# An update on Lean NOx trap modeling in PSAT

Zhiming Gao, Kalyana Chakravarthy, Dean Edwards & Stuart Daw
Oak Ridge National Laboratory

**11th DOE CLEERS workshop**
**May 13, 2008**
**University of Michigan, Dearborn, MI**

# 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

# 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

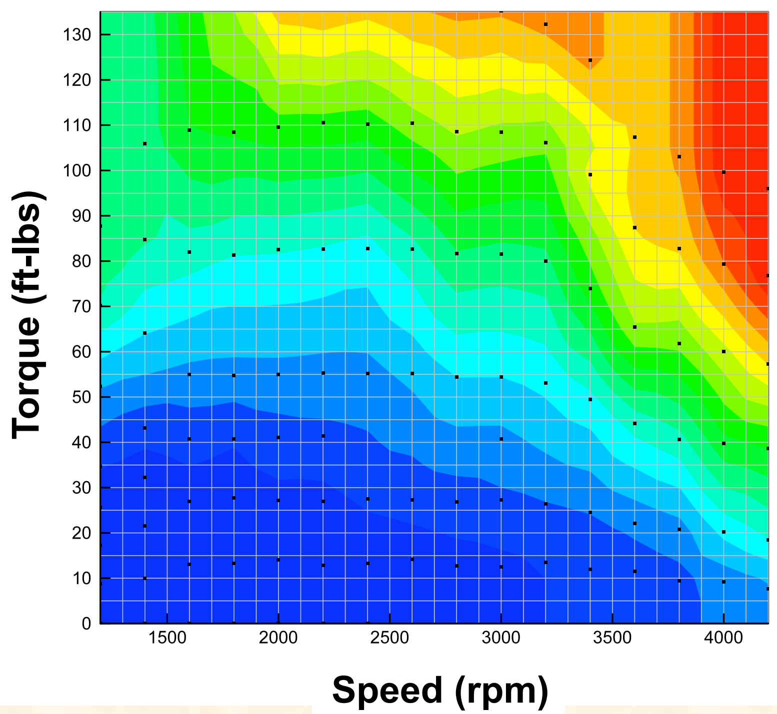
# Recent Accomplishments

- 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, $C_3H_8$ 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

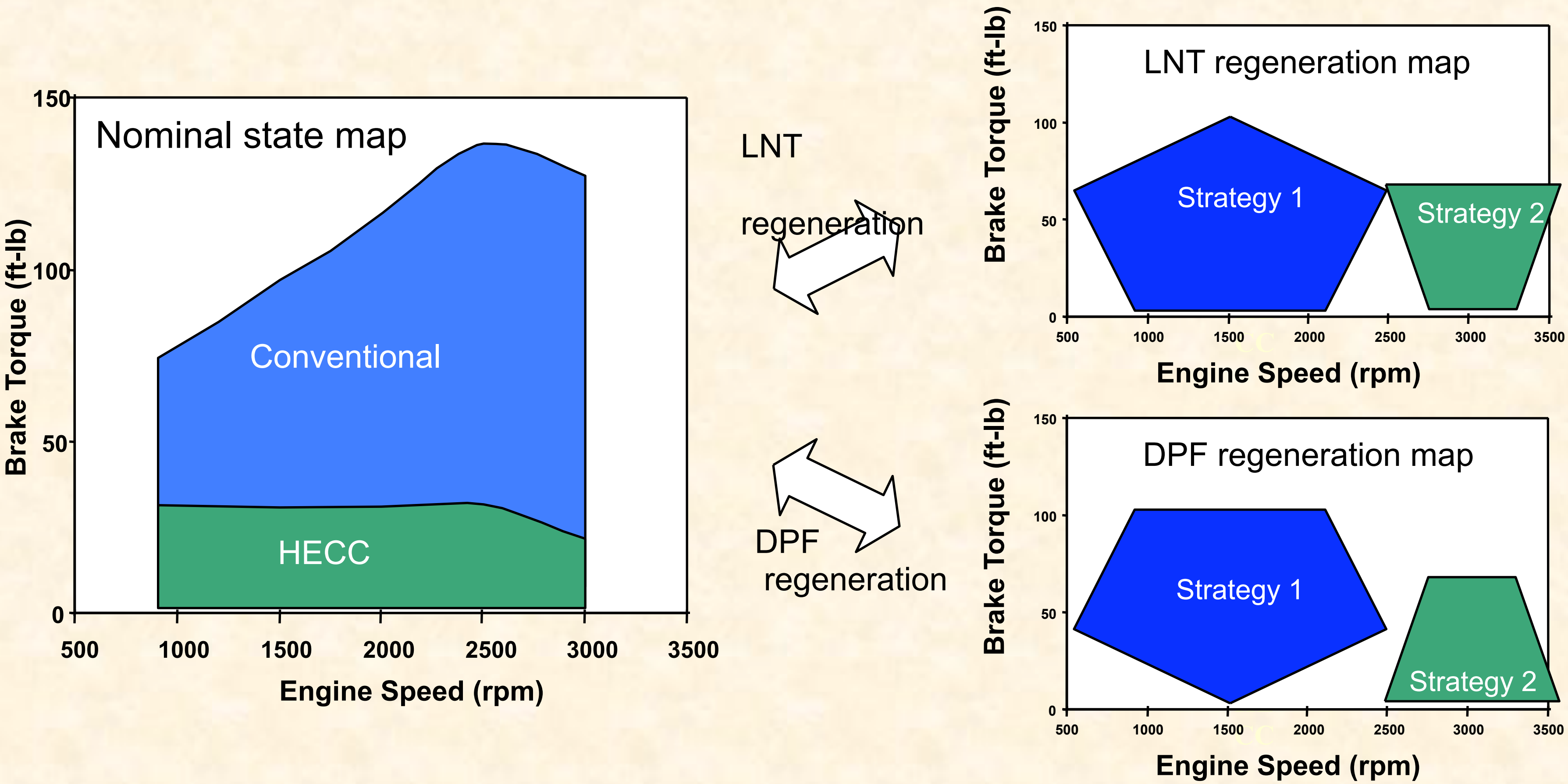
# Standard Engine Mapping Approach for PSAT Relies on Experimental Data Tabulation

- **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**

**Example $NO_x$ Map**

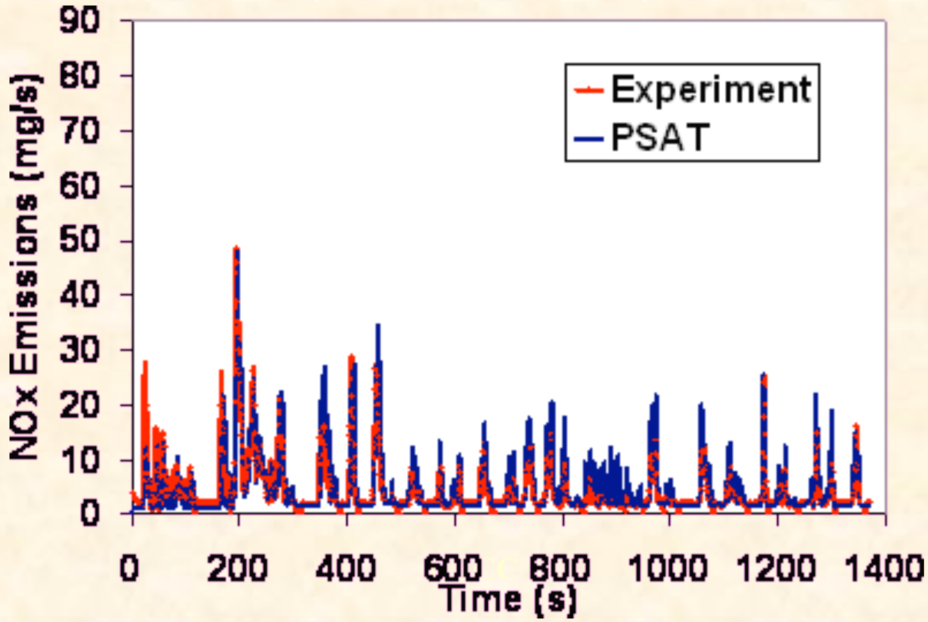


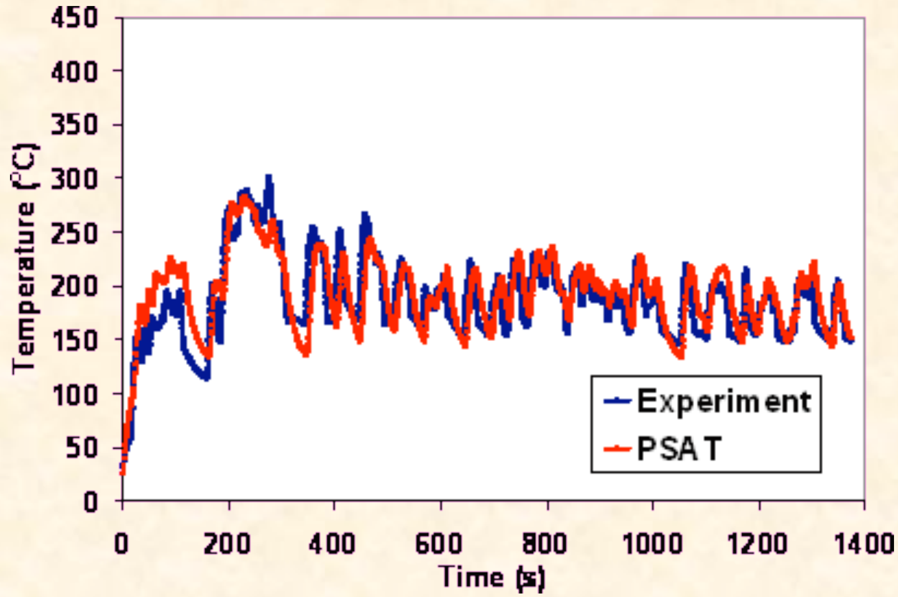
# LNT and DPF Regeneration States




- **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

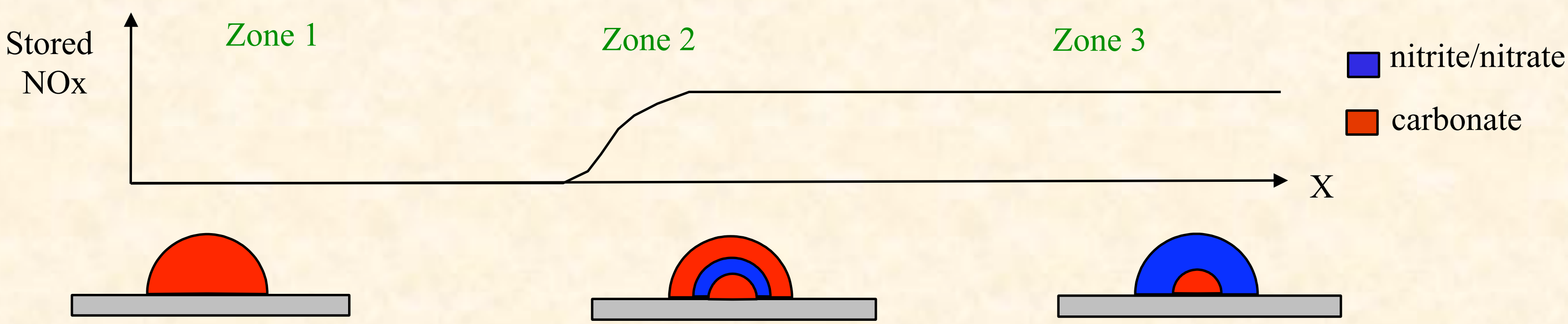
# LNT Simulink Model

- Based on a Chalmers/GM model (Ind. Eng. Chem. Res. 2005, 44, 3021)
  - NOx capture in nitrite/nitrate form and $C_3H_6$ based regeneration
  - NO<=>$NO_2$ inter-conversion
  - Diffusion resistance to bulk nitrite/nitrate storage (shrinking core)
- Extensions
  - CO/$H_2$ 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

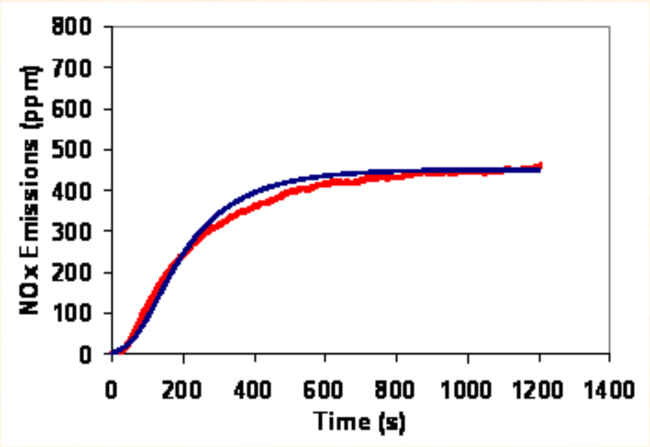


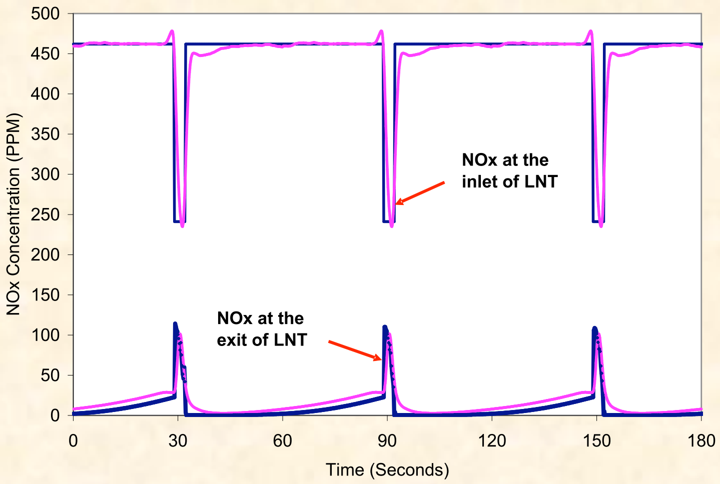

**Zone 1: fully regenerated**

**Zone 2: bulk nitrates remain**

**Zone 3 : does not encounter reductant (no regeneration at all)**

# Simulation of a MECA catalyst performance in engine tests

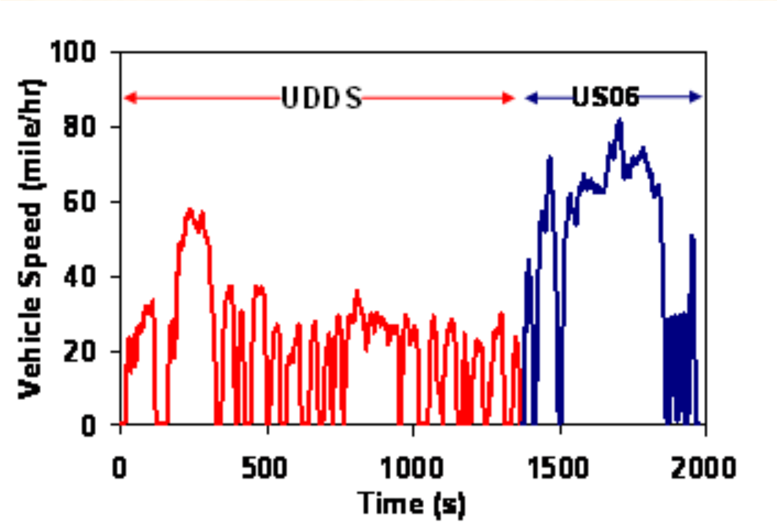


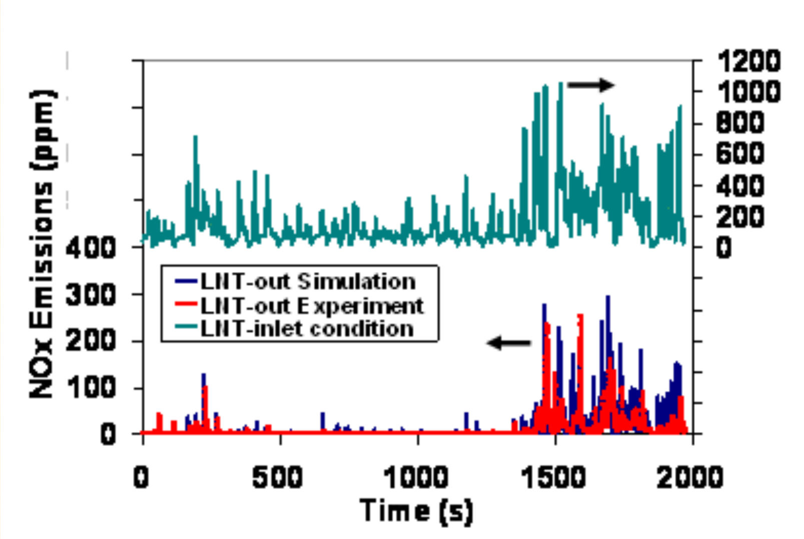




**Predicted and experimental NOx profiles**

- **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**

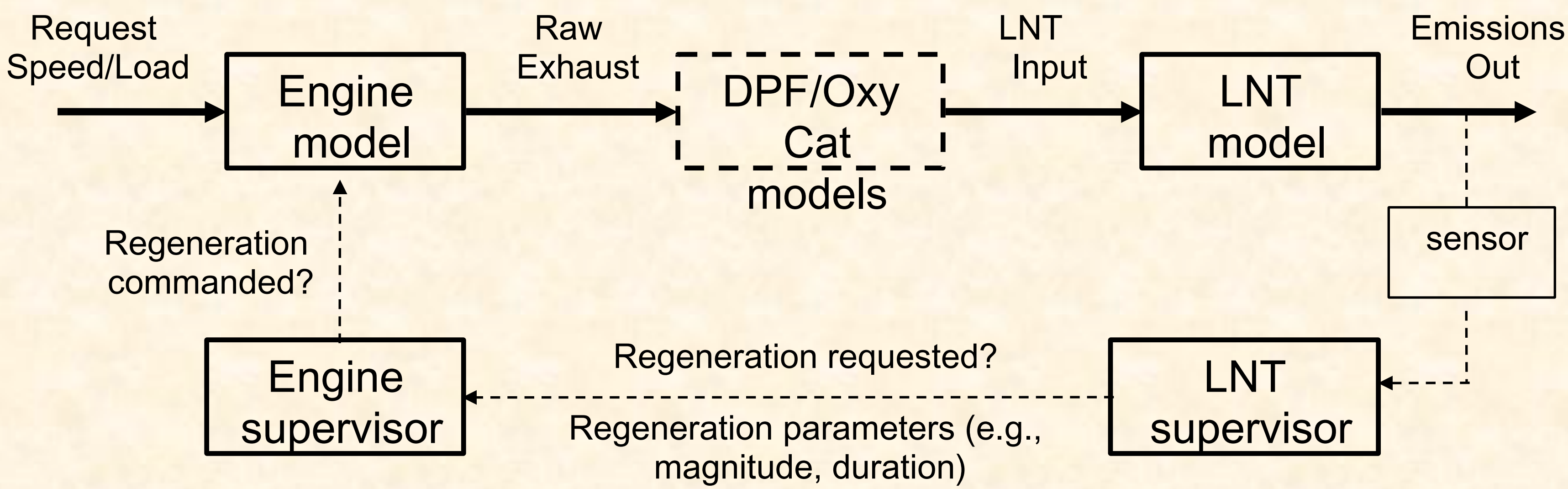
# Simulation of a MECA catalyst performance in FTP tests




- 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 < 150$^o$C
- 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

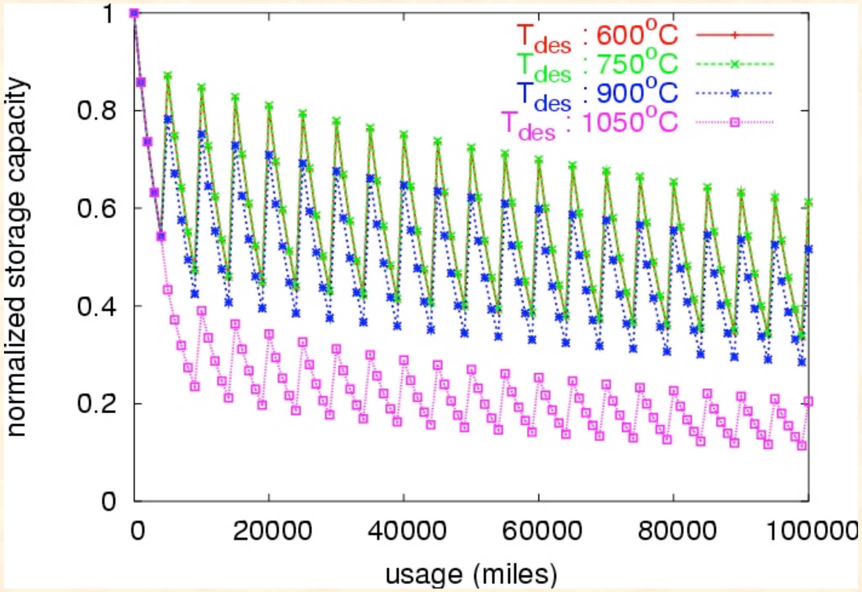
# Additions to the LNT Simulink model

- $NH3_{out} \sim 0.1\ CO_{in}\ (CO_{in} - CO_{out})/\exp(9.3CO_{in})$
  - derived from CLEERS test protocol data generated for Umicore catalyst
  - NH3 breakthrough possible only is there is a deficit of CO across the reactor
- Convective heat loss model
  - heat transfer coefficient $h_{conv} = Nu_{conv}$ (thermal conductivity)/$D_{cat}$
  - $Nu_{conv} = [Nu_{forced}^4 + Nu_{free}^4]^{1/4}$
  - $Nu_{forced} = 0.0297\ Re^{4/5}Pr^{1/3}$, $Nu_{free} = 0.6 + 0.387\ Ra^{1/6}/[1+(0.6/Pr)^{9/16}]^{8/27}$
  - $h = 40\ W/(m^2K)$ 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

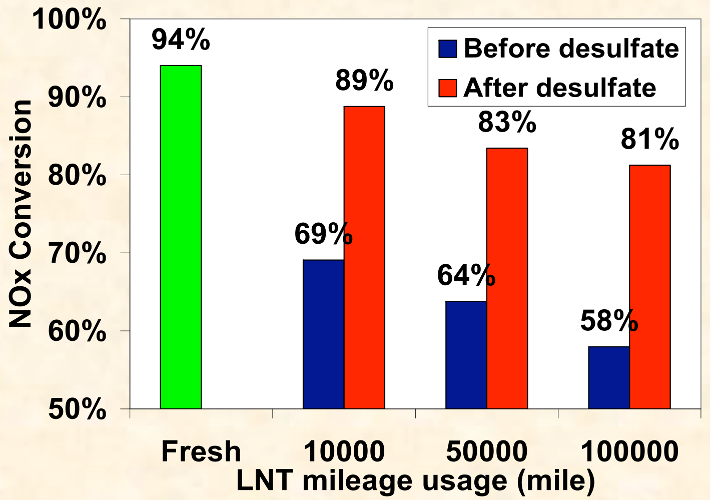
- **Aging, sulfation/desulfation effects**
  - Initial NOx storage capacity is multiplied by a factor $\chi$ to account for aging, sulfation/desulfation based on mileage ($M_{usage}$)
  - assuming 30-40ppm fuel sulfur level
  - $\chi = \exp(-3\times10^{-6}\ M_{usage})\ \exp\{-\ F_1(T_{des}, N_{des}) - F_2[\mathrm{mod}(M_{usage}/M_{des})]\}$
  - $M_{des}$ : 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/deS
  - $\alpha = G_1(T_{des}, N_{des})\ G_2\ [M_{des}, \mathrm{mod}(M_{usage}/M_{des})]$
  - $\beta = 0.92\ G_1(T_{des}, N_{des}) + 0.08$
  - 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)

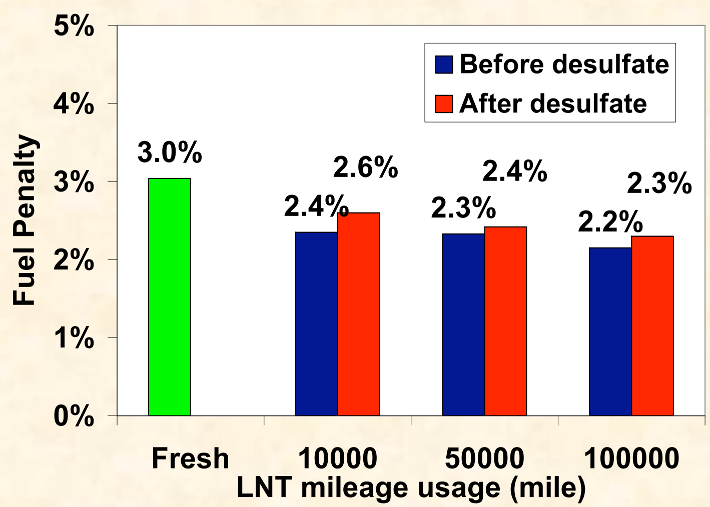
# Effects of rapid aging at various temperatures on storage capacity




- NOx storage capacity falls rapidly once catalysts are exposed to T exceeding 900°C

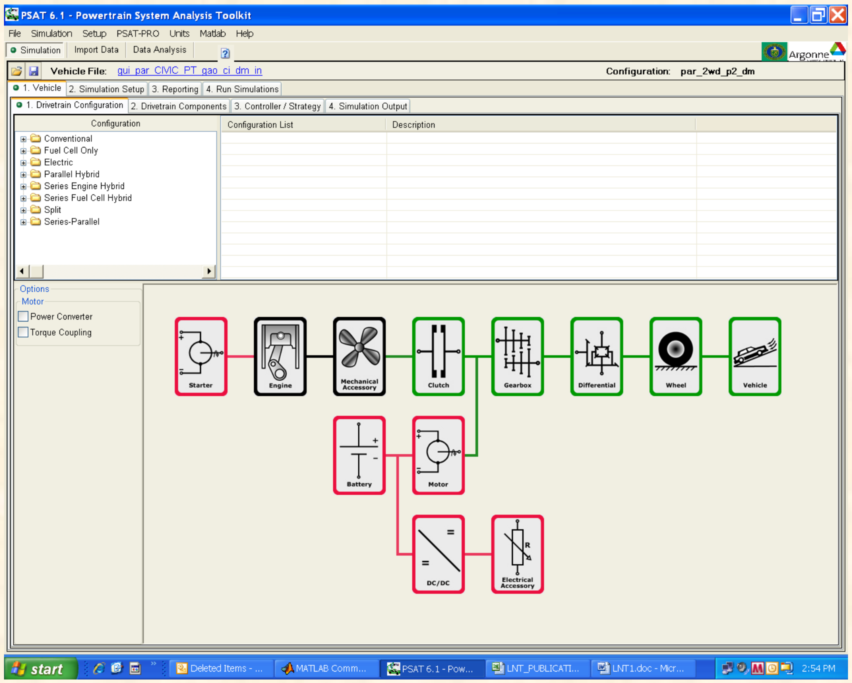
# Effects of Sulfation/desulfation on performance




- 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

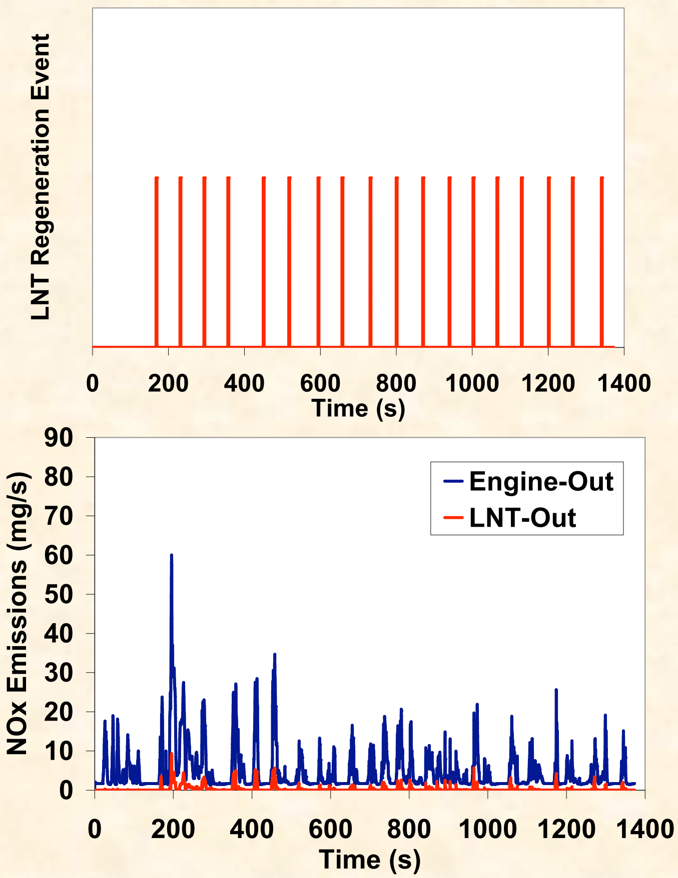
# Simulation of LNT on a hybrid vehicle




Powertrain configuration of a parallel 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

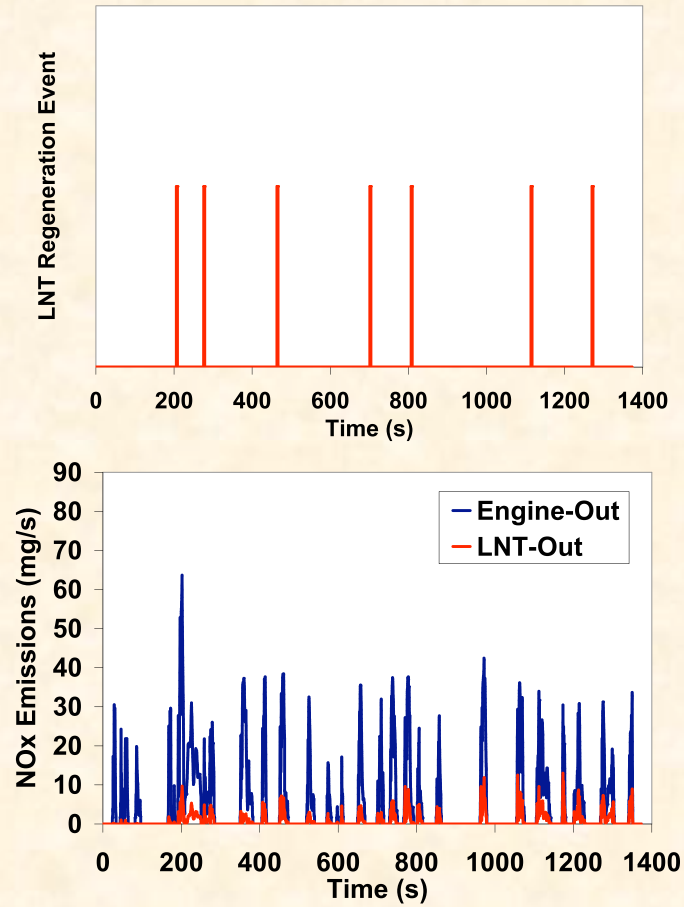



conventional configuration

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

# 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)

# Contact information

- **PSAT**
  - Aymeric Rousseau (arousseau@anl.gov)
- **Engine & aftertreatment models**
  - Stuart Daw (dawcs@ornl.gov)
- **Model details**
  - Kalyana Chakravarthy (chakravartvk@ornl.gov)
  - Zhiming Gao (gaoz@ornl.gov)