Design, Modeling, and Validation of a Flame Reformer for LNT External Bypass Regeneration

Shawn Midlam-Mohler
Ohio State University
Center for Automotive Research

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Presentation Overview

• Brief Overview of LNT Systems
• Overview of Work-to-Date
  – Goals of Bypass Regeneration System
  – Bypass System Configuration Options
  – Regeneration Options – What is a Flame Reformer?
  – Exotherm Analysis
  – Control Development
  – Experimental Validation of Control
  – Vehicle Simulation Studies of System
• Conclusions and Possible Next Steps

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Conventional LNT Regeneration

- Engine management provides rich conditions for NO$_x$ regeneration and de-SO$_2$
- A Pre-catalyst upstream of LNT is typically required for oxygen removal during rich phase because of rich combustion inefficiencies
- DPF position is variable, here it is shown at the rear to promote rapid light-off of LNT system
- Engine-based systems are capable of achieving Tier 2, Bin 5 emissions in lab tests
Bypass Regeneration Systems

- Allow engine runs continuously in lean mode
- Regeneration occurs on the catalyst with most or all of exhaust diverted from the catalyst
- Only locally rich conditions are necessary
- Reductant delivery achieved with an external device
  - Diesel injector or a fuel reformer
- In order to justify higher system cost, a bypass system must provide increased benefit or reduced cost elsewhere.

![Bypass Regeneration Systems Diagram]
Sources of Bypass System
Fuel Economy Penalty

It is worth looking at where fuel goes in a bypass regeneration system:

**Unwanted Effects:**
1. Reductant production losses: a function of the reductant generation technique (straight diesel has no loss here)
2. Reductant used for gaseous oxygen reduction: best case is to divert 100% of exhaust from catalyst during regeneration
3. Reductant used for stored oxygen reduction: a function of catalyst formulation; typically >50% of fuel goes to oxygen reduction
4. Reductant slip: through proper control, this is minimized

**Desired Effect:**
5. Reductant used for reduction of stored NO$_x$; the only desired outcome

To minimize fuel penalty, the system (hardware and control) must be optimized to minimize 1 through 4 and maximize 5.
System Configurations

Single-Catalyst Bypass (SCB)

Dual-Catalyst Asymmetric (DCA)

Dual-Catalyst Symmetric (DCS)

Simulation is for mid-size SUV, 3 to 6 L of LNT, 5 to 20 sec regeneration time, city cycle shown.

System Configuration Simulation Study: varying catalyst size, regeneration threshold, required regeneration time.

US06 is not shown, but it kills the performance of the SCB system because of high average NOx.
Best Cases from Batch Simulations

- If one picks out the best performers, the NO$_x$ conversion-fuel penalty trade-off is roughly the same
- DCS system was selected for this work
  - Most insensitive to catalyst volume (cost)
  - Most insensitive to regeneration time
  - Slight edge in FE penalty vs. NOx conversion

Upper = FHDS, Lower = UDDS
Reductant Flow Rate Requirements

- It is possible to measure experimentally the maximum rate of reductant consumption of a particular LNT for specified conditions.
- It makes practical sense for the reductant delivery system to be capable of operating near this level, so that regenerations occur as rapidly as possible
  - Fast regenerations mean that the catalyst is taken offline for a shorter period of time.
  - This allows both catalysts to be operating in parallel for the majority of the time
  - Which allows for the reduction of the required LNT system volume (cost)
- Bypass regeneration systems that operate at a 50% duty cycle are nearly double the size required of a system that operates at a 95% duty cycle

Since a bypass regeneration system already has a cost disadvantage, it is impractical to have any extra catalyst volume than absolutely necessary.
Current Reductant Delivery Systems

1. **Exhaust Fuel Injection**: Poor performance at low temperatures
2. **Catalytic Reformers**: High yield of $H_2$, require a catalyst, generally have marginal dynamic response
3. **Plasma Reformers**: High yield of $H_2$ and CO, require power electronics and sometimes a catalyst, typically have marginal dynamic response

The last two options are viable, however, they are relatively complex and an alternative solution was sought.

Two Key Points Regarding Alternatives:

1. An LNT is **not** a fuel cell: It will gladly accept CO and light chain HC; pristine syngas is overkill.
2. Reductant production efficiency is **not** a major factor due to low duty cycle of operation and low fuel usage.
Flame Reforming for LNT Regeneration

- The alternative method developed is referred to as “Flame Reforming”
- The goal of this method is to overcome deficiencies in other LNT management methods:
  - Marginal dynamic response
  - Marginal warm-up characteristics
  - High system cost
  - High system complexity
  - High scalability to higher flow rates

- Flame Reforming Concept:
  - Uses a rich, premixed Diesel flame to generate carbon monoxide, hydrogen, and lighter chain hydrocarbons
  - A potential low-cost, low-tech competitor to more complicated reformer methods

The concept replaces a high-cost, high complexity solution with a low-cost technology with a proven track record of several thousand years: fire
Flame Reformer Prototype

- 2.5” OD, 12” long, low-pressure fuel inlet, low-pressure air inlet
- Ignition and flame stabilization is accomplished with a Diesel glowplug
- Has sub 1-second ignition time and fast dynamic response
- Can “process” up to 0.5 g/s of diesel fuel
Prototype FR Output –
Data from Multiple Fuel and Air Inputs

- Output roughly agrees with theory; saturation of CO and H₂ as THC is formed
- 9% CO and 4% H₂ are produced
- Overall, satisfactory results for a first-generation prototype
- PM emissions were not measured, but expected to be present but manageable
Flame Reformer Efficiency

- When at high temperatures, LNTs can utilize Flame Reformer HC’s for NO\textsubscript{x} reduction.

- Above 350 deg. C, the catalyst tested uses over 90% of the Flame Reformer HC’s.

**Formula:**

\[
\eta_{FR} = \frac{m_{CO, out, adj} \cdot Q_{HHV, CO} + m_{H_2, out} \cdot Q_{HHV, H_2} + m_{HC, usable, out} \cdot Q_{HHV, HC}}{m_{fuel, in} \cdot Q_{HHV, fuel}}
\]
Summary of Flame Reformer Performance

- Prototype is capable of regenerating 2.5L LNT in <10 seconds
- Capable of regenerating down to 200°C
- Requires < 2 grams of fuel per regeneration
- < 0.05 grams of THC slip per regeneration

- System simulations for modern engine yield < 2% fuel economy penalty for Bin 5 emissions for varying levels of sulfur poisoning and catalyst size.

- Satisfactory results were obtained for experimental testing from 200°C to 450°C
Benefits of Flame Reforming

- **Low hardware Costs**: no catalyst required, no power electronics
- **High Durability**: no impact from sulfur, no danger of coking, minimal service requirements
- **Fast Dynamic Response**: rapid startup, excellent dynamic response
- **Acceptable Efficiency**: Not as good as more sophisticated methods (40% typical versus 60% to 80% for reformers.); not a major drawback
- **Excellent Scalability**: By shear simplicity, scaling the device is guaranteed
- **Synergies with other systems**:
  - **Sulfur Regeneration**: SO$_2$ regeneration is difficult with engine-based methods; the flame reformer can provide a low continuous flow of hydrogen rich gas
  - **Rapid Catalyst Light-Off**: The prototype flame reformer can function as a 40 kW heater within seconds of engine-start
  - **DPF Regeneration**: Depending on the configuration, it is possible to use the flame reformer for DPF regeneration rather than using the engine
Control and Diagnostics of Bypass Systems

• Even the best system will have poor results if the control algorithm is lacking
• LNTs are a particularly tricky plant to control, since they are highly non-linear and have constantly changing parameters due to aging and sulfur poisoning

• To address these issues, the following tasks were undertaken:
  – Development of a novel measurement technique for LNT analysis and control
  – Development of control-oriented models for the entire LNT system
  – Use of the above models to design and validate adaptive control and closed-loop controls
  – Demonstrating the above through a combination of dyno tests and system simulations

The end result is a model-based, adaptive NO\textsubscript{x} management algorithm that performs high-level regeneration scheduling as well as low level control of actuators.
Exotherm Analysis

• During the regeneration event, it is possible to correlate the observed temperature rise to the various chemical reactions occurring in the catalyst.

• This correlation exists only in the low-flow rate, bypass regeneration system.

• This allows time and spatially resolved measurements of reductant usage, NO\textsubscript{x} storage, and oxygen storage in the catalyst.

• Provides useful information for:
  – Model data collection
  – Feedback control
  – Sulfur poisoning detection
  – Catalyst condition monitoring

• Offers a low cost way of seeing the reactions inside the catalyst for research.

• If viable for production, could reduce the need for expensive gas sensors.
Correlation to Mass of NO\textsubscript{x} Stored

• Total mass of NO\textsubscript{x} stored correlates very well to the processed temperature measurements.
• This method essentially provides a “measurement” of the mass of NO\textsubscript{x} and O\textsubscript{2} regenerated from the catalyst.
Sulfur Poisoning Detection with Exotherms

- The exotherms detect the distribution of $\text{NO}_x$ in the catalyst
- Sulfur poisoning manifests itself as a change in distribution
- Poisoning happens from the front of the catalyst back
  - Depression of front exotherms
  - Increase in rear exotherms
Adaptive LNT Storage Estimator

- The error between the measured NO\textsubscript{x} storage and the estimated NO\textsubscript{x} storage is used to drive changes in the catalyst model.
- A gain matrix produces an incremental change in parameters which is added into the previous parameter values.
- The adapted parameters are low pass filtered for noise rejection.

An adaptive model is critical for a model-based control, otherwise the ECU “thinks” that the catalyst is better shape than it really is. This leads to increased NO\textsubscript{x} emissions.
Experimental Results for LNT Model Adaptation

- Offline experiment conducted using SO₂ poisoning data
- Only the gains and filter coefficient were tuned
- Adaptive estimator tracks the efficiency decrease with acceptable error
Optimal Regeneration Control

- Based on the control-oriented modeling which was supported by exotherm analysis, it is possible to develop an optimal closed-loop regeneration control.
- Optimal is defined as: minimum regeneration time, minimum reductant slip, and maximum NO$_x$ reduction
- For the purpose of this work, a temperature sensor was used as the feedback sensor, however, the method could be extended for use of a UEGO sensor.
- The control is formulated from a linearized version of the control-oriented model:
  - The linearized version has acceptable performance on the real plant
  - For slightly better performance, a gain-scheduled version could be used

For optimal regeneration, the reductant flow rate must be tapered to zero as the regeneration proceeds.

This requires a regeneration actuator with good dynamic response.
Regeneration Scheduling

- It can be shown that system efficiency is greater if the two traps are kept out of phase for regenerations.
- An algorithm was developed which accomplishes the above, while minimizing the frequency of regenerations.
- The algorithm utilizes the adaptive storage model to compensate for plant variation.

With the adaptive control, the system will automatically compensate for high levels of sulfur poisoning and maintains the desired NO$_x$ conversion.
System Simulation for Performance and Control

• The last phase of the work involved evaluating the potential of the control methods and calibrations in simulation
• The sensitivity of the algorithms to plant changes and various faults were evaluated, including:
  – SO$_2$ poisoning
  – Estimation errors
• Vehicle simulations were conducted for a passenger car with a modern diesel engine

• There is not sufficient time to present these results here
• For additional info, contact me and I can provide some publications

• Overall, simulations point to Bin 5 compliance with < 2% fuel economy penalty with a wide range of catalyst sizes and sulfur poisoning levels.
Can the Bypass Regeneration System Compete with Engine-Based Systems?

- **Engine Calibration Effort:**
  - Engine-based LNTs require a normal engine cal, a catalyst warm-up cal (for Bin 5), a NO\textsubscript{x} regeneration cal, a sulfur regeneration cal, and a DPF regeneration cal.
  - Each vehicle platform (i.e. engine/transmission/chassis) will require some additional calibration; possibly extensive recalibration.
  - A single bypass regeneration system and calibration could be suitable for a range of platforms since it is engine independent.

- **Fuel Economy Benefit:**
  - A properly designed and controlled bypass regeneration system will have improved fuel economy over engine-based methods.
Can the Bypass Regeneration System Compete with Engine-Based Systems?

• **Happier Catalysts:**
  – Because of the more refined regeneration actuator, it seems reasonable that bypass regenerations will not age the catalyst as rapidly as engine-based systems
  – This allows for reductions in catalyst volume and cost

• **System Synergies:**
  – DPF regeneration, De-SO$_2$, and rapid catalyst light-off are built in

• **Exotherm Analysis:**
  – If exotherm analysis can be applied, costly gas sensors can be reduced or eliminated

Although it isn’t a sure bet, there seems to be some chance of overcoming the additional hardware cost of the bypass regeneration system.
Future Work

The following are suggestions for future work:

– Extension of closed-loop control techniques to the use of the more commonly used UEGO and NO\textsubscript{x} sensors
– Development and demonstration of de-SO\textsubscript{2} algorithm using the Flame Reformer
– Scale-up of system and control methods to HDV
– Evaluation of exotherm techniques for mass production
– Implementation of the system on a vehicle

• We are currently seeking opportunities to continue this work:
  – All LNT Control and Flame Reformer IP belongs to OSU

• The OSU Challenge-X team is seeking sponsors to continue this work:
  – DOE/GM Sponsored Student Engineering Competition
  – Platform is a Chevy Equinox Diesel HEV
  – The primary need is for donation of LNTs, DOCs, and DPFs
  – Please see/contact me if you think your company may be able to help them out