An update on Lean NOx trap modeling in PSAT

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Introduction

• **PSAT : Powertrain System Analysis Toolkit**
  - sponsored by DOE, effort led by ANL
  - contributions from various auto companies
  - package of modular simulation tools to test various powertrain configurations (e.g., hybrid concepts, HCCI/PCCI combustion engines)
  - written mostly in MATLAB, Simulink
  - ORNL is tasked with generating experimental data on engines and after-treatment devices and developing models
  - For more information, visit PSAT website at [www.transportation.anl.gov/software/PSAT/index.html](http://www.transportation.anl.gov/software/PSAT/index.html)
Engine and Aftertreatment Model Development

- Engine models/maps
  - performance, fuel costs, emissions
  - conventional and advanced combustion modes (HCCI, PCCI, LTC etc.)
  - regular and emerging fuels (gasoline, diesel, ethanol etc.)

- After treatment models
  - performance, costs (fuel penalty, aging etc.)
  - systems integration and control
  - failure modes
Recent Accomplishments

- Generated engine maps for GM 1.9L engine operating in regular and HECC (PCCI) modes
- Engine warmup model to simulate transient behavior following a cold/warm start using steady state maps (particularly important for simulating hybrid vehicles where engine stops, cools down and then restarts)
- Model for a Pd/Rh based 3-way catalyst for stoic engines
  - contains BaO (improves WGS activity, CO, C$_3$H$_8$ conversion)
  - Possibility of NOx storage
- Vehicle speed based heat loss models for after-treatment devices (critical for simulating hybrid vehicles)
- Aging and desulfation effects in LNT model
- Simulation of a parallel hybrid vehicle (Honda-Civic configuration) exhaust after treatment using a LNT
Standard Engine Mapping Approach for PSAT Relies on Experimental Data Tabulation

- Detailed speed-load sweep provides data to map engine (e.g., 109 operating conditions for MB 1.7-L)
- Data includes fuel consumption, exhaust temperature, exhaust mass flow rate, and regulated pollutants
- Square matrix generated by nearest-neighbor interpolation based on measured data
LNT and DPF Regeneration States

- Regeneration maps derived from limited data, simulations
- Engine switching triggered by LNT/DPF state indicators, engine supervisor assessment
Prediction of transients using steady state maps for the Mercedes 1.7L engine

- Transient profiles of most species are predicted well
- Engine-out temperature predictions (made using steady state maps and engine thermal model) matches well with the experimental data
LNT Simulink Model

  - NOx capture in nitrite/nitrate form and C₃H₆ based regeneration
  - NO<=>NO₂ inter-conversion
  - Diffusion resistance to bulk nitrite/nitrate storage (shrinking core)

- Extensions
  - CO/H₂ based regeneration (as in CLEERS protocol)
  - CO equivalent to H₂ in terms of reducing capacity
  - Oxygen storage
  - calibrated using CLEERS protocol data for a Umicore catalyst
  - Effects of aging, sulfation/desulfation
  - Heat loss model
  - NH₃ breakthrough model – empirical, qualitative (quantitative tracking may be needed for simulating LNT-SCR combinations)
LNT Simulink Model: deficiencies

- Nitrites are not converted to nitrates (approximation works well for short capture times)
- Bulk nitrition/nitration histories are destroyed while simulating regeneration (shrinking core model is not applicable to model bulk nitrition/nitration in zone 2)
- Zone 2 length as a fraction of the reactor length should be low for the model to be accurate

State of the catalyst immediately at the beginning of lean phase after partial regeneration

- Zone 1: fully regenerated
- Zone 2: bulk nitrates remain
- Zone 3: does not encounter reductant (no regeneration at all)
Simulation of a MECA catalyst performance in engine tests

- Model was calibrated using a long NOx capture experiment
  - adjust NOx storage capacity
  - all other model parameters (kinetic rates) fixed at values determined for the Umicore catalyst
- Calibrated model predicts the steady state engine data well

Predicted and experimental NOx profiles

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Simulation of a MECA catalyst performance in FTP tests

- Combination of a UDDS and US06 cycles
- Regeneration done using syn-gas (CO+H2) injection into the exhaust
- Predicted overall NOx conversion (93%) compares well against experimentally determined value (94%)
LNT-out NOx feedback based regen: optimal performance

- LNT supervisor monitors LNT state and requests regeneration when needed.
- Engine supervisor commands regeneration when speed/load/other constraints permit.
- Regeneration command switches engine to LNT regeneration map for specified period.
- Engine supervisor must also prioritize LNT regeneration relative to DPF regeneration and other emission control requests.
Regeneration schemes

- No regeneration when LNT-out T < 150ºC
- Minimum period of lean operation between regenerations
- Downstream NOx sensor based engine control
  - regenerate if LNT-out NOx conc exceeds a user-specified level
  - fixed regeneration interval (user-specified)
  - Optimal but not currently practical (NOx sensors are expensive, hard to measure NOx at low concentrations)
- Downstream UEGO sensor based engine control
  - regenerate at fixed intervals
  - stop regen when A/F drops below a specified value (e.g., 14.1)
  - reductant breakthrough unavoidable
- Engine map based control : no feedback
  - Integrating NOx influx into the LNT
  - start a regeneration when the integrated NOx exceeds a given fraction (say 25%) of the storage capacity
  - Controller needs good estimate of storage capacity
Additions to the LNT Simulink model

- $\text{NH}_3_{\text{out}} \sim 0.1 \text{ CO}_{\text{in}} (\text{CO}_{\text{in}} - \text{CO}_{\text{out}})/\exp(9.3\text{CO}_{\text{in}})$
  - derived from CLEERS test protocol data generated for Umicore catalyst
  - NH3 breakthrough possible only if there is a deficit of CO across the reactor

- Convective heat loss model
  - heat transfer coefficient $h_{\text{conv}} = \text{Nu}_{\text{conv}}$ (thermal conductivity)/$D_{\text{cat}}$
  - $\text{Nu}_{\text{conv}} = [\text{Nu}_{\text{forced}}^4 + \text{Nu}_{\text{free}}^4]^{1/4}$
  - $\text{Nu}_{\text{forced}} = 0.0297 \text{ Re}^{4/5}\text{Pr}^{1/3}$, $\text{Nu}_{\text{free}} = 0.6 + 0.387 \text{ Ra}^{1/6}/[1+(0.6/\text{Pr})^{9/16}]^{8/27}$
  - $h = 40 \text{ W/}(\text{m}^2\text{K})$ is often used in 3-way catalyst modeling
  - Re is based on vehicle speed and catalyst can dimensions
  - Vehicle speed available from PSAT
Additions to the LNT Simulink model

- **Aging, sulfation/desulfation effects**
  - Initial NOx storage capacity is multiplied by a factor $\chi$ to account for aging, sulfation/desulfation based on mileage ($M_{usage}$)
  - assuming 30-40ppm fuel sulfur level
  - $\chi = \exp(-3 \times 10^{-6} M_{usage}) \exp\{- F_1(T_{des}, N_{des}) - F_2[\text{mod}(M_{usage}/M_{des})]\}$
  - $M_{des}$: miles between desulfation events
  - $T_{des}$: max desulfation T
  - $N_{des}$: number of desulfation events
  - Nitrate/nitrite formation reaction rates and noble metal surface area are multiplied by $\alpha$ and $\beta$ to account for aging, sulfation/desulfation
  - $\alpha = G_1(T_{des}, N_{des}) G_2 [M_{des}, \text{mod}(M_{usage}/M_{des})]$
  - $\beta = 0.92 G_1(T_{des}, N_{des}) + 0.08$
  - correlations obtained from experimental data (Theis et al., SAE paper 2004-01-1493; Nguyen et al., SAE paper 2007-01-0470; Toops et al., Cat. Today, 123, pp 285-292)
Effects of rapid aging at various temperatures on storage capacity

- NOx storage capacity falls rapidly once catalysts are exposed to T exceeding 900°C
Effects of Sulfation/desulfation on performance

- UDDS cycle simulation with regen strategy based on downstream NOx sensor (i.e., optimal regen strategy)
- Desulfation done at 5000 miles intervals
- NOx reduction efficiency drops rapidly with sulfation
- Post desulfation NOx conversion seems to level off with increasing mileage
- Desulfation results in increased NOx conversion with out a big change in fuel penalty
Simulation of LNT on a hybrid vehicle

- Parallel hybrid (Honda Civic configuration) with a 1.7L Mercedes engine
- Fuel efficiency of the hybrid configuration is nearly 50% higher than in case of conventional configuration (using the same engine in both cases)
- Compare LNT performance on a hybrid vehicle to its performance on a conventional vehicle
  - identify potential problem when using LNTs on hybrid vehicles which have intermittent engine operation
Simulation of LNT (with optimal regen strategy) on a hybrid vehicle

Conventional configuration
NOx reduction efficiency: 94%
fuel penalty: 3.0%
NOx emission: 0.052g/mile

Hybrid configuration
NOx reduction efficiency: 85%
fuel penalty: 2.1%
NOx emission: 0.145g/mile

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Future Plans

- Update and supplement LNT model
  - Other regeneration schemes (suggestions welcome)
  - NH$_3$ formation kinetics (to simulate LNT+SCR combinations)
- Expand engine maps
  - DPF regeneration states=> full FTP capability
  - Alternative and conventional fuels (e.g., ethanol, biodiesel)
- Update the 3-way catalyst model for stoic engines
  - Current version based on guestimated precious metal loading and O$_2$ storage capacity
  - Chemical analysis being done at present
- Complete the SCR model
  - Dosing strategies (suggestions welcome)
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