

Optimization of Purge Air-to-Fuel Ratio Profiles for Enhanced Lean NOx Trap Control

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Abstract—Lean NOx Traps (LNT), as a critical aftertreatment device for lean burn engines, require active control to manage its storage and purge cycles. In this paper, optimal air-to-fuel ratio profiles are pursued in LNT operation cycles with focus on the purge phase in which the stored NOx is neutralized by a rich air-to-fuel ratio mixture. It is shown that allowing the AFR to vary during the purge phase can provide a substantial leverage in improving LNT performance, in comparison to the fixed AFR purge strategy. Our findings also demonstrate a fundamental trade-off between the NOx and HC emissions and the fuel consumption with different purge AFR profiles.

I. INTRODUCTION

FUEL economy and exhaust emissions are the two primary considerations in automobile engine control design. More often than not, the objectives of optimizing fuel economy and meeting the stringent emission regulations are conflict to each other. Trade-off has to be made to balance the competing requirements. The advent of new engine and aftertreatment technologies has made more options available to achieve low emissions and high fuel economy, in terms of both hardware and control strategies.

Lean burn technology for gasoline engines has emerged as a viable technology to improve fuel economy and reduce CO₂ emissions [4,7]. Compared to the conventional port fuel injection (PFI) engine, the gasoline lean burn engine represents a new set of challenges to the engine control community. Exhaust NOx emission control has been recognized as one of the primary hurdles for the lean burn engine technology. Since the conventional three-way catalyst (TWC) system is no longer effective in reducing NOx pollutants under lean conditions, a special catalyst known as lean NOx trap (LNT) is utilized for NOx treatment [1,5,6,11]. During the lean operation, NOx in the feedgas is stored in the LNT. When its stored NOx reaches a certain level, the LNT must be purged to recover the storage capacity and efficiency. This is accomplished by

switching to rich operation for a short period of time. The NOx released from the LNT during this period are converted into non-polluting nitrogen by the rich air/fuel mixture [1,6,11,14].

Properly managing the storage and purge cycles is critical for achieving the fuel economy and NOx emission control targets of the lean burn gasoline engine. LNT purge control, with the objectives of optimizing fuel economy while satisfying emission constraints, has been addressed by several researchers [8,9,12]. Dynamic programming [2,14] has been effectively used to deal with the numerical optimization problem for this dynamic system. Other control design aspects, such as dealing with aging and sulfur poisoning, have also been addressed using adaptive control techniques [15].

Most of the results in open literature [8,9,12] on LNT control have focused on the trade-off between the fuel economy and NOx emission. However, recent laboratory data and vehicle work [1,11] suggest that HC also represents a great, if not greater, challenge and deserves more attention. Especially during the LNT purge phase when rich engine operation is required to deliver the needed reductants (primarily the CO) for NOx conversion, the feedgas HC, as the by-products of the rich operation, could cause tailpipe emission problems if it is not properly treated by the emission control system. Since the conventional aftertreatment system using the three-way catalyst is not effective in reducing HC during the rich operation, the issue of HC emissions must be resolved by improving LNT purge control strategies to minimize feedgas HC emissions.

In this paper, we investigate LNT purge control strategies that optimize fuel economy with active constraints on both HC and NOx emissions. The variables defined by LNT control strategies usually include the air-to-fuel ratio, the storage time, purge threshold, and purge duration. In this paper, we concentrate on the impact of AFR control on LNT performance. During the storage phase when the engine is operating under the lean condition, the AFR is selected to (i) meet the driver's demand, (ii) maximize the fuel economy benefits, and (iii) satisfy other constraints, such as the lean burn limit. These requirements often dictate the set-point selection, and the optimal choice for the AFR usually is rather straightforward because of the over-

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constrained conditions. During the purge phase, however, the AFR has the greatest impact on both the emissions and fuel economy. No obvious choice exists that will maximize the fuel economy benefits with minimum negative emission impact. Therefore, our investigation of AFR control for the LNT will be focused on the purge phase.

Most purge control strategies select a fixed air-to-fuel ratio, presumably for its implementation simplicity. However, the following observations imply potential benefits of purge AFR trajectory optimization (which will also be referred to as AFR profiling in this paper):

- Oxygen and NO_x storage capacities co-exist in most production LNT. At the initial purge phase, the released NO_x and the released oxygen will both compete for reductant. This large demand for the reductant, if not been met by richer AFR, will lead to deficit in neutralizing agents for the NO_x and therefore cause large NO_x spikes during this time interval. This phenomenon has been observed both in vehicle data and model simulations [11].
- The oxygen storage capacity for an LNT is often substantially less than the NO_x storage capacity. As a result, the stored oxygen is depleted quickly. The demand for the reductant is then reduced. If the constant rich AFR mixture is supplied after the stored oxygen is depleted, the over-supply of the reductant will lead to excessive HC emission in the tailpipe.
- The release rate of NO_x decreases substantially (in some model structures, it decreases exponentially) during purge phase, rendering a requirement of gradually reduced feedgas reductants.

These observations suggest that an AFR profile that starts with a richer AFR and gradually changes towards the stoichiometric value can potentially provide a better purge performance. This seemingly rather intuitive strategy however will complicate the LNT control strategy calibration process, if no formal process can be used to tune the parameters and provide design guidelines. What remains unclear is how this AFR profiling can be optimally selected, and how significant the benefits of this trajectory optimization are, in comparison to fixed purge AFRs and in terms of fuel economy, NO_x and HC emissions. This paper is focused on answering these questions.

In this paper, dynamic programming is utilized to search for optimal purge AFR profiles. Two types of optimization performance are employed: (1) The trade-off among fuel economy, NO_x emission, and HC emission is explicitly contained in the performance index with adjustable weightings; (2) A fuel economy performance index with emission constraints from HC and NO_x. The first approach is more suitable for understanding the fundamental trade-off among fuel economy and emissions; while the second index can be used to derive a strategy under a given NO_x and HC

emission limits, such as the current federal requirements. The findings of this analysis will show that AFR trajectory optimization can indeed provide a substantial improvement on the fundamental trade-off. For example, for the specific lean-burn engine and LNT configuration used in our evaluation, a reduction of over 30% HC emission is observed while maintaining the same fuel economy and NO_x emission. These results indicate that despite the higher complexity in purge strategy developments, AFR trajectory optimization should be an important strategy consideration in LNT control.

The paper is organized as follows: The problem of LNT control will first be described in Section II. The motivating issues for the problems addressed in this paper will be further detailed. The LNT models used in this study will be briefly summarized. Section III presents the dynamic programming approach for purge AFR profiling. The key findings of the paper are described in Section IV. Section V provides some concluding remarks on the insights that might be derived from our results and potential utility of them in LNT control design and calibration.

II. LEAN NO_x TRAP (LNT) MODELS

A typical aftertreatment system for a lean burn engine with a commonly used sensor configuration is shown in Figure 1. It consists of a conventional three-way catalyst (TWC) (usually in a closely-coupled location with the engine for optimal cold start performance) and an underbody special TWC or LNT, with oxygen and temperature sensors in various locations.

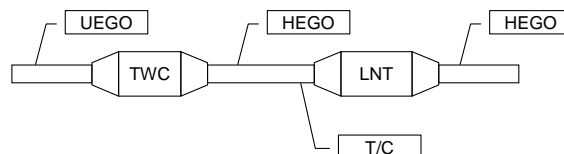


Figure 1. After-treatment systems

The key chemical processes in an LNT operation can be briefly described as follows. When the exhaust gas is leaner than stoichiometric, NO_x is oxidized to NO₂ in the gas phase and the resulting NO₂ is then adsorbed on storage sites as barium nitrate. This process is termed as *NO_x storage*. As the NO_x stored in the LNT increases, the storage efficiency drops and the trap needs to be purged to regenerate its capacity once the stored NO_x reaches a certain level. The purge can be accomplished by providing a rich exhaust environment to the trap. The nitrate, Ba(NO₃)₂ for the LNT under consideration, becomes thermodynamically unstable under stoichiometric or rich exhaust conditions and releases NO₂ and BaO. BaO then becomes BaCO₃, thereby regenerating the storage sites.

This step is referred to as *NOx release and trap regeneration*. The released NO₂ is converted to N₂ by the reductants, such as CO, H₂ and HC over the precious metal sites (platinum for example). This process, consisting of NOx release, trap regeneration, and NOx conversion is termed as *LNT purge*.

A control-oriented model which characterizes the storage and purge process at the phenomenological level is described below. The model is derived from the early work described in [10,16] and extended with our experiments and data analysis in [15].

A. NOx Storage

By mass conservation, assuming low and negligible NOx conversion efficiency during lean operation, the NOx accumulated in the LNT during the storage phase is

$$\dot{m}_{NOx,stored} = \dot{m}_{NOx,in} - \dot{m}_{NOx,out} \quad (1)$$

where the rates are the derivatives of the following variables: $\dot{m}_{NOx,stored}$ is the NOx storage rate [g/sec], $\dot{m}_{NOx,in}$ is the NOx flow rate into the LNT [g/sec], and $\dot{m}_{NOx,out}$ is the NOx flow rate leaving the LNT [g/sec]. The storage instantaneous efficiency, defined as

$$\eta_s = (\dot{m}_{NOx,in} - \dot{m}_{NOx,out}) / \dot{m}_{NOx,in} \quad (2)$$

provides a measurement of the effectiveness of the trap in treating NOx in the storage phase. Also, by expressing

$$m_{NOx,stored} = C_{LNT} \cdot x \quad (3)$$

where C_{LNT} is LNT NOx storage capacity [g] and x is the fraction of utilized LNT capacity (or the fraction of occupied storage sites), we have

$$\dot{x} = -\frac{1}{C_{LNT}} \frac{dC_{LNT}}{dt} x + \frac{1}{C_{LNT}} \eta_s \dot{m}_{NOx,in} \quad (4)$$

The storage capacity C_{LNT} can be modeled as a Gaussian function of the temperature T that has a center at T_m

$$C_{LNT} = C_m \exp \left[-\left(\frac{T - T_m}{T_s} \right)^2 \right] \quad (5)$$

where T_m , T_s , C_m are parameters characterizing a specific LNT.

The instantaneous storage efficiency η_s changes as a function of the LNT state x and the trap temperature, and can be described by

$$\eta_s = \frac{e^{-\alpha x} - e^{-\alpha}}{1 - e^{-\alpha}} \quad (6)$$

where α is a parameter that incorporates the effects of the trap temperature on storage efficiency.

B. NOx Purge

During the purge phase, the stored NOx is released from the storage sites. By mass conservation we have:

$$\dot{m}_{NOx,stored} = -\dot{m}_{NOx,released} \quad \text{where } \dot{m}_{NOx,released} \text{ is the NOx release}$$

rate. The release rate, $\dot{m}_{NOx,released}$, depends on how much NOx is stored in the trap at the moment considered and the trap capacity. For the work described in this paper, the normalized release rate, defined as:

$$k_r = \frac{\dot{m}_{nox,released}}{C_{LNT}}$$

is identified by the following function:

$$k_r = \frac{1 - e^{-\beta x}}{1 - e^{-x}} (1 - x_{oxy}) f_r(\lambda_{in}, MAF, T) \quad (7)$$

where x_{oxy} is the oxygen storage level in the LNT, λ_{in} is the relative air-to-fuel ratio at the LNT entrance, MAF is the mass air flow rate, and β is a parameter depending on the physical properties of the catalyst under consideration, such as its formulation, geometry, etc. The second factor on the right hand-side ($1 - x_{oxy}$) captures the interactions between NOx and oxygen storage mechanisms.

The last step in trap regeneration is to convert the released NOx into non-pollutant species, primarily by the reductants, such as HC and CO. The efficiency of this process, defined as

$$\eta_c = (\dot{m}_{NOx,r} - \dot{m}_{NOx,out}) / \dot{m}_{NOx,r} \quad (8)$$

is modeled by equation

$$\eta_c = \frac{e^{\gamma x} - e^{\gamma}}{1 - e^{\gamma}} f_c(\lambda_{in}, MAF, T) \quad (9)$$

where γ is a parameter and $f_c(\lambda_{in}, MAF, T)$ accounts for the effects of the air-to-fuel ratio, temperature and mass flow rate (or space velocity) of the exhaust gas. By using the indication function $I_{\{A\}}$ ($I_{\{A\}}=1$ if A is satisfied and $I_{\{A\}}=0$ otherwise), the dynamics of the LNT can be described by

$$\dot{x} = -\frac{1}{C_{LNT}} \frac{dC_{LNT}}{dt} x + I_{\{\lambda_{in}>1\}} \eta_s \frac{\dot{m}_{NOx,in}}{C_{LNT}} - I_{\{\lambda_{in}\leq 1\}} \frac{\dot{m}_{NOx,r}}{C_{LNT}} \quad (10)$$

The NOx flow rate leaving the LNT, is

$$\dot{m}_{NOx,out} = I_{\{\lambda_{in}>1\}} (1 - \eta_s) \dot{m}_{NOx,in} + I_{\{\lambda_{in}\leq 1\}} (1 - \eta_c) \dot{m}_{NOx,r} \quad (11)$$

C. Oxygen Storage and Purge

The oxygen storage model used here is adopted from [3]. The dynamics of oxygen storage are described, in either lean (storage) or rich (release) operations, as

$$\dot{x}_{oxy} = \begin{cases} 0.21 \alpha_L \rho_L(x_{oxy}) MAF (1 - \lambda_{in}^{-1}) C_{oxy}^{-1}, & \lambda_{in} \geq 1 \\ 0.21 \alpha_R \rho_R(x_{oxy}) MAF (1 - \lambda_{in}^{-1}) C_{oxy}^{-1}, & \lambda_{in} < 1 \end{cases} \quad (12)$$

where $x_{oxy} = m_{oxy} / C_{oxy}$ (m_{oxy} being the total oxygen stored) is the relative amount of stored oxygen with respect to the available oxygen storage capacity C_{oxy} . Here, α_L and α_R are constants and ρ_L and ρ_R are nonlinear functions indicating the relative storage and release rates, respectively as shown in Figure 2.

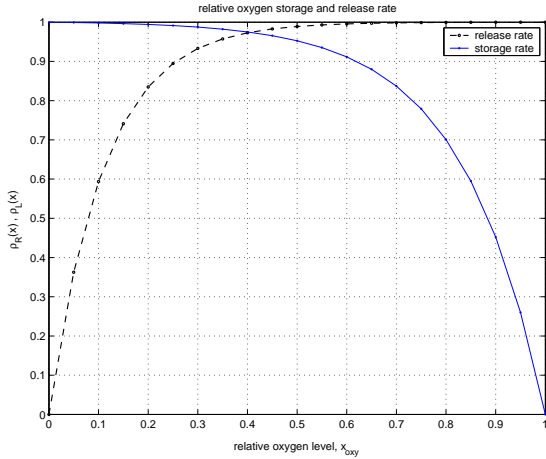


Figure 2. Oxygen storage and release rates

III. AIR-TO-FUEL RATIO TRAJECTORY OPTIMIZATION

A. Fuel Economy and Tailpipe Emissions

To attain the best fuel economy, a lean burn engine must operate in the lean mode as long as possible, since that is where the fuel saving benefits are achieved. However, the fuel economy cannot be achieved at the expense of higher NOx and/or HC emissions. The trade-off between fuel economy and NOx/HC emissions is determined by the LNT purge strategy, including the conditions under which the purge will start and end; and the purge air-fuel ratio.

AFR is the most significant variable influencing system performance during the purge operation, since it determines the oxygen deficiency level (which affects the release rate and therefore the purge duration) and the amount of available reductants for converting the released NOx. With a near stoichiometric exhaust gas, the purge duration will be extended over a long period and the NOx conversion efficiency will be very low. As the AFR becomes richer, the purge will end faster and NOx conversion efficiency will increase. Further enriching AFR beyond a certain point, however, does little to improve the performance in terms of the purge duration and NOx conversion efficiency. Rather it will incur HC breakthrough.

The challenge is to select the proper AFR that will minimize the fuel consumption while meeting the emission requirements. To make our LNT purge control problems amenable to existing numerical optimization tools, we first need to define proper performance indices.

B. Optimization Indices

There are two feasible approaches in defining optimization performance indices for AFR profiling during a purge operation.

1) Weighted Optimization

In this approach, the fundamental trade-off among fuel economy, NOx emission and HC emission is formulated in

a weighted performance index

$$J(\lambda, t_f) = \int_0^{t_f} (w_1 h_{fuel}(\lambda) + w_2 h_{NOx}(\lambda) + w_3 h_{HC}(\lambda)) dt \quad (13)$$

where the normalized AFR $\lambda(t)$ is optimized and the purge termination time t_f is derived when the stored NOx reaches a certain lower threshold or when the tailpipe HEGO sensor switches. By choosing different weightings, one can adjust relative penalties on fuel economy and emissions. This allows us to study fundamental relations between achievable fuel economy and corresponding emission costs, and to select appropriate purge operating conditions.

2) Constrained Optimization

One may elect to define a constrained optimization problem with the cost function and constraints defined as:

$$J(\lambda, t_f) = \int_0^{t_f} h_{fuel}(\lambda) dt; \quad (14)$$

$$s.t. \int_0^{t_f} h_{NOx}(\lambda) dt \leq d_{NOx}; \int_0^{t_f} h_{HC}(\lambda) dt \leq d_{HC}$$

Typically, the NOx and HC limits are defined based on the government emission requirements.

C. Dynamic Programming

After selecting a performance index, the optimization process is numerically performed by dynamic programming [9]. In this method, the purge phase is divided into uniformly spaced time intervals. Then, the normalized AFR, the LNT NOx amount, oxygen level, are all quantized into limited precisions. Then, the finite-state discrete-time constrained dynamic programming is performed to find optimal AFR profiles and optimal NOx and oxygen trajectories. Since the generic structure of this dynamic programming procedure is well known, we will not indulge in further details.

IV. RESULTS AND DISCUSSIONS

To evaluate the fundamental trade-off among competing performance requirements in this problem, we conducted a set of simulation evaluations using the lean-burn engine and LNT configuration reported in [15]. The weighted optimization is employed. By repeated search of suitable weightings, we obtained purge operating conditions under which NOx and HC emissions are closely clustered around their limits. These conditions are of essential practical interests since these are practical boundaries for LNT calibration. For comparison with constant purge AFR strategies, we also simulated achievable fuel economy, NOx and HC emissions under a set of constant purge AFR values. A typical set of simulation results corresponding to the optimal solution with different weights is obtained using dynamic programming, and is illustrated in Figures 3, 4.

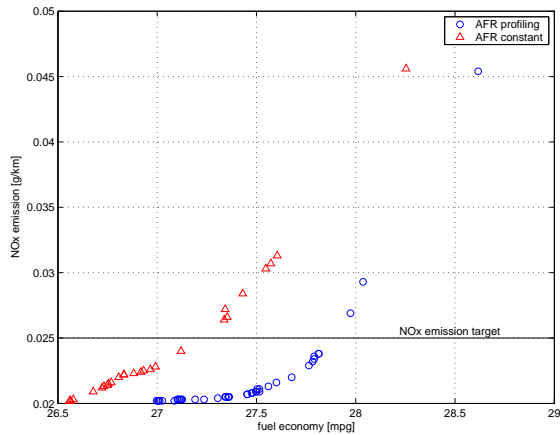


Figure 3. Trade-off between fuel economy and NOx emission

The essential relations between achievable fuel economy and corresponding penalty on NOx emissions are depicted in Figure 3. The NOx emission target is set at 25mg/km, corresponding to the Europe Stage V standard with an engineering margin. By comparing the AFR profiling with constant AFR purge, it is observed that for the comparable NOx emission level, appreciable fuel economy improvement can be achieved with AFR trajectory optimization. A typical optimal AFR profile is shown in Figure 5. The profile suggests that when the AFR is allowed to vary during the purge phase, it tends to go richer initially. This rich AFR mixture at the initial purge phase will play a dual role: (1) It substantially reduces the NOx spike; and (2) it speeds up the purge process. As a result, the purge time will be shortened and fuel economy improved. As shown in the second plot of Figure 5, the purge time can be shortened by approximately 1.5second. This is a substantial improvement considering that the total purge time is about 10 second.

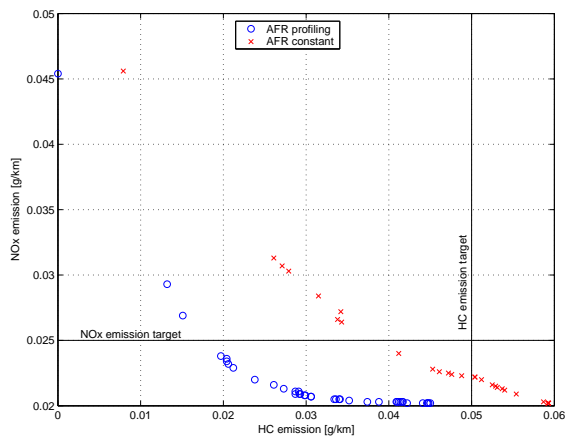


Figure 4 Trade-off between HC and NOx emissions

HC emission reduction is even more dramatic with the

AFR profiling when compared to the fixed AFR case. This is demonstrated by Figure 4. With the same NOx emission level, the AFR trajectory optimization can reduce the HC emission almost by 50%. It should be pointed out this number is not obtained over the standardized drive cycle, but is evaluated over the repeated store/purge cycle, for which the HC emission is almost negligible during the storage phase. As the secondary reductant (the primary reductant is CO), the HC in the exhaust stream usually does not get sufficiently converted during the purge phase except at the initial stage, when the stored oxygen is purged out of the system. With AFR trajectory optimization, the richer mixture will lead to higher feedgas HC initially. However, during this phase, the stored oxygen will be purged out of the system and react with the HC. In the second half, when the oxygen in the system has been depleted and the HC can no longer be efficiently converted, the leaner AFR (compared to the constant AFR case) is used and the feedgas HC is reduced. We can see from fourth plot of Figure 5 that even though the AFR is further enriched at the initial stage compared to the constant AFR purge, the tailpipe HC is only increased slightly. But for the later stage, when the AFR gets leaner, the tailpipe HC emission is much lower compared to the constant AFR case. Therefore, the total HC emission is reduced.

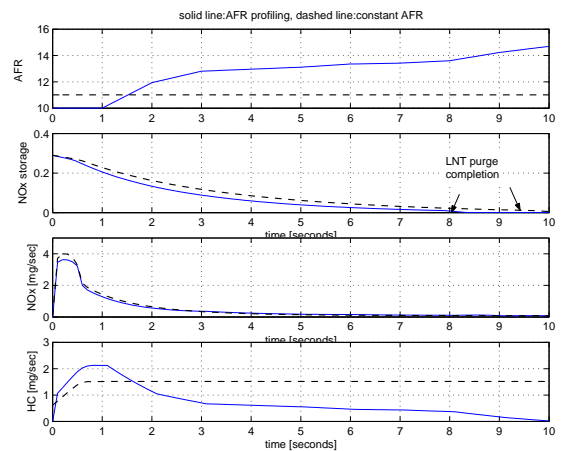


Figure 5. Comparison of the trajectories with (solid lines) and without (dashed lines) AFR profiling: optimal AFR profiles , NOx in the LNT, tailpipe NOx and HC responses

Figures 6 and 7 demonstrate further details pertinent to the above analysis. Given the NOx emission target of 25mg/km and HC emission target of 50mg/km, all feasible trajectories with AFR trajectory optimization are shown in Figure 6, and the optimal solution with the best fuel economy is the point on the right of plot. Without AFR trajectory optimization, there are fewer feasible points that can meet both the NOx and HC emission targets, as shown in Figure 7.

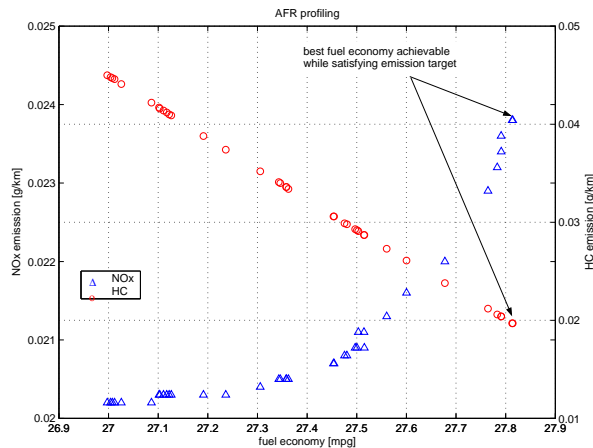


Figure 6. Trade-off among Fuel economy, HC and NOx emissions with purge AFR trajectory optimization

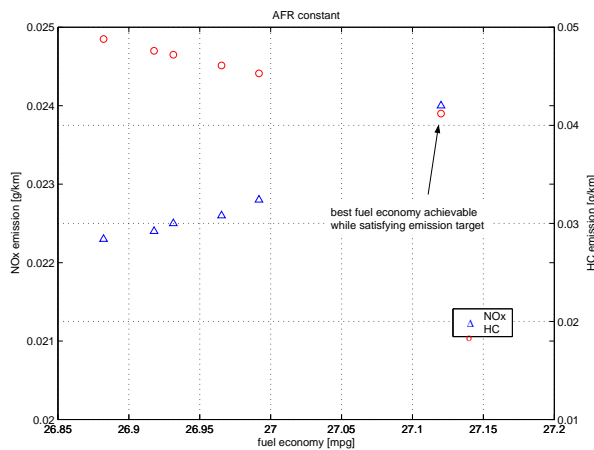


Figure 7. Trade-off among Fuel economy, HC and NOx emissions with constant purge AFR

V. CONCLUSIONS

Optimal purge AFR profiling is shown to be of significant potential in improving trade-off between fuel economy and emissions. In particular, it is revealed that AFR trajectory optimization can provide substantial leverage in reducing both HC and NOx emissions. While this understanding is obtained by rigorous dynamic programming in this paper, for practical utility of this approach, it is desirable to seek simplified calibration procedures that will achieve near-optimal AFR profiles, but carry much lower computational complexity. Furthermore, to realize this potential benefit, it is necessary to incorporate purge AFR profiling into overall LNT control strategies that involve many other LNT control variables and constraints, such as purge thresholds, prediction of LNT internal states, estimation of feedgas contents and flow rates, sensor selections and locations, as well as efficient algorithms.

This algorithm of AFR trajectory optimization also requires a well-engineered off-stoichiometric AFR control. These are worthwhile research directions towards enhanced LNT performance.

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