DEVELOPMENT OF A FAST RUNNING LEAN NOx TRAP MODEL FOR SIMULATION OF REAL CUSTOMER DRIVE CYCLES
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SUMMARY

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BACKGROUND
Renault NOx Trap Technology

- First application: Renault Espace dCi 175 Euro 5
  - Sold in Europe since mid 2009

- A technology that will be applied on Euro 6 high-end vehicles.
Design of the NOx Trap system (1/2)

1/ Architecture: NOx Trap position in the exhaust line
Design of the NOx Trap system (2/2)

2/ Catalyst characteristics:
   - NOx Trap catalyst volume,
   - NOx Trap coating, ...

3/ Constraints:
   - Emissions on NEDC / resp. FTP75 – US06 test cycles
   - Compatibility with real customer use (city, road, highway) and serviceability targets
Real Customer use

- Real customer use = various drive cycles
  - City (including heavy traffic conditions & slow average speed)
  - Road
  - Highway
  - Mixed

- A challenge for simulation experts:
  - Even at a real-time speed simulation duration is prohibitive!
  - Accuracy and numerical efficiency are often conflicting requirements

=> A methodology is needed that is capable of simulating at speeds exceeding $10^3 \times$ Realtime sacrificing minimum accuracy.
02
PROCEDURE
=> Neural Network reduction of a detailed model, based on previous Gamma Technologies’ experience (with DOC and SCR – cf FISITA 2010 paper).

1/ Creation of the detailed model of a Lean NOx Trap.

2/ Model validation and calibration by LMM, based on Renault experimental data.

3/ Definition of operating ranges of the input parameters and creation of a design of experiments. Training of a set of static neural network to reproduce the kinetic behavior of the catalyst using the resulting data.

4/ Training of the NN models to predict the catalyst output conditions given the inlet conditions and the catalyst state (temperature and NOx coverage)
Procedure (2/2)

- Catalyst states could not be trained by the static Neural Network as they depend on past history. Dynamic Neural Network is ruled out as it cannot be easily made autonomous.

- State variables are deduced from two physical models that rely on outputs from the Neural Network models.
03

NEURAL NETWORK MODEL

HYBRID NEURAL NETWORK & ARCHITECTURE
Detailed Model Overview

- The considered detailed model consists in a Lean NOx Trap catalyst operating under lean and rich conditions.
Detailed Model Overview

- The LNT detailed model behavior is characterized by the following 12 reactions:

1. \( \text{NO} + \text{BaO} + \frac{1}{2} \text{O}_2 \rightarrow \text{BaONO}_2 \)
2. \( \text{NO}_2 + \text{BaO} \rightarrow \text{BaONO}_2 \)
3. \( \text{BaONO}_2 \rightarrow \text{NO}_2 + \text{BaO} \)
4. \( \text{C}_{10}\text{H}_{22} + 15.5 \text{BaONO}_2 \rightarrow 15.5\text{BaO} + 7.75\text{N}_2 + 11\text{H}_2\text{O} + 10\text{CO}_2 \)
5. \( \text{C}_3\text{H}_6 + 4.5\text{BaONO}_2 \rightarrow 4.5\text{BaO} + 2.25\text{N}_2 + 3\text{H}_2\text{O} + 3\text{CO}_2 \)
6. \( \text{C}_7\text{H}_8 + 9\text{BaONO}_2 \rightarrow 9\text{BaO} + 4.5\text{N}_2 + 4\text{H}_2\text{O} + 7\text{CO}_2 \)
7. \( 10\text{CO} + 5\text{BaONO}_2 \rightarrow 5\text{BaO} + 2.5\text{N}_2 + 10\text{CO}_2 \)
8. \( \text{C}_{10}\text{H}_{22} + 15.5\text{O}_2 \rightarrow 10\text{CO}_2 + 11\text{H}_2\text{O} \)
9. \( \text{C}_3\text{H}_6 + 4.5\text{O}_2 \rightarrow 3\text{CO}_2 + 3\text{H}_2\text{O} \)
10. \( \text{C}_7\text{H}_8 + 9\text{O}_2 \rightarrow 7\text{CO}_2 + 4\text{H}_2\text{O} \)
11. \( \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \)
12. \( \text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2 \)
Methodology - Neural Network Architecture

- The proposed neural network architecture is a three-layer feed-forward neural network with 2 hidden layers whose activation functions are tan-sigmoid and 1 output layer with linear activation.
LNT NOx Coverage

- The used approach consists in using a NN to predict derivative of coverage and then to integrate it along the simulation. Thus the coverage calculation during transient simulation is equal to:

\[
\text{Coverage } \Theta = \Theta_{\text{init}} + \int_{t}^{t} \left( \frac{d\Theta}{dt} \right)_{NN}
\]

where

- \(\Theta_{\text{init}}\) is the initial coverage
- \(\left( \frac{d\Theta}{dt} \right)_{NN}\) is the coverage derivative predicted by the static NN.

- This procedure can be improved by using conservation principles.
LNT wall temperature

- The LNT mass is treated as a single mass
- Model is considered to be adiabatic with respect to the heat loss to the environment
- Calculation based on the heat flux of energy entering/leaving the catalyst wall predicted by a NN

\[ T_{\text{wall}} = T_{\text{wall,init}} + \int \frac{dT}{dt} \]

with

\[ \frac{dT}{dt} = \frac{Q_{\text{NN}}}{m \cdot C_p} \]

Where \( T_{\text{wall,init}} \) is the initial wall temperature and \( Q_{\text{NN}} \) is the heat flux energy predicted by the NN.
Methodology - DoE Setup

- Two DoE models were set up (each 5,000 experiments): one for lean and one for rich conditions
- Results are used to train Neural Network: 8 input variables, 11 predicted quantities

<table>
<thead>
<tr>
<th>Inlet variables</th>
<th>Lean conditions</th>
<th>Rich conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate [kg/s]</td>
<td>Min 0.001</td>
<td>Max 0.08</td>
</tr>
<tr>
<td>Inlet gas temperature [K]</td>
<td>Min 280</td>
<td>Max 700</td>
</tr>
<tr>
<td>Catalyst Wall temperature [K]</td>
<td>Min 280</td>
<td>Max 800</td>
</tr>
<tr>
<td>CO mass fraction</td>
<td>Min 0</td>
<td>Max 8.0e-3</td>
</tr>
<tr>
<td>NO₂ mass fraction</td>
<td>Min 0</td>
<td>Max 4.0e-4</td>
</tr>
<tr>
<td>O₂ mass fraction</td>
<td>Min 0.04</td>
<td>Max 0.23</td>
</tr>
<tr>
<td>Total HC's mass fraction</td>
<td>Min 0</td>
<td>Max 3.0e-3</td>
</tr>
<tr>
<td>Coverage</td>
<td>Min 0</td>
<td>Max 0.5</td>
</tr>
</tbody>
</table>

Table 1. DoE ranges for LNT inlet conditions

<table>
<thead>
<tr>
<th>Neural Networks outlet variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄ mass fraction</td>
</tr>
<tr>
<td>C₃H₆ mass fraction</td>
</tr>
<tr>
<td>C₇H₈ mass fraction</td>
</tr>
<tr>
<td>C₁₀H₂₂ mass fraction</td>
</tr>
<tr>
<td>CO mass fraction</td>
</tr>
<tr>
<td>NO₂ mass fraction</td>
</tr>
<tr>
<td>O₂ mass fraction</td>
</tr>
<tr>
<td>Coverage derivative (dΘ/dt)</td>
</tr>
<tr>
<td>Gas temperature at the LNT middle point</td>
</tr>
<tr>
<td>Gas temperature at the LNT outlet</td>
</tr>
<tr>
<td>Heat flux to LNT wall (Q)</td>
</tr>
</tbody>
</table>

Table 2. NN outputs: dependent variables
Neural Network model setup

- During the driving cycle transient simulation, the appropriate NN model is activated (switching from lean NN model to rich NN model and vice versa) based on the inlet condition.
04

NEURAL NETWORK MODEL RESULTS
Neural Network Model Results - Hydrocarbon (inst. and cumul.)

CH\textsubscript{4} Mole Fraction

CH\textsubscript{4} Cumulative Mole Fraction

C\textsubscript{10}H\textsubscript{22} Mole Fraction

C\textsubscript{10}H\textsubscript{22} Cumulative Mole Fraction
Neural Network Model Results – NO₂ and CO

NO₂ Mole Fraction

CO Mole Fraction

NO₂ Cumulative Mole Fraction

CO Cumulative Mole Fraction

Inlet (measured)
Detailed model results
Neural Network results
Neural Network Model Results – Temperatures and NOx Coverage

LNT Wall Temperature
- Inlet gas temperature
- Detailed
- NN

Gas Temperature (LNT middle point)
- Inlet temp. (measured)
- Detailed model results
- Neural Network results

Gas outlet temperature
- Inlet gas temperature
- Detailed
- NN

NOx Coverage
- Detailed
- NN

Time [sec]
0 250 500 750 1000 1250

Inlet temp. (measured)
Detailed model results
Neural Network results
CONCLUSION
Conclusion (1/2)

- Detailed After-treatment models can be reduced to very fast running Neural Network model with a more than acceptable loss of accuracy.

- Neural Network model was improved using a hybrid methodology that improved the fidelity of the system model.

- For an overall duration of about 33h of real time. The computational time on a laptop with Intel 2.53 GHz CPU and 3 GB ram (using a single core) were:
  - Detailed model: 10’ 15”
  - NN model: 01’ 25”
Conclusion (2/2)

- It was noted that the Neural Network model runs 1300 times faster than real time which is about 7 times faster than detailed model.

- It should be pointed out that the performance of the Neural Network model depends on the number of independent variables (look ups) and the number of dynamic physical models. Thus, the numerical efficiency of the NN model will be maintained even in cases where the detailed model numerical efficiency degrades due to stiffer and/or more complex kinetics.

- Further improvements in computation speed can be expected, e.g. by using parallelized computing.
END