Development of Numerical Simulink Model to Predict Tail Pipe NOx Emissions of a BSVI Vehicle with Lean NO\textsubscript{x} Trap

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Objective and Motivation

Objective:
The objective of the current modelling is to estimate the Tail Pipe NO$_x$ emissions in order to understand the feasibility of meeting BSVI emissions norms & RDE Compliance factors with LNT as an after treatment system for NO$_x$ reduction.

Motivation:

Effects of NO$_x$:
- Acid Rain
- Global Warming
- Ground level Ozone (SMOG)
- Visibility
- Respiratory Diseases

BS VI - April, 2020
RDE compliance

Less time available for the OEMs to be BSVI ready

HC
CO
PM
NO$_x$
+ other gases
Current OEM challenges for BSVI

- Less development time to be ready with BSVI
- Complexity of RDE
- Cost increase due to after treatment systems
- Durability of after treatment components
- Customer acceptance (Not to compromise on FE, driveability due to addition of after treatment systems)
Importance of Real driving Emissions:

- Real Driving Emissions (RDE) is critical in BSVI.
- RDE will have a mixture of driving conditions of:

  City
  - Critical bumper to bumper traffic
  - Very less exhaust temperature
  - Critical for after treatment systems light off

  Rural
  - High Engine out NO\textsubscript{x}
  - High accelerations

  Highway
  - Very high exhaust temperatures
  - Very high Engine out NO\textsubscript{x}
  - High exhaust flow rate

Critical factors:
- Critical bumper to bumper traffic
- Very less exhaust temperature
- Critical for after treatment systems light off
Diesel Engine NO\textsubscript{x} control:

Typical Engine configuration till BSIV

Addition of After treatment devices is the way forward to meet BSVI norms.

BSVI and Beyond: NO\textsubscript{X} reduction Technologies

- SCR
- LNT

**SCR**

- Dosing Unit
- AdBlue Tank
- Exhaust Gases Containing NO\textsubscript{X}
- Exhaust Gases + NH\textsubscript{3} + CO\textsubscript{2} + H\textsubscript{2}O
- SCR-Cat
- N\textsubscript{2} + CO\textsubscript{2} + H\textsubscript{2}O

**LNT**

- Adsorption (lean)
- Regeneration (rich)
- NO, NO\textsubscript{2}
- MeNO\textsubscript{3}
- CO
- N\textsubscript{2}, CO\textsubscript{2}
LNT vs. SCR

- LNT is efficient at low temperatures whereas SCR’s best operating temperatures tend to be higher.

Features comparison:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Packaging Constraints</th>
<th>Reductant Fluid</th>
<th>Fuel Penalty</th>
<th>NOx Conversion Efficiency</th>
<th>Desulphation</th>
</tr>
</thead>
<tbody>
<tr>
<td>LNT</td>
<td>-</td>
<td>0</td>
<td>-</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>SCR</td>
<td>--</td>
<td>--</td>
<td>0</td>
<td>++</td>
<td>0</td>
</tr>
</tbody>
</table>
Introduction to Lean NO\textsubscript{x} Traps (LNT)

- NO\textsubscript{x} is adsorbed onto a catalyst during lean engine operation. When the catalyst is saturated, the system is regenerated in short periods of fuel-rich operation during which NO\textsubscript{x} is catalytically reduced.

- The two phases of operation of LNT are:

  **Storage**

  - $\text{NO} + 0.5 \text{O}_2 \leftrightarrow \text{NO}_2$
  - $\frac{1}{2} \text{BaCO}_3 + \text{NO}_2 + \frac{1}{4} \text{O}_2 \leftrightarrow \frac{1}{2} \text{Ba(NO}_3)_2 + \frac{1}{2} \text{CO}_2$. 

  **Purge/Regeneration**

  - $\text{Ba(NO}_3)_2 \leftrightarrow \text{BaO} + 2\text{NO}_2 + \frac{1}{2} \text{O}_2$.
  - $\text{BaO} + \text{CO}_2 \rightarrow \text{BaCO}_3$.
Phases of LNT

I. NO\textsubscript{x} - storage  
\[ \lambda > 1 \]  
\[ 150 \degree \text{C} < T < 450 \degree \text{C} \]

II. NO\textsubscript{x} - reduction  
\[ \lambda < 1 \]  
\[ 200 \degree \text{C} < T < 500 \degree \text{C} \]

III. Desulphurization  
\[ \lambda < 1 \]  
\[ T > 700 \degree \text{C} \]

In lean mode, NO is converted to NO\textsubscript{2} on PGM and is further stored by Barium as Barium Nitrate.

In rich mode, NO\textsubscript{2} is released by Barium and it is converted into N\textsubscript{2} on PGM.

Sulphur, owing to high affinity, requires very high temperatures to be removed. Hence, a desulphation is conducted periodically.
LNT Characteristics

**Temp (deg C)**
At different Space Velocities and at constant filling and NO\textsubscript{x} ppm

**Efficiency**

**SV(1/hr)**
At different Temperatures and at constant filling and NO\textsubscript{x} ppm

**Efficiency**

**For different Temperatures and at constant Space Velocity and NO\textsubscript{x} ppm**

**Efficiency**

**For different Temperatures and at constant Space Velocity and Stored NO\textsubscript{x} ppm**
Traditional Procedure

- The traditional procedure would take approximately 1.5-2 years.
- By simulating LNT behavior, we are able to take a call on the suitable after treatment technology in a short span of time (2 months)

1. Obtain LNT prototypes from suppliers
2. Calibrate the Engine to reduce Engine out NO\textsubscript{x}
   - LNT rich mode calibration
   - LNT Desulphation calibration
   - LNT Vehicle level calibration
3. Employ vehicles with LNT and obtain the Tail Pipe Emissions
4. Decide if LNT will satisfy BSVI norms
5. Select the right technology
Approach

Lab testing for LNT characterization

On road testing
RDE data collection

Tests conducted:
- Obtain engine operating conditions
- Obtain engine out emissions data using condensed cycle run on Chassis Dynamometer
- Obtain temperatures of exhaust at various locations

Tests conducted:
- NO\textsubscript{x} conversion efficiency wrt temperate & Space velocity
- Maximum NOx storage limit at different temperatures
- NO\textsubscript{x} conversion efficiency with different filling levels of the cat
- Efficiency of regeneration at different temperatures & filling level
- Temperature transient slip
Components of LNT Modeling

**Efficiency**
- Steady State Efficiency maps are obtained from Test Bed.
- The Efficiency maps provide the dependence of Efficiency on Temperature, Space Velocity and filling.
- A sample efficiency map is shown below:

The above maps represent the efficiency maps obtained for different fillings; the right picture is for higher filling.
Components of LNT Modeling

- **Regeneration**
  - Regeneration of LNT requires the engine to switch to rich mode for a small period of time (6-10 sec).

  - Efficiency of Regeneration:

    - Regeneration requires certain operating conditions and if the conditions are not met, regeneration is not performed or will be interrupted. The regeneration conditions are:
      - Minimum exhaust temperature needed: 230°C
Components of LNT Modeling

- **Regeneration**
  - Brake mean effective pressure (bmep) requirements for regeneration are:
    - Regeneration at higher bmep leads to high cylinder pressure and noise of the engine.
    - At low bmep and high rpm, the engine would have to risk unstable combustion during regeneration and thus not feasible.
    - Regeneration at high bmep and high engine speed can lead to a risk of turbine damage owing to high gas temperatures.
Components of LNT Modeling

- **Temperature Transient Slip**
  - During temperature ramps, Tail Pipe NO\textsubscript{x} slip is observed and the corresponding effects are included after analysis.

![Graphs showing Exh_tOxiCatDs °C, Temperature Ramp, and Extracted Data](image)

A deviation from Steady State efficiencies, an extra slip of NO\textsubscript{x}, is observed during temperature gain ramps. The corresponding differences are extracted by conducting tests at different starting temperatures and extra slip data is extracted.
Components of LNT Modeling

Storage Capacity

- Storage Capacity = f(T,SV)
- Storage Capacity is high at medium temperatures and drops at either extremities
- Storage Capacity has very less dependency on SV; hence not considered.

Due to transient temperature, a small increase of it can change the storage capacity of CAT drastically

- If the currently stored value of NO\textsubscript{x} equals the storage capacity at the current temperature condition, the efficiency reaches 0 and further storage is not possible.

- Similarly, if the current stored NO\textsubscript{x} is higher than the storage capacity at the current temperature, LNT desorbs NO\textsubscript{x}. 

Storage Capacity vs. Temperature

![Graph showing Storage Capacity vs. Temperature](image-url)
Creation of Simulink Model

Physical System:

- Engine Exhaust
- Engine Operating Conditions
- Sensory Signals
- Regeneration Mode
- LNT: Stores NOx & Regenerates
- Engine Control Unit
- Exhaust gases to Tail Pipe
- Tail Pipe Emissions

Mathematical Model:

- Engine Out Emissions measured on Test Bed
- Simulink Model
- Calculated Tail Pipe NOx after LNT

Engine

LNT: Stores NOx & Regenerates

Engine Control Unit

Tail Pipe Emissions

O₂ – in & out

NOₓ - in
Simulink Model

Inputs:
- Exhaust Flow rate
- Exhaust Temperature
- Engine Out NO\textsubscript{x}
- Engine rpm
- BMEP

Storage Capacity Calculation

Tail Pipe NO\textsubscript{x} Calculations

Result: Tail Pipe NO\textsubscript{x}

Temperature Transient Slip

Efficiency map & Regeneration Calculations

Regeneration Conditions

Regeneration Strategy

Tail Pipe NO\textsubscript{x} Calculations

Storage Capacity Calculation

Efficiency map & Regeneration Calculations

Regeneration Conditions

Regeneration Strategy

Temperature Transient Slip

Result: Tail Pipe NO\textsubscript{x}

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Storage Capacity Calculation

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Result: Tail Pipe NO\textsubscript{x}

Tail Pipe NO\textsubscript{x} Calculations

Storage Capacity Calculation

Efficiency map & Regeneration Calculations

Regeneration Conditions

Regeneration Strategy

Temperature Transient Slip
Background of the model

- Engine Out NO\textsubscript{x}
- Efficiency
- Tail Pipe NO\textsubscript{x}

- Temperature
- Space Velocity
- Temperature Transient Slip
- Storage Capacity
- Detect Ramp
- LNT Load

- NO\textsubscript{x} flow
- Sensory Signal

- Regeneration Trigger
- Regeneration Conditions
Correlation with New European Driving Cycle (NEDC)

- NEDC Simulation results are compared to Test’

![Graph showing NOx and Temperature correlation]

Correlation: 99%
Application to Real Driving Emissions:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>City Conditions</th>
</tr>
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<tbody>
<tr>
<td>Time (s)</td>
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<tr>
<td>Distance (km)</td>
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<tr>
<td>Avg. Speed (kmph)</td>
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<tr>
<td>CF (-)</td>
<td>0.50</td>
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Regeneration

Very less Downstream NO\(_x\) compared to upstream NO\(_x\).

CF of 0.5 implies that LNT will satisfy the emission requirements in city conditions.
Application to Real Driving Emissions:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Highway Conditions</th>
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<tbody>
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<td>Distance (km)</td>
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</tr>
<tr>
<td>Avg. Speed (kmph)</td>
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</tr>
<tr>
<td>CF (-)</td>
<td>2.61</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Very high number of regenerations owing to suitable regeneration conditions and high Engine Out NOx.

High Downstream NOx because of less efficiency

CF of 2.61 implies that LNT will not satisfy the emission requirements in highway conditions for this vehicle application. But increasing the regeneration frequency can improve the CF.
Change of approach

Traditional approach

- Obtain LNT prototypes from suppliers
- Calibrate the Engine to reduce Engine out NOx
- LNT rich mode calibration
- LNT Desulphation calibration
- LNT Vehicle level calibration
- Employ vehicles with LNT and obtain the Tail Pipe Emissions
- Decide if LNT will satisfy BSVI norms
- Select the right technology

The traditional procedure would take approximately 1.5-2 years.

By simulating LNT behavior, we are able to take a call on the suitable after treatment technology in a short span of time (2 months)

Simulation based approach

Requires a lot of time and effort

Able to correlate well with tests and requires very less time

Tests conducted:
- NOx conversion efficiency with tail temperate & Space velocity
- Maximum NOx storage limit at different temperatures
- NOx conversion efficiency with different filling levels of the cat
- Efficiency of regeneration at different temperatures & filling level
- Temperature transient step
Summary

- OEMs have to select the best technology to satisfy BSVI emission norms for all the vehicle variants within the limited time period.
- In this scenario, using a simulation model helps in reducing the precious time and effort.
- In order to study the feasibility of LNT for the given vehicle application, LNT characteristics are obtained along with engine out on-road emissions separately.
- MATLAB Simulink model is created successfully and feasibility study is performed for legislative cycles and RDE conditions.
- The created Simulink model can be used for different vehicle and engine variants and their applications in various RDEs.
Advantages of LNT Simulink model

• The feasibility of LNT meeting the emission requirements in a given cycle even before the vehicle level testing
• An idea of the size required
• An idea of required technology to meet the emission norms
• Comparison between different LNT suppliers
• An estimate of reduction of Engine-out emissions required
• Compliance factor in different RDE cycles can be predicted
• Same model can be used for different vehicle applications
• Time saving of approx. 1.5 years
• Cost saving
• Effort saving
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Thank you for your attention!