Case C delayed the first regeneration to the point where the LNT temperature increased to the normal operating range. In this situation, unnecessary regenerations were prevented. The tailpipe NO\textsubscript{x} emission comparisons in Figure 22 explain the “unnecessary” regenerations. Even though Case A and Case B had more regenerations before the first regeneration of Case C, as shown in Figure 20, they all had higher NO\textsubscript{x} emissions at the beginning of the cycle. It was primarily due to the low regeneration NO\textsubscript{x} conversion efficiency at low temperature. Regenerations in such a low temperature environment can release NO\textsubscript{x} but cannot efficiently convert the released NO\textsubscript{x} to nontoxic gases such as nitrogen. Essentially, the NO\textsubscript{x} was released to tailpipe by regenerations without conversion, and the fuel penalties were wasted on releasing NO\textsubscript{x} and oxygen. On the other hand, even though Case C had higher NO\textsubscript{x} emissions when the LNT reached the normal operating temperature, the NO\textsubscript{x} emissions quickly converged below the maximum emission constraint of 0.07 g/mile and the fuel penalty was much lower than that of Case B. The results showed the NMPC ability of minimizing fuel penalty with respect to temperature variations.
Figure 20. Comparison of the regeneration triggers during the FTP 75 cycle. The conventional control strategy and the MPC control strategy without temperature consideration triggered regenerations at temperatures below 150 degree C.

Figure 21. Comparison of the cold start fuel consumptions at the end of the FTP 75 cycle.
Figure 22. Comparison of the cold start tailpipe NO\textsubscript{x} emissions during the FTP 75 cycle, the high values of NO\textsubscript{x} emission at the first few seconds were due to the low mileage at the start of the cycle that leads to small denominators of g/mile.

![Graph showing comparison of LNT NO\textsubscript{x} storages during FTP cycle]

Figure 23. Comparison of the cold start LNT NO\textsubscript{x} storages during the FTP cycle

Table VI: Comparison of fuel consumption and NO\textsubscript{x} emission at the end of the FTP 75 cycle with cold start

<table>
<thead>
<tr>
<th>Controller</th>
<th>Fuel Consumption (g)</th>
<th>Fuel Penalty (g)</th>
<th>Tailpipe NO\textsubscript{x} Emission (g/mile)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A</td>
<td>1169.4</td>
<td>20.05</td>
<td>0.096</td>
</tr>
<tr>
<td>Case B</td>
<td>1164.2</td>
<td>14.85</td>
<td>0.064</td>
</tr>
<tr>
<td>Case C</td>
<td>1161.2</td>
<td>11.85</td>
<td>0.069</td>
</tr>
</tbody>
</table>

6.4 Simulations with Uncertainties

Model predictive control is essentially a model-based control algorithm. Many studies about MPC robustness have been proposed for linear systems [12][21][25][19][36]. Due to the high complexity of the LNT model, in this section, simulations with uncertainties introduced in the key reaction rates and sensor are presented to show the system robustness.

In the following simulation cases, uncertainty factors were applied to the different LNT reaction rates of NO\textsubscript{x} release, of NO\textsubscript{x} storage, and of NO\textsubscript{x} conversion, and mass air flow rate (MAF) measurement, i.e. \(N_{\text{rel}}=1.1\) implies the NO\textsubscript{x} release rate is 10% faster than the actual rate, \(N_{\text{red}}=0.9\) implies the NO\textsubscript{x} reduction rate is 90% of the actual value, \(N_{\text{con}}=1.1\) implies the NO\textsubscript{x} conversion rate is 110% of the actual rate, and \(N_{\text{MAF}}=1.1\) indicates the mass air flow rate sensor reading is 1.1 times of the actual value.
Figure 24. Comparison of AFR controls during the first regeneration as in Figure 12 with different NOx release rate and MAF sensor uncertainties

Figure 25. Comparison of total fuel cost at the end of the FTP cycle with different NOx release/storage/conversion rates and MAF sensor uncertainties
Figure 26. Comparison of regeneration triggers with different NO\textsubscript{x} release/storage/conversion rates and MAF sensor uncertainties

Figure 27. Comparison of tailpipe NO\textsubscript{x} emission with different NO\textsubscript{x} release/storage/conversion rates and MAF sensor uncertainties
Note that because NO\textsubscript{x} reduction and conversion rates do not have effect on the LLC NMPC for regeneration AFR control, only uncertainties of NO\textsubscript{x} release rate and MAF are discussed in Figure 24. Based on the foregoing comparisons, it was observed that the ±10% uncertainties did not result in evident divergences from the original results. The uncertainty associated with the MAF sensor induced small variations on the regeneration AFR profile control. Even though differences between cases with and without model/sensor uncertainties can still be identified, the performance of the regeneration AFR control and regeneration trigger control as well as the NO\textsubscript{x} emissions and fuel consumptions were close. They still clearly outperformed the conventional controller.

7. Conclusions

In this paper, a two-level nonlinear model predictive control scheme for LNT regeneration control was proposed using a physically-based experimentally-validated LNT model. The control objective is to minimize the fuel penalty for LNT regenerations while keeping the tailpipe NO\textsubscript{x} emission below the legislated regulations. Grounded in the physical insights into the LNT operational characteristics, a higher-level NMPC was designed for regeneration trigger/timing control and a lower-level NMPC controls the AFR profile during regenerations triggered by the higher-level NMPC. The prediction capability of NMPC enables regenerations being triggered at high efficiency points instead of passively triggered by the NO\textsubscript{x} emission saturation. The receding horizon control strategy can control the AFR profile to minimize the fuel penalty in the horizon during regenerations. Different NMPC designs and a conventional LNT control algorithm were compared and analyzed base on an experimentally-validated diesel engine aftertreatment vehicle simulator. From the simulation results, 26.6% reduction of unit NO\textsubscript{x} fuel penalty was observed during a single regeneration. Moreover, 28.1% of tailpipe NO\textsubscript{x} reduction and 40.9% of fuel penalty reduction were achieved for the entire FTP75 cycle. It is believed that for other high-speed-high-load and aggressive test cycles such as US06, the benefits of the proposed control scheme will be more pronounced. The LNT operational efficiency is greatly increased by using the proposed two-level NMPC control strategy. The results indicated the potentials and benefits of the two-level MPC scheme for diesel engine LNT system applications.

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