Dynamic Modeling of a Lean NO_x Trap for Lean Burn Engine Control

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Abstract

A control oriented dynamic model of the Lean NO_x Trap (LNT) behavior has been developed in SIMULINK™. The model simulates the trapping and purging phenomena and includes the important parameters which affect the LNT behavior. These include the trap temperature, trapping and purging duration, air fuel ratios and the mass flow rates of the exhaust gases. Engine dynamometer test data have been used to identify the model parameters and to validate the model structure. There is good agreement between the simulation results and test data. The model is suitable for control and fuel / emission tradeoff analysis.

1. Introduction

With the increased emphasis on fuel economy improvements, especially in Europe, automotive research and engineering efforts are refocused on Lean burn (LB) and Direct Injection (DI) engines. Lean burn engines typically operate at air fuel ratios of 20:1, while DI engines are operated at air fuel ratios as high as 40:1 during stratified charge mode of operation. The three way catalytic converter (TWC) removes CO and HC efficiently at lean air fuel ratios, but has a low removal efficiency for nitrogen oxides (NO_x). Research has focused on the catalytic decomposition of NO_x, but to date a suitable catalyst with a significant activity in real exhaust gas has not been identified [1,2]. A promising technique under investigation for NO_x removal is the placement of an LNT after the TWC in the exhaust system. Under lean operating conditions, the NO_x is accumulated or "trapped" in the LNT. The trapped NO_x is periodically released or "purged" by operating at a stoichiometric or rich air fuel ratio. The released NO_x is reduced to N_2 by reductants present in the exhaust gas such as CO and H_2.

The possible reaction mechanisms during the storage and purging phases have been well documented in the literature [3]. Under lean conditions, NO is oxidized to NO_2 in the gas phase over platinum. The resulting NO_2 is adsorbed on an oxide surface as barium nitrate. Typical adsorbents include oxides of [1]potassium, calcium, cerium, zirconium, lanthanum, calcium and barium [4,5]. The sequence of steps is:

<u>Step I:</u> $NO + \frac{1}{2}O_2 \Leftrightarrow NO_2$

<u>Step II:</u> $BaCO_3 + 2\,NO_2 \Leftrightarrow Ba(NO3)_2$

At rich air fuel ratios, the adsorbed barium nitrate is released from the trap as barium oxide. In the presence of reducing agents such as CO, HC and H_2 and Pt/Rh catalyst, the NO_x is converted to nitrogen and the trapping constituent, barium carbonate is restored. The sequence of steps is:

<u>Step III:</u> $Ba(NO_3)_2 \Leftrightarrow BaO + 2\,NO_2$

<u>Step IV</u>: $2\,NO_2 + 2\,CO/HC \xrightarrow{Pt/Rh} N_2 + 2\,CO_2$

<u>Step V</u>: $BaO + CO2 \rightarrow BaCO3$

Sulfur present in the fuel acts as a poisoning agent. In the combustion process, the sulfur is oxidized to sulfur dioxide (SO_2). The sulfur dioxide is oxidized to sulfur trioxide in the presence of platinum. The sulfur trioxide is trapped as barium sulfate at the trap operating conditions

Based on experimental and model results, the trapping efficiency is a function of trap temperature, catalyst loading, fuel sulfur content, space velocity, feedgas concentration and trap regeneration frequency. It has also been noted that using a richer A/F ratio for purging allows the trap to be run lean for a longer period of time. But purging at a richer A/F ratio not only has a larger impact on fuel economy but also increases the likelihood of converting the trapped sulfate to hydrogen sulfide [6], which would be unacceptable.

It is clear that in order to improve fuel economy and minimize NO_x emissions, the storage/purge control

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SIMULINK™ is a registered trademark of The Mathworks Inc., 24 Prime Park Way, Natic, MA 01760 strategy must be well designed and optimized. To assist the strategy development, a control oriented dynamic model of the trap behavior has been developed. The model captures the LNT trapping and purging phenomena and includes the important parameters which affect it's behavior.

2. Control-Oriented LNT Model

The trap storage and purging characteristics are captured using parameter identification methodology. The model shown in Figure 1, can be used as a stand-alone model or be combined with the TWC model [7] to provide an integrated after-treatment model. In the first case, the inputs to the model would include the mid-bed (post-TWC) concentrations of NO_x, HC and CO, exhaust gas temperature and flow rate. In the latter case, the inputs would include feedgas (pre-TWC) concentrations of NO_x, CO and HC, feedgas temperature and flow rate. The mid-bed concentrations and exit gas temperature would be calculated by the TWC model. The exhaust gas flow rate was approximated by the air mass flow rate because that was the only measured flow rate.

Although the model structure is similar to the TWC model [7], their characteristics are very different. NO_x is either being stored or purged from the trap at any instant. The state of the LNT is dynamic in the sense that the trap efficiency is not constant, until it is saturated. It was observed from the engine dynamometer results that even after extended periods of lean operation, the NO_x trap efficiency was around 15-20%, as shown in Figure 2. It is speculated that the NO_x entering the LNT at lean conditions is removed through two mechanisms: a majority through the trapping process and a smaller quantity through the gas phase catalytic reduction of NO_x. Similar observations have been reported in the literature. The catalytic reduction phenomena is incorporated in the model.

Under lean conditions, the storage capability of the LNT is modeled by a limited integrator with the storage rate of NO_x being a monotonically decreasing function of the state of the integrator. The NO_x mass flow rate leaving the LNT is the mass flow rate of NO_x entering the LNT, less the NO_x removed from the exhaust stream through the phenomena of trapping and catalytic gas phase reduction. When the exhaust air fuel ratio is rich, the trapped NO_x is purged and subsequently reduced by the reducing agents present in the exhaust such as CO, HC, and H_2. The model only considers CO as the reducing agent because it is present in larger quantities than the hydrocarbons. The purged and subsequently reduced NO_x is not a constituent of the tailpipe exhaust stream.

The efficiency of the LNT is a complex function of many factors. The important factors are trap capacity, temperature, and sulfur content of the fuel. The maximum storage capacity of the LNT varies with temperature, peaking at a value between 300 C and 400 C depending on the catalyst, and decreasing on either side of this temperature. High LNT temperatures can cause the NO_x stored in the trap to be released back into the exhaust stream, while low LNT temperatures cause the reactions to cease, effectively reducing the trap capacity to zero. The fuel used in the dynamometer had a low sulfur content and hence the effect of sulfur is ignored in the current representation of the model.

Let λ be the relative air fuel ratio of the exhaust entering the LNT; let ρ represent the mass of NO_x stored in the trap during lean operation or the mass of NO_x released from the trap under rich or stoichiometric conditions; let c be the equivalent maximum capacity of the LNT, in term of grams of NO_x; and let $\dot{NOx}$ and $\dot{CO}$ be the mass flow rates of NO_x and CO into the LNT. The equations are:

$$\frac{d\rho}{dt}=\begin{cases} f_L(\rho,\dot{NOx},c) & \lambda\geq 1 \ \& \ 0\leq\rho\leq c \\ f_R(\rho,\dot{CO}) & \lambda<1 \ \& \ 0\leq\rho\leq c \\ 0 & \text{otherwise} \end{cases}$$

The functions f_L and f_R model the lean and rich operation of the LNT, respectively, and are expressed as:

$$f_L(\rho,\dot{NOx},c)=(1-\beta)\times\dot{NOx}\times\mu\times\varepsilon(\alpha,x)$$

$$f_R(\rho,\dot{CO})=\rho-\gamma\times\dot{CO}$$

where

- β is the fraction of the entering NO_x that is catalyzed in the gas phase
- μ is the maximum empty trap storage efficiency
- $\varepsilon(\alpha,x)$ represents the trapping possibility function
- $1\leq\gamma\leq 2$ is the number of moles of CO it takes to reduce a mole of NO_x

The maximum capacity of the LNT, c, is modeled by a rational function of temperature (see Figure 3), i.e,

$$c=\frac{1}{\left(a+b\times T_{LNT}+c\times T_{LNT}^2+d\times T_{LNT}^3+e\times T_{LNT}^4\right)}$$

where a,b,c,d and e are regression coefficients derived from dynamometer results.

The trapping possibility function is modeled as $\varepsilon(\alpha,x)=\frac{e^{-\alpha x}-e^{-\alpha}}{1-e^{-\alpha}}$, with values of 1 when $x={}^{\rho}\!/_{c}=0$ and 0 when $x={}^{\rho}\!/_{c}=1$. This function models the phenomena that as the trap gets filled with NO_x, it is increasingly difficult to trap additional NO_x entering the trap. The temperature effect on the maximum trap capacity is modeled due to the fact that α is a function of the trap temperature and has different values at the different temperatures. Based on dynamometer data, α is represented by a fifth order polynomial equation.

The trapping possibility function is plotted as a function of LNT temperature in Figure 4. It can be seen that the capacity to store incoming NO_x peaks around 400 ^{o}C. When the temperature is higher or lower than 400 ^{o}C, the storage capability decreases. Thus maintaining the trap temperature around 400 ^{o}C is critical to maintaining a high trap efficiency.

The mass flow rate of NO_x out of the LNT, y, is

$$y=\begin{cases}(1-\beta)\times N\dot{O}x-f_L(\rho,N\dot{O}x,c) & \lambda\geq 1\\ (1-\beta)\times N\dot{O}x-f_R(\rho,\dot{C}O) & \lambda<1\end{cases}$$

3. Results

The model predictions were validated against dynamometer data from a 1.8L 4V Zetec engine. The after treatment system included a close-coupled three way catalyst (TWC) and a two-brick LNT. Two speed/load points of 1950 rpm/26.5 ft-lb and 1875 rpm/21.2 ft-lb were used. They were chosen as being representative of common driving conditions. At each speed, load, and trap temperature point, experiments were conducted with varying trapping and purging durations, the lean and rich air-fuel ratios being maintained at 19.5:1 and 11:1. The LNT brick temperature was maintained at the desired value by wrapping insulation tape around the pipe between the TWC and the LNT. The model was parameterized at one operating point, and validated against the experimental results at other temperatures and operating points. Figure 5 compares the model prediction with the dynamometer results and there is good agreement at the four trap temperatures ranging from 300 ^{o}C to 450 ^{o}C.

Figure 6 is a comparison of the model prediction and the dynamometer results for an experiment with filling and purging durations of 47.5 and 3 seconds respectively. Although there are some differences in the instantaneous values between the model and the experiments, the integrated values of the trap capacity are in good agreement. The bottom plot in Figure 6 represents the simulated LNT state. The figure indicates that for the selected storage and purge durations, about 60% of the trap's capacity is filled up with incoming NO_x. If the trap filling duration were increased, this would result in lower trap efficiencies; this is evident from Figure 4 where the trapping possibility function falls off rapidly when ρ/C is larger than 0.6.

4. Conclusions/Recommendations

A control oriented model of an LNT has been developed and the model predictions are in good agreement with test data from a 1.8L Zetec engine. Trap temperature, purging frequency and duration are important factors which impact the LNT efficiency. The model because of its simple structure, is suitable for LNT strategy design and fuel economy and emission optimization studies. It is recommended that the TWC and LNT be considered as an integrated after-treatment system for lean burn and DI engine systems. This would facilitate studies to maximize the performance of both devices with a proper choice of catalyst formulation and oxygen storage capacities in the LNT and TWC.

Acknowledgment

The work of J.W. Grizzle was supported in part by an NSF GOALI grant, ECS-9631237, and in part by matching funds from Ford Motor Company.

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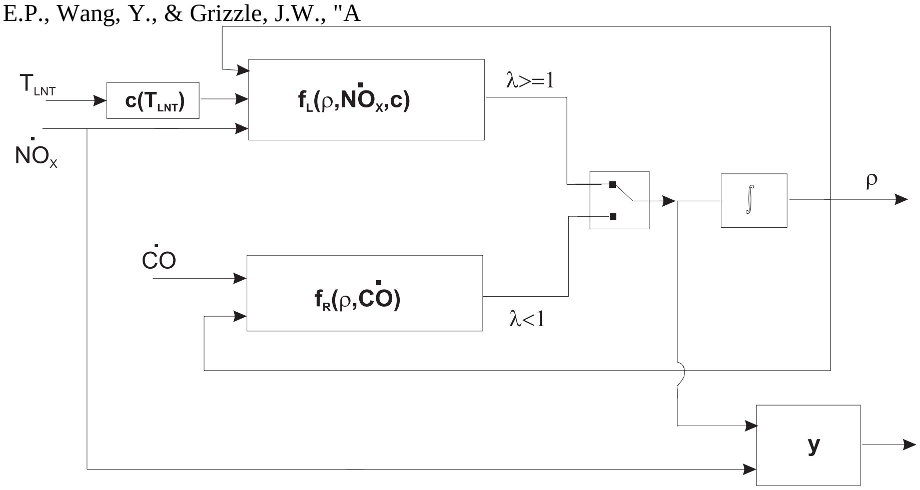

Figure 1: Structure of the LNT Model

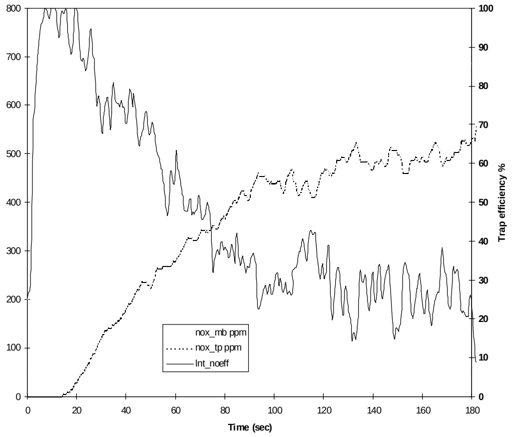

Figure 2: LNT trapping characteristics

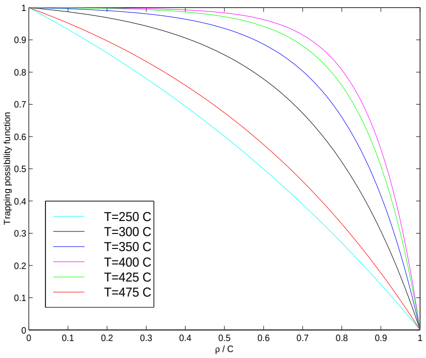

Figure 4: Trapping possibility as a function of LNT state

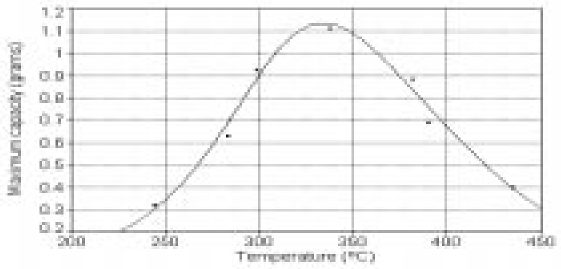

Figure 3: Maximum capacity of the LNT

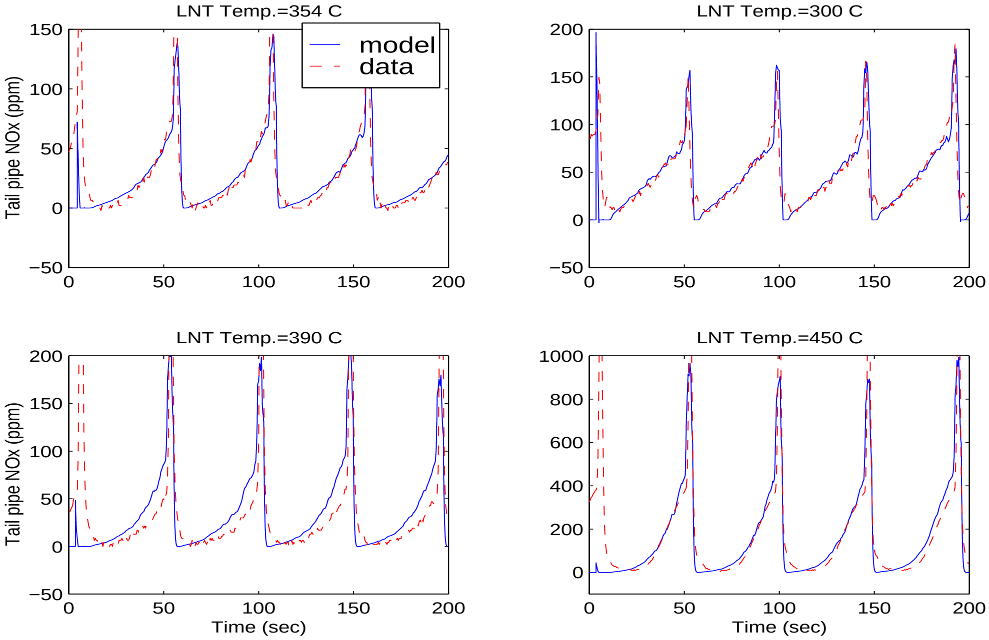

Figure 5: Tail pipe NO_x validation results for different trap temperatures

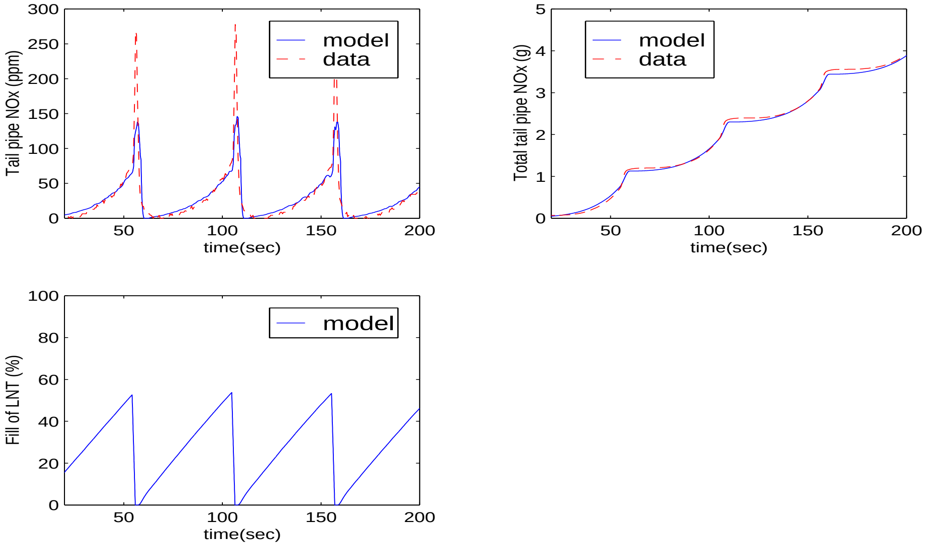

Figure 6: Simulation results