Model-Based Performance Assessment of a Lean-Burn System

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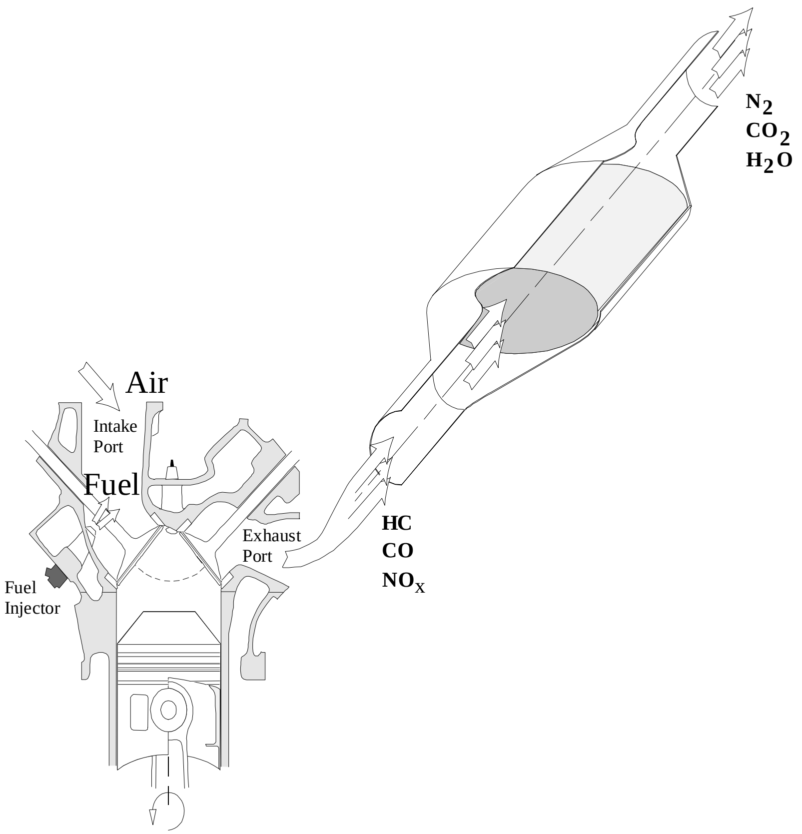
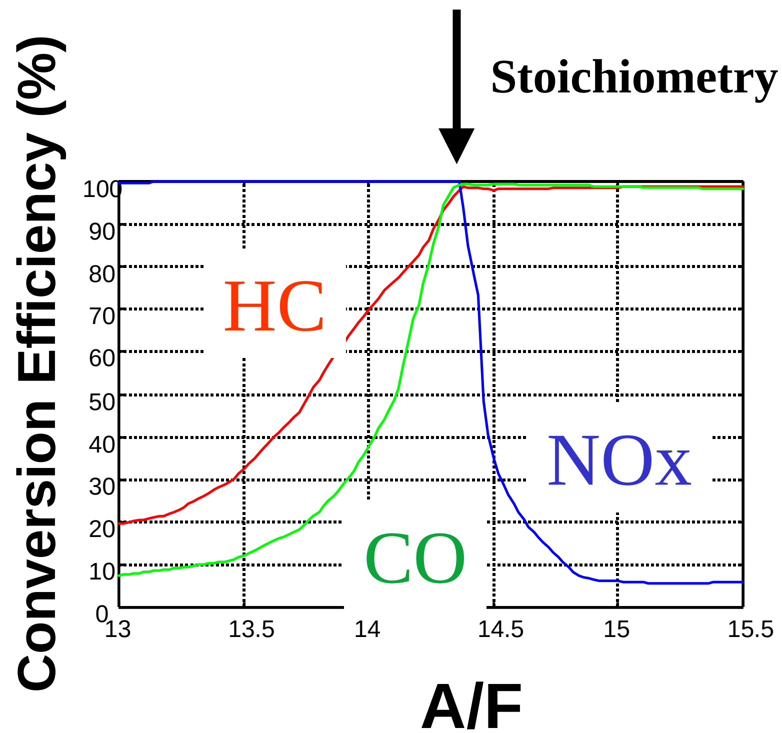
Outline

- Performance Assessment Problem Statement
- Relevant Models
  - DISC Engine
  - Three-way Catalytic Converter
  - Lean NOx Trap
- Results of the Performance Assessment

Classic Engine and Emissions Treatment System





Remarks

- To-date, we have been able to essentially ignore after-treatment system dynamics in feedback design

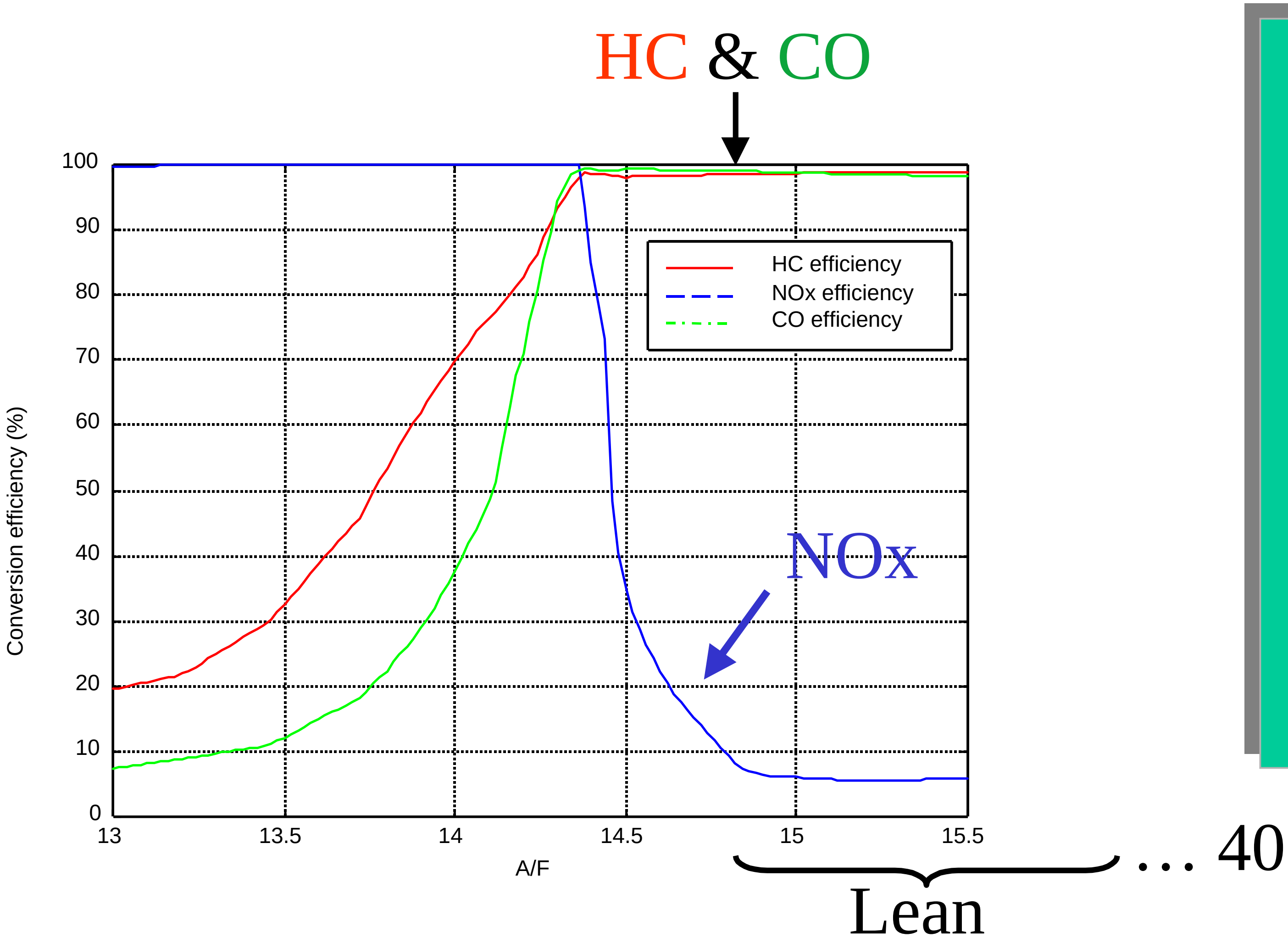
- Create an emissions pseudo-objective:
  - $\rightarrow$ maintain A/F at stoichiometry
  - $\rightarrow$ main focus becomes engine dynamics

- Rare exception: feedback of post-TWC A/F

Lean Burn Basics

- Fuel economy → run SI engine like a diesel:
  - reduce pumping losses with high manifold pressure
  - requires combustion of high air fuel ratios
  - stratified charge engines: 40:1 A/F
- Must also worry about emissions
  - HC & CO easy
  - NOx hard!

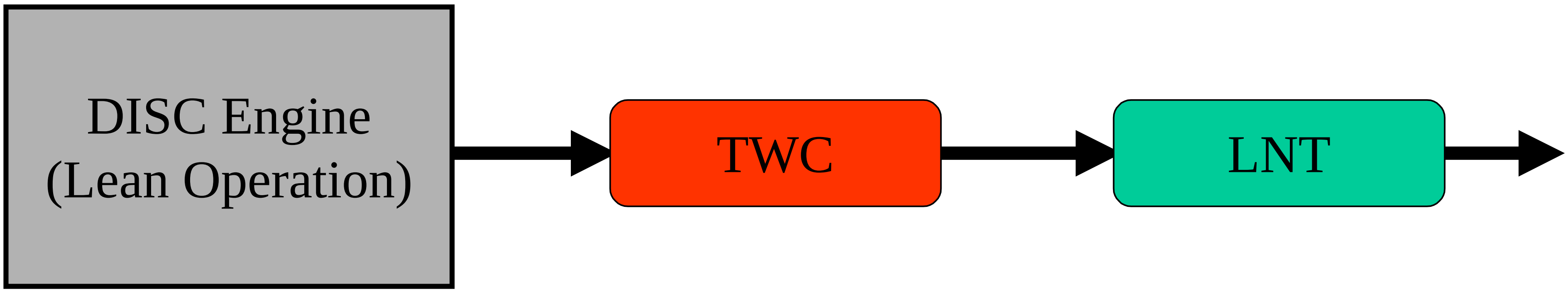
TWC Alone Inadequate for Treating NOx in Lean Operation



Poor NOx conversion for lean mixtures

Must do something else!

Potential Solution: Lean NOx Trap



LNT Basics:

1) Store NOx under lean conditions…. …until device saturates

2) Empty device by reducing NOx under rich conditions

3) Thus, even for constant “speed and load”, steady state system operation unlikely to be acceptable!

Goal: Make Initial Performance Assessment w/o Assembling the Overall System

- Evaluation of fuel economy versus NOx emission trade-off
  - intrinsically a dynamic problem
  - evaluate over an emission test cycle, for example
  - determine how to operate the system (e.g., when to purge?)
  - assess relative effects of component parameters
    - size
    - temperature sensitivity, etc.

Approach

- Dynamic Models
  - DISC engine
  - TWC
  - LNT

\+

•Dyn. Prog.

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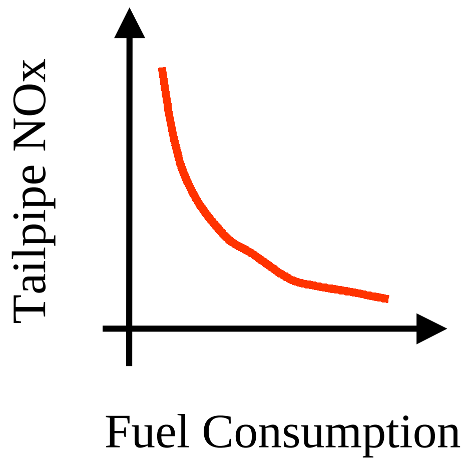
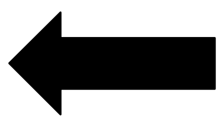
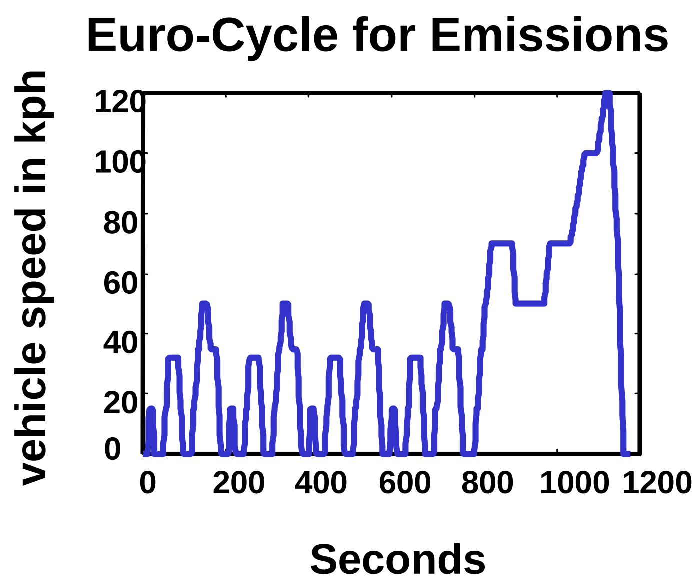






Later step: approximate the optimal control by a causal feedback ….

Engine Model

- 1.8 L, Direct Injection, Stratified Charge
  - homogeneous mode: from 12:1 to 20:1 (A/F)
  - stratified mode: from 25:1 to 40:1 (A/F)
- Model built in standard fashion
  - regression against steady state mapping data
  - insertion of dynamic elements
    - intake manifold
    - EGR
    - fuel injection timing delays
    - transport delays

Engine Model (cont.)

- Inputs:
  - throttle
  - fuel
  - EGR
  - spark
- Injection timing was fixed
- Primary Outputs:
  - torque
    - brake & indicated
  - manifold pressure
  - in cylinder A/F, etc.
  - emissions
    - HC
    - NOx
    - CO
    - feedgas temperature

Control-Oriented TWC Model

- Steady-state conversion efficiency curves are like the steady-state gain of the system
- Would like to get a good approximation of a "time constant" of the TWC
- Possible approaches
  - deduce from existing PDE models
  - measure "it" in a dynamometer test cell
  - propose a phenomenological mechanism/model and fit to data

TWC Basic Chemistry (in the Presence of Pd, Rh and/or Pt)

- Typical Oxidation Reactions

$$2C_3H_6 + 9O_2 \rightarrow 6CO_2 + 6H_2O$$

$$2CO + O_2 \rightarrow 2CO_2$$

- Typical Reduction Reactions

$$2NO_2 \rightarrow N_2 + 2O_2$$

- Combined

$$2CO + 2NO \rightarrow N_2 + 2CO_2$$

TWC Basic Chemistry (cont.)

- Additional key reactions

$$2PdO \underset{\rightarrow}{\leftarrow} 2Pd + O_2$$

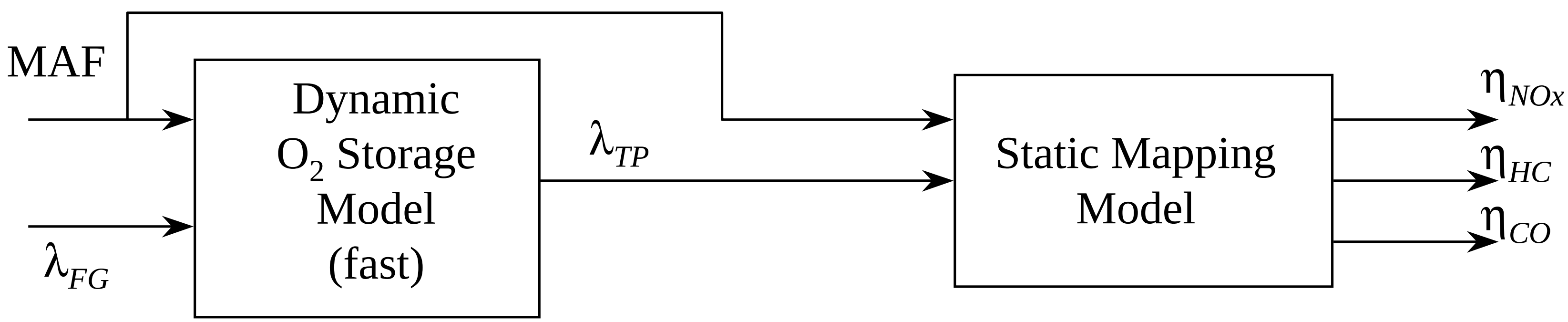
$$4CeO_2 \underset{\rightarrow}{\leftarrow} 2Ce_2O_3 + O_2$$

- Referred to as ‘oxygen storage’

Phenomenological Basis for Model

- **Observation:** A/F through TWC can change only through oxidation and/or reduction reactions
- **Hypothesis:** "time constant" of A/F is rough indicator of "time constants" of underlying chemistry
- **Idea:** Dynamic conversion efficiencies can be approximated by applying standard TWC static curves to A/F at output of TWC

Phenomenological Model Structure for Dynamic TWC (Warm)



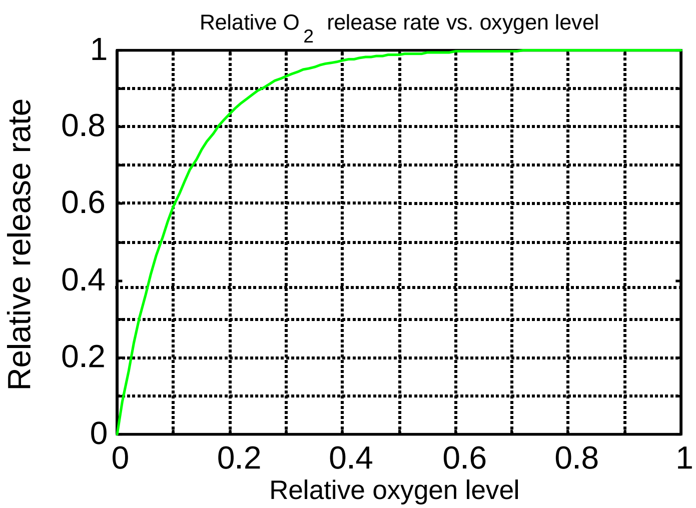
- Accurate to within experimental error on dynamic emission measurements
- Motivates development of a dynamic A/F model for TWC [Shafai et al. (1996)]

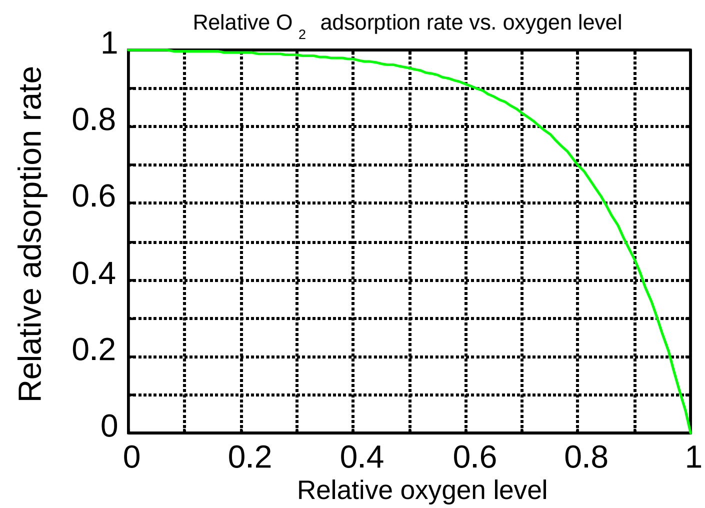
Oxygen Storage Sub-model

"sticking" fraction

Oxygen excess/deficit

$$\dot{\Theta} = \begin{cases} \frac{1}{C} \times \rho(\lambda_{FG}, \Theta, MAF) \times 0.21 \times MAF \times (1 - \frac{1}{\lambda_{FG}}) & 0 \leq \Theta \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

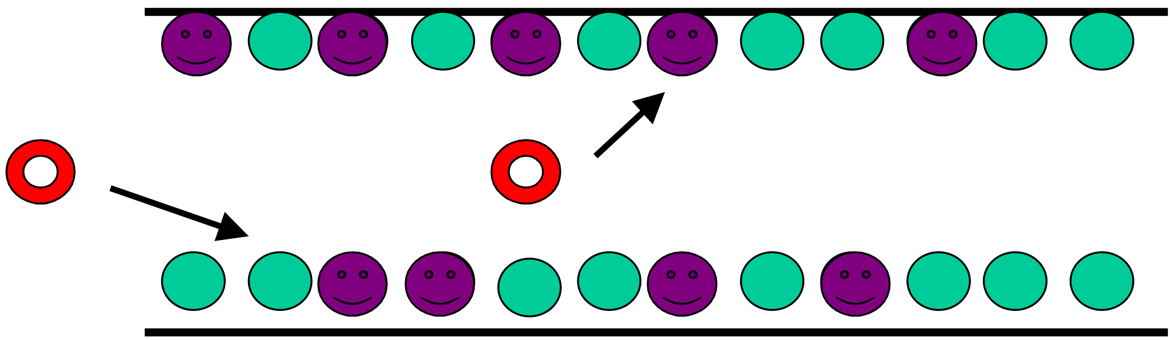




$\Theta = \text{Relative } O_2 \text{ level}$

$\lambda_{TP} = \lambda_{FG} + (O_2 \text{ storage effect})$

Storage and Release Rates Depend on Number of Available Pd or Ce Sites

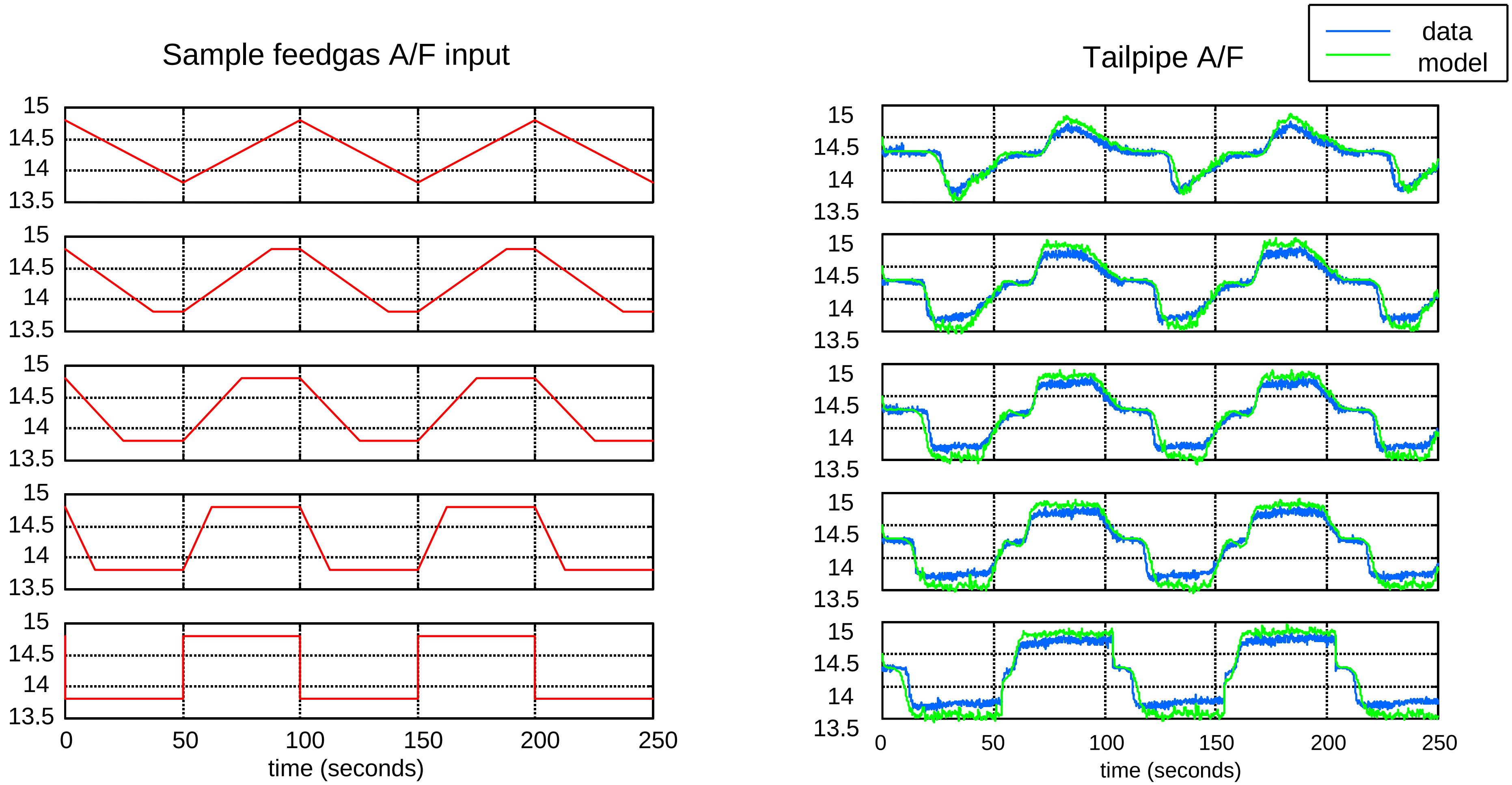


= O_2

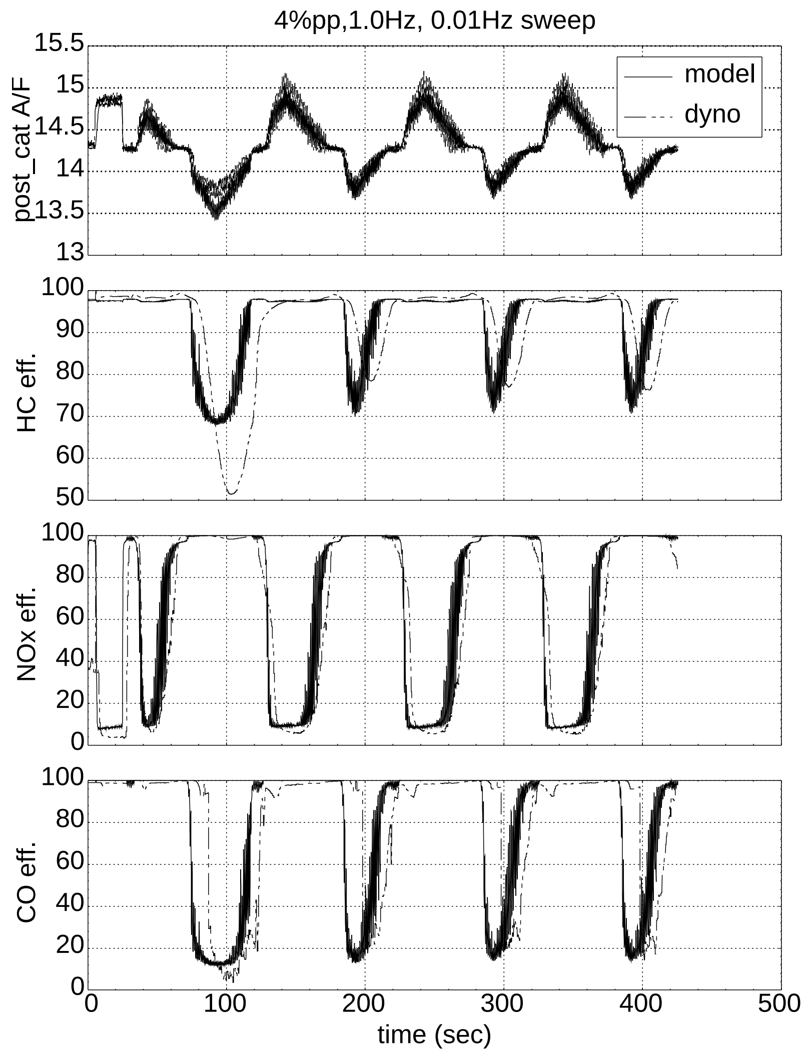
= Pd or Ce

= **PdO or CeO_2**

Dynamic A/F Validation



Dynamic Emissions Validation



LNT Storage Chemistry

- Under lean conditions, NO is oxidized to NO_2 in the gas phase over platinum.
- The resulting NO_2 is adsorbed on barium carbonate surface as barium nitrate.

$$NO + \frac{1}{2} O_2 \overset{\text{Pt}}{\Leftrightarrow} NO_2$$

$$BaCO_3 + 2NO_2 \Leftrightarrow Ba(NO_3)_2$$

Surface saturates and must be renewed….by running rich (purging)!

LNT Purge Chemistry

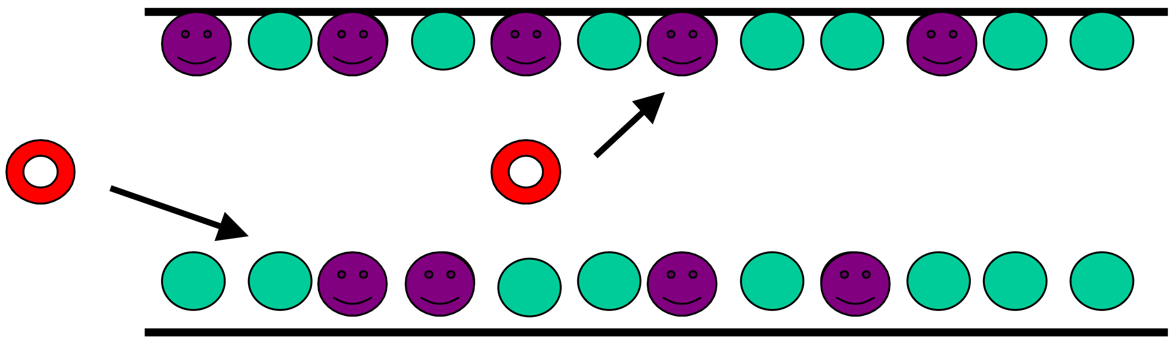
- At rich air fuel ratios, the adsorbed barium nitrate is released from the trap as barium oxide.
- In the presence of reducing agents (such as CO, HC and H2) and the platinum/rhodium catalyst, the NO_x is converted to nitrogen.

$$Ba(NO_3)_2 \Leftrightarrow BaO + 2NO_2$$

$$BaO + CO_2 \longrightarrow BaCO_3$$

$$2NO_2 + 2CO \xrightarrow{Pt/Rh} N_2 + 2CO_2$$

Key Feature: State Dependent Storage Efficiency



= NOx

= Ba CO3

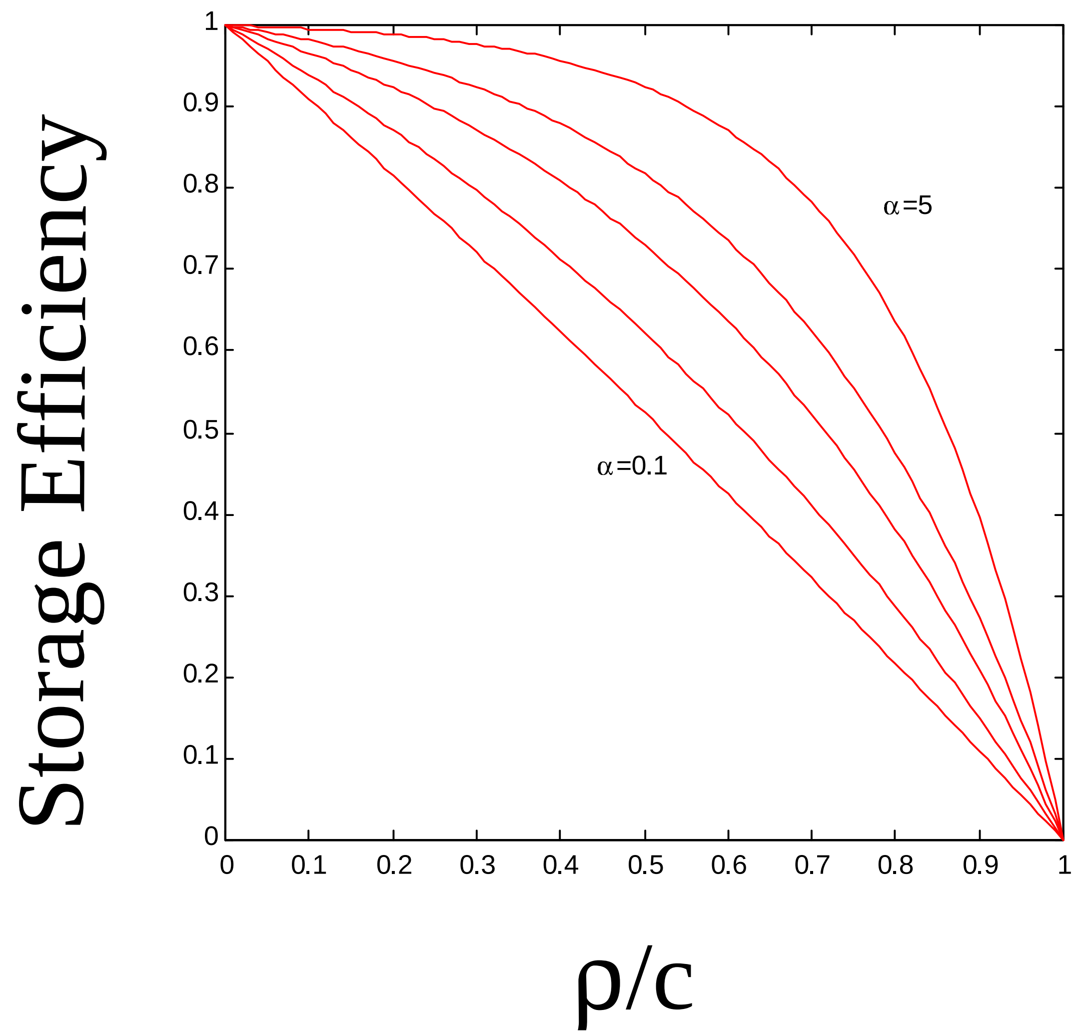
= **$Ba(NO_3)_2$**

"Probability of sticking" depends of how full the trap is

Storage efficiency versus the ratio of trap state to capacity

$$\varepsilon(x) = \frac{e^{\alpha x} - e^{\alpha}}{1 - e^{\alpha}}$$

x = ρ/c



Nomenclature for Trap Model

- λ relative air fuel ratio of exhaust entering the LNT
- ρ mass of NOx stored in the LNT (g)
- c maximum capacity of the LNT (g)
- $\dot{NOx}$ and $\dot{CO}$ flow rates of NOx and CO into LNT (g/s)
- β is the reduction rate of NOx in the LNT (fraction)
- μ is the maximum empty trap storage efficiency (fraction)
- γ moles of CO needed to reduce one mole of NOx

Phenomenological Trap Model
"Mass Balance"

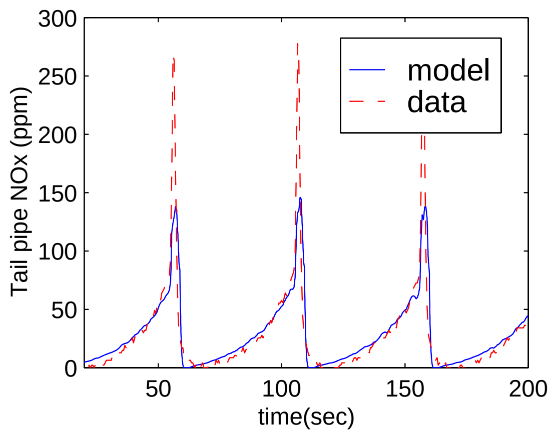
$$\frac{d\rho}{dt} = \begin{cases} f_L(\rho, N\dot{O}x, c) & \lambda \geq 1 \,\&\, 0 \leq \rho \leq \mathrm{c} \\ f_R(\rho, C\dot{O}) & \lambda < 1 \,\&\, 0 \leq \rho \leq \mathrm{c} \\ 0 & \text{otherwise} \end{cases}$$

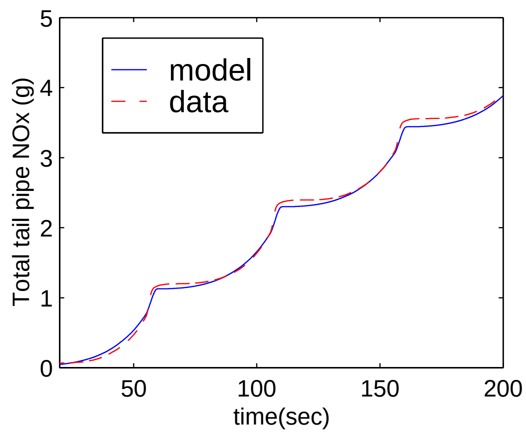
$$f_L(\rho, N\dot{O}x, c) = (1-\beta) \times N\dot{O}x \times \mu \times \varepsilon(\rho / c)$$

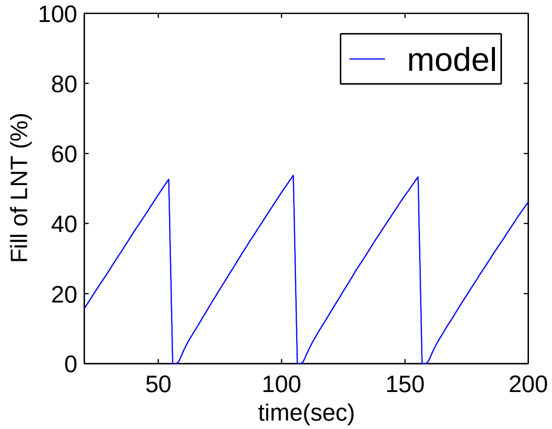
$$f_R(\rho, C\dot{O}) = -\gamma \times C\dot{O}$$

$$y = \begin{cases} (1-\beta) \times (N\dot{O}x - f_L(\rho, N\dot{O}x, c)) & \lambda \geq 1 \\ 0 & \lambda < 1 \end{cases}$$

Model versus Data







← Not a measurable quantity

Qualitative Analysis

- Time-scales
  - LNT nominally 30 sec to 1 minute to “fill”; 1 to 3 seconds to “purge”
  - TWC nominally a few secs to “empty-fill”
  - Intake manifold nominally 4 to 6 engine revolutions to “empty-fill”, or 100 ms

⇒Dynamics of exhaust system are dominant

⇒Can start with a static engine model

⇒Optimization complexity determined by exhaust system models

Optimization Problem

- Overall Model of Engine + Exhaust System

$$x_{k+1} = f(x_k, u_k)$$

$$u = \begin{cases} \text{throttle} \\ \text{fuel} \\ \text{spark} \\ \text{EGR} \\ \cdots \end{cases}$$

- Cost

$$J = \sum_{k=1}^{N} g(x_k, u_k)$$

$$g(x_k, u_k) = \text{fuel}_\text{k} + \mu \text{NOx}_\text{k}$$

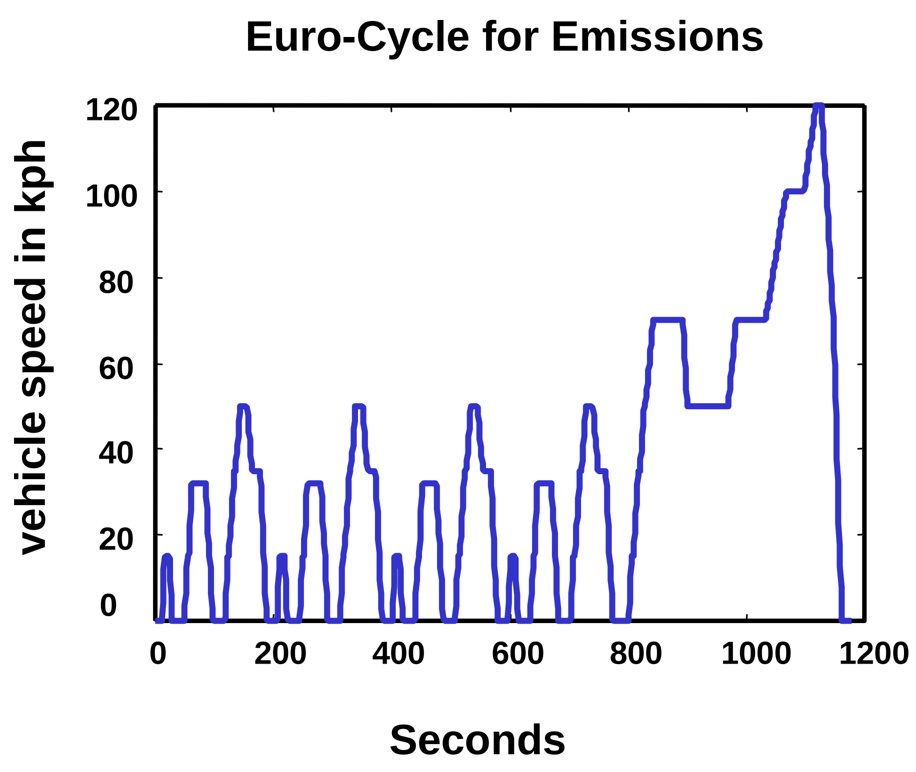
Optimization Problem (cont)

$$\min_{u_k} \quad J = \sum_{k=1}^{N} g(x_k, u_k)$$

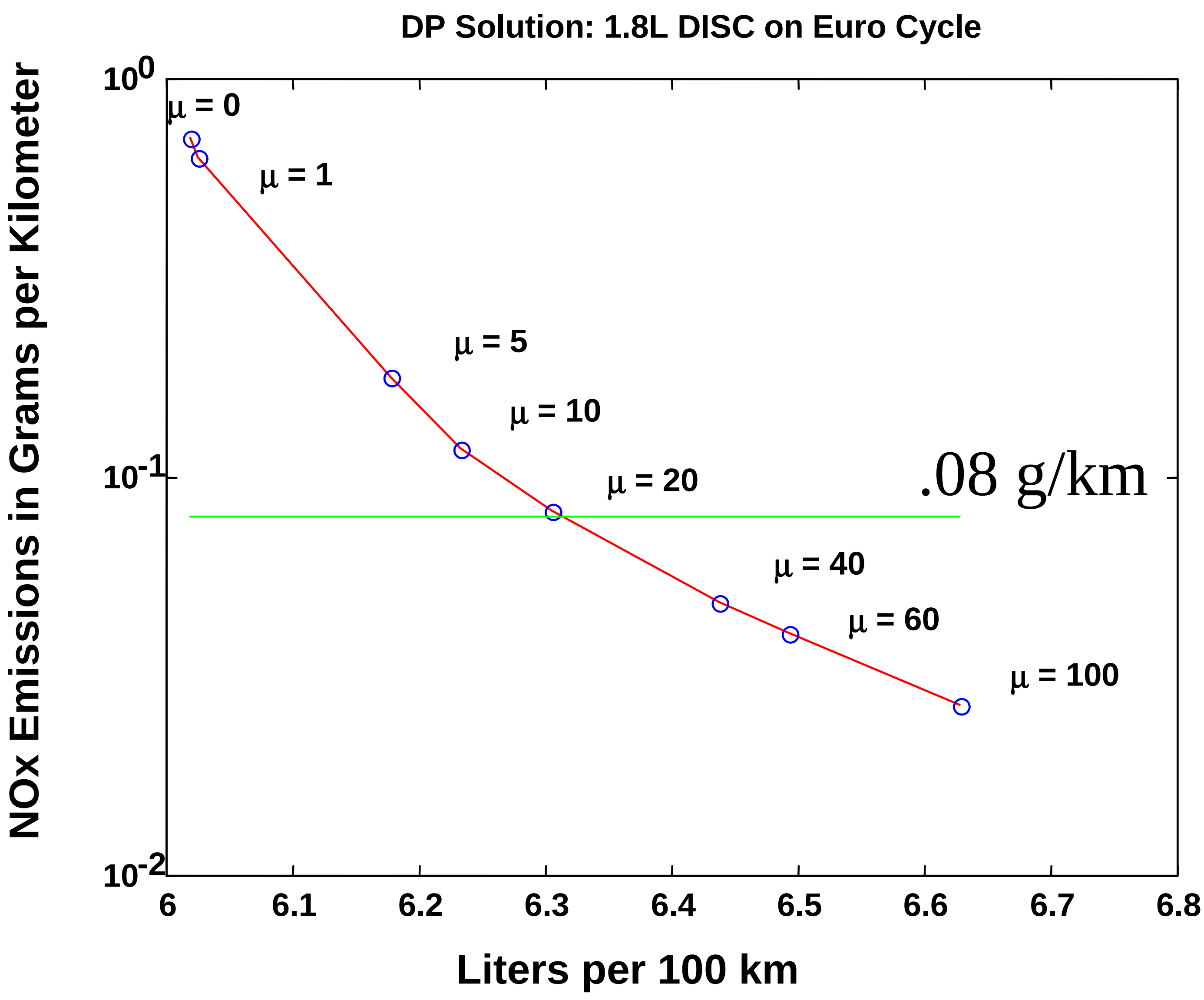
Subject to:

•Physical limitations on actuators, states ….

• Drive a given emissions cycle (Euro-Cycle)



Nominal Trade-off Curve



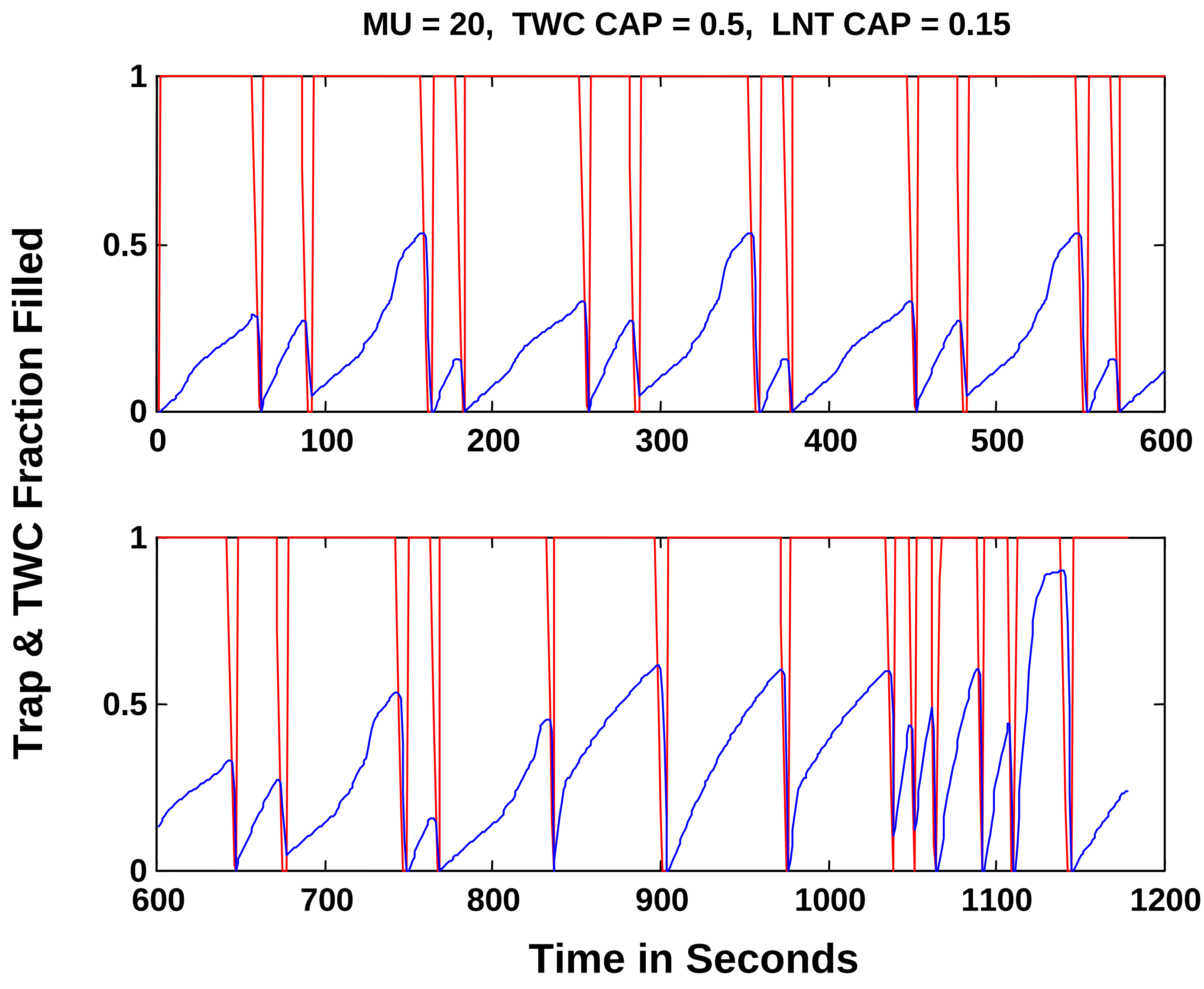
TWC Cap = 0.5 g

LNT Cap = 0.15g

FE = 6.3 l/100 km

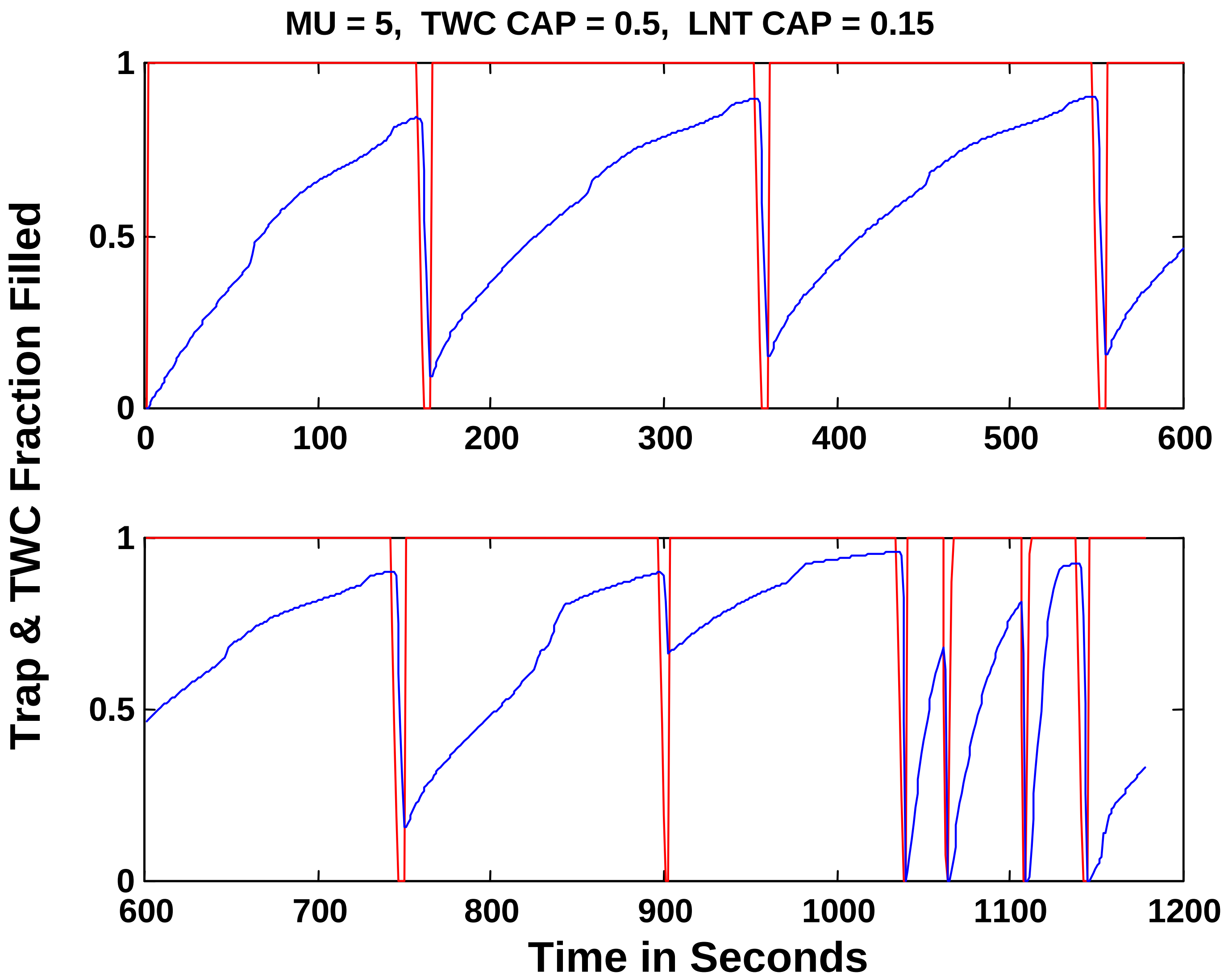
= **37.3** mpg

Nominal Optimal Dynamic Response



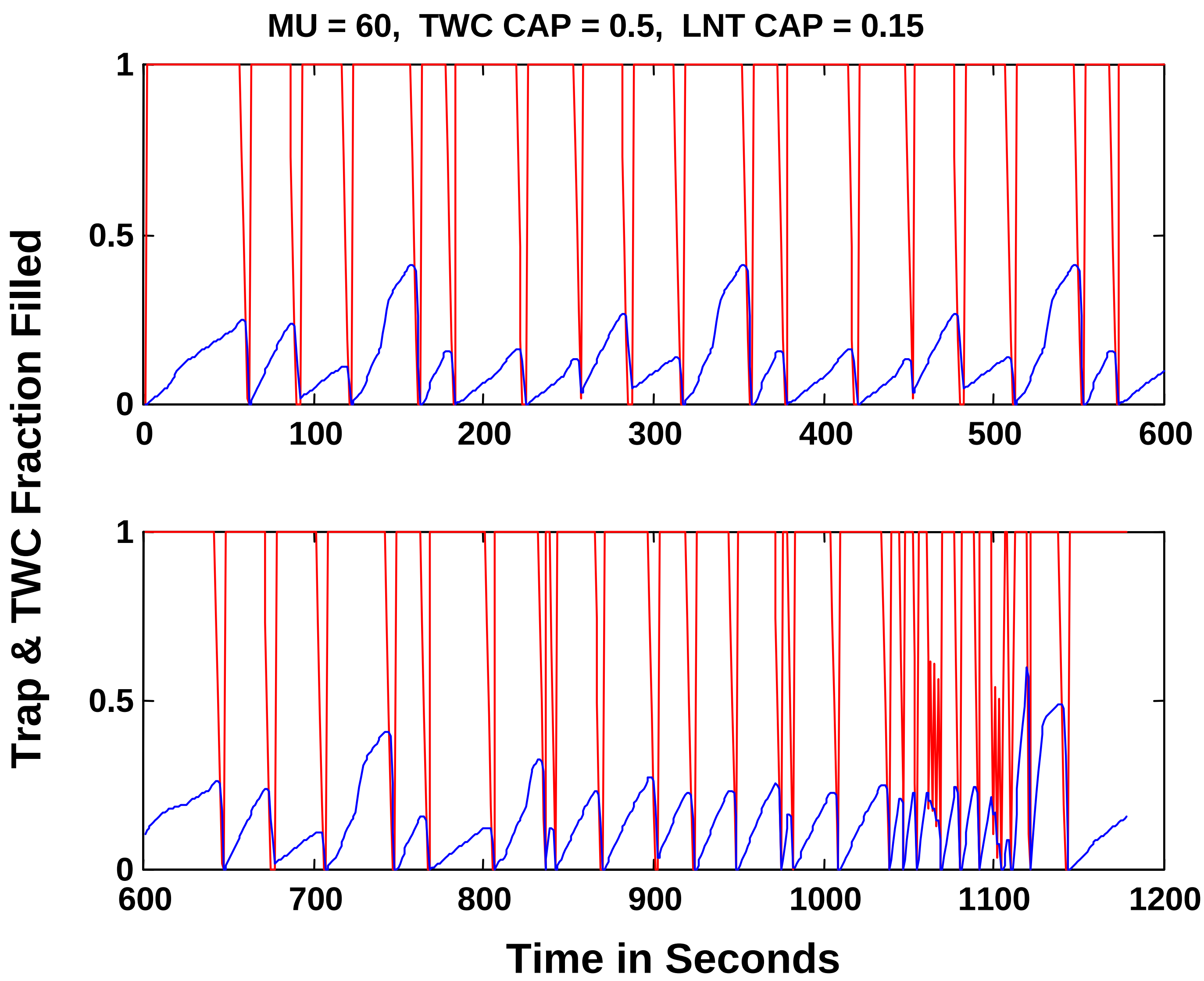
High Fuel Economy Dynamic Response

(infrequent purging)

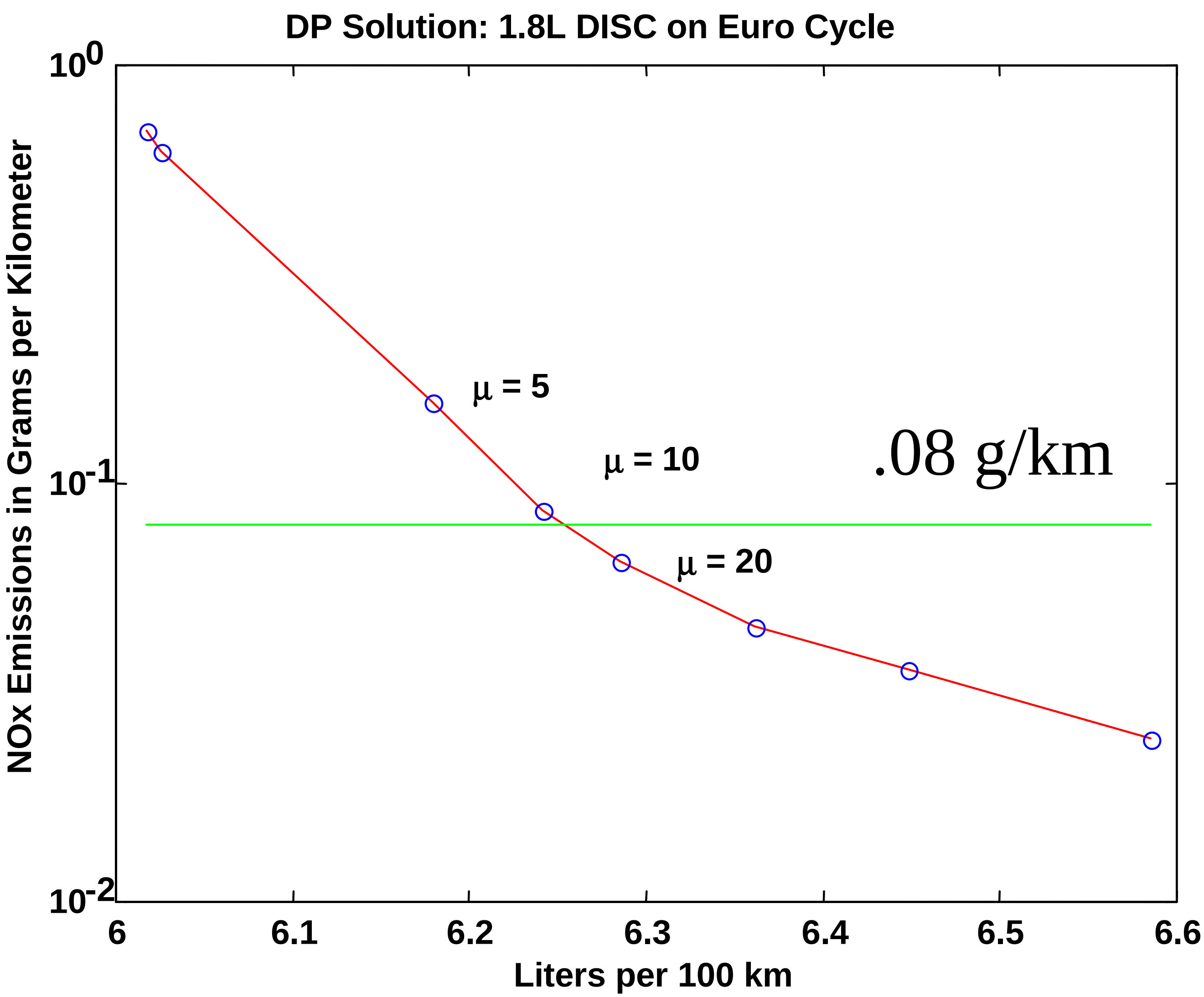


Lower NOx Dynamic Response

(more frequent purging)



Trade-off Curve w/ 200% LNT Cap.



TWC Cap = 0.5 g

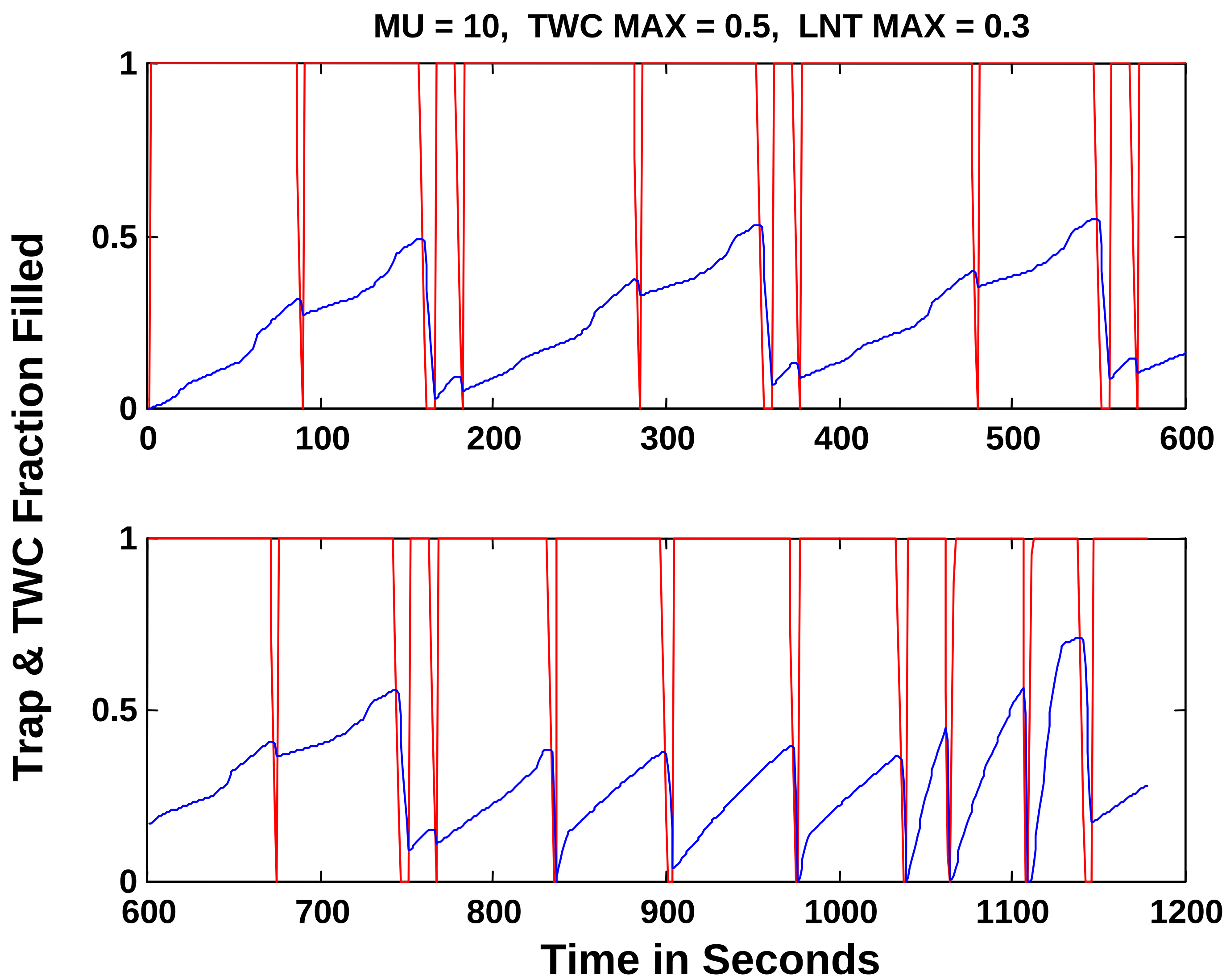
LNT Cap = 0.3g

FE = 6.25 l/100 km

= **37.6 mpg**

Nominal = **37.3** mpg

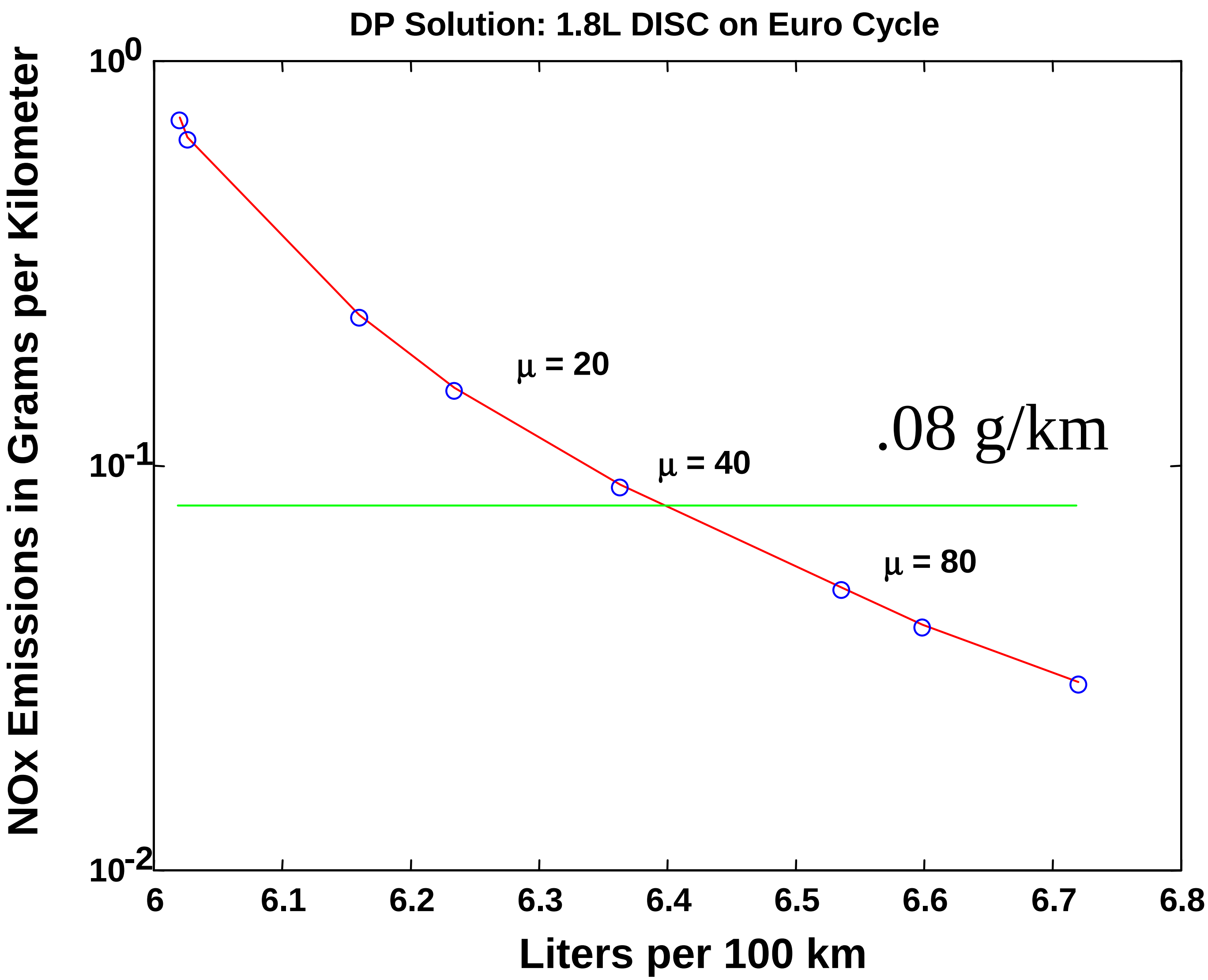
Optimal Dynamic Response w/ 200% LNT Capacity



Remarks

- Doubling the LNT capacity has improved the fuel economy by less than 1%
- However, it has yielded an ‘easier’ closed-loop purge control problem
  - less frequent purging
  - less sensitive to errors in the purge time schedule

Trade-off Curve w/ 50% LNT Cap.



TWC Cap = 0.5 g

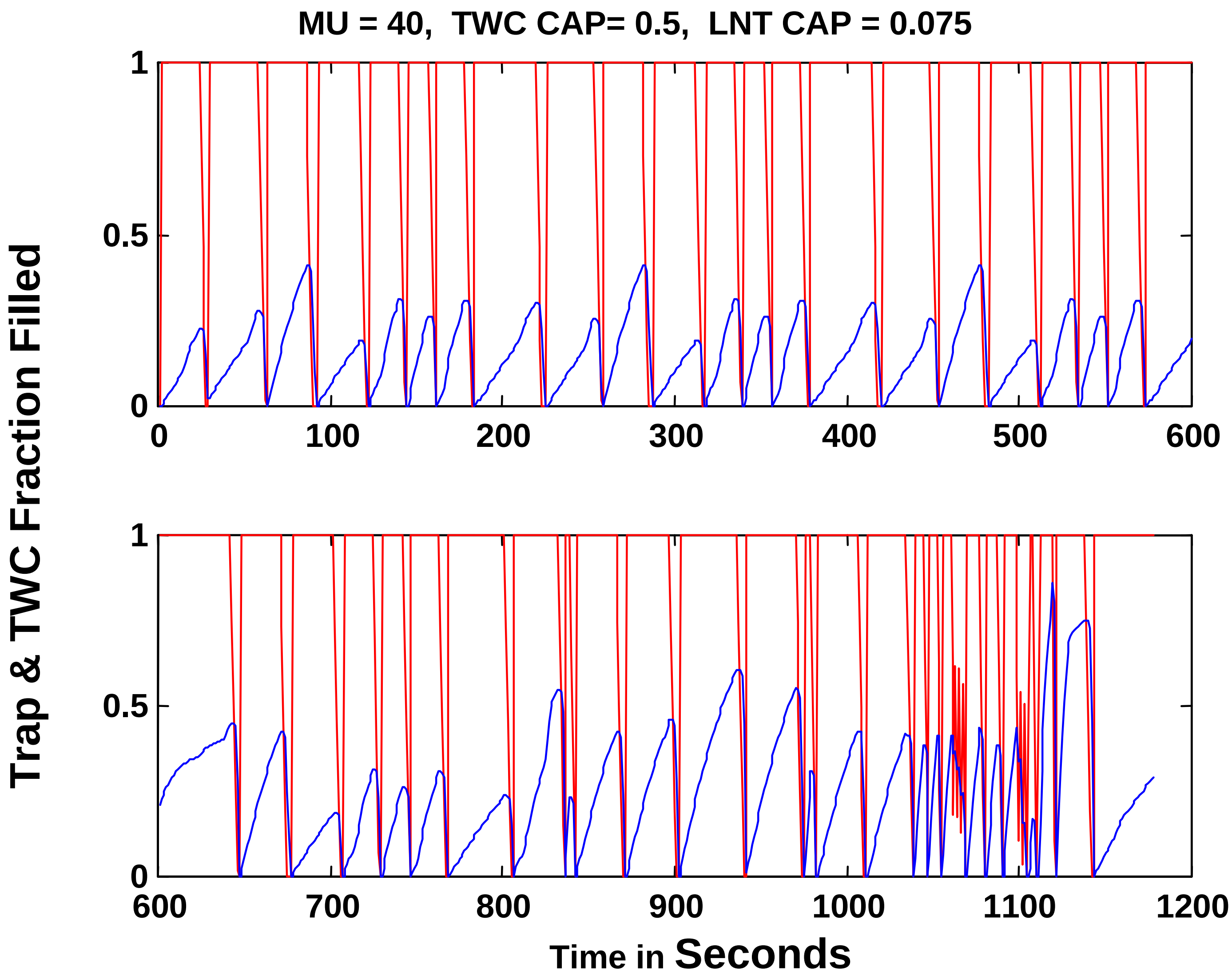
LNT Cap = 0.075 g

FE = 6.54 l/100 km

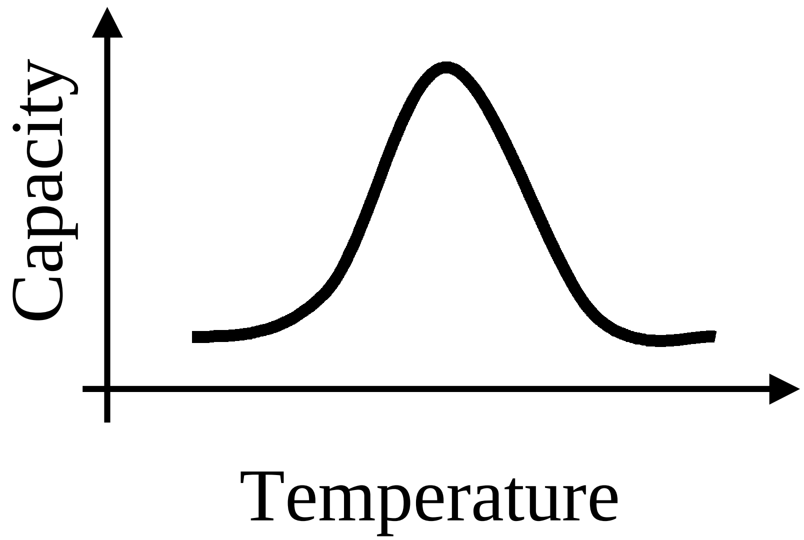
= **36.0 mpg**

Nominal = **37.3** mpg

Optimal Dynamic Response w/ 50% LNT Capacity

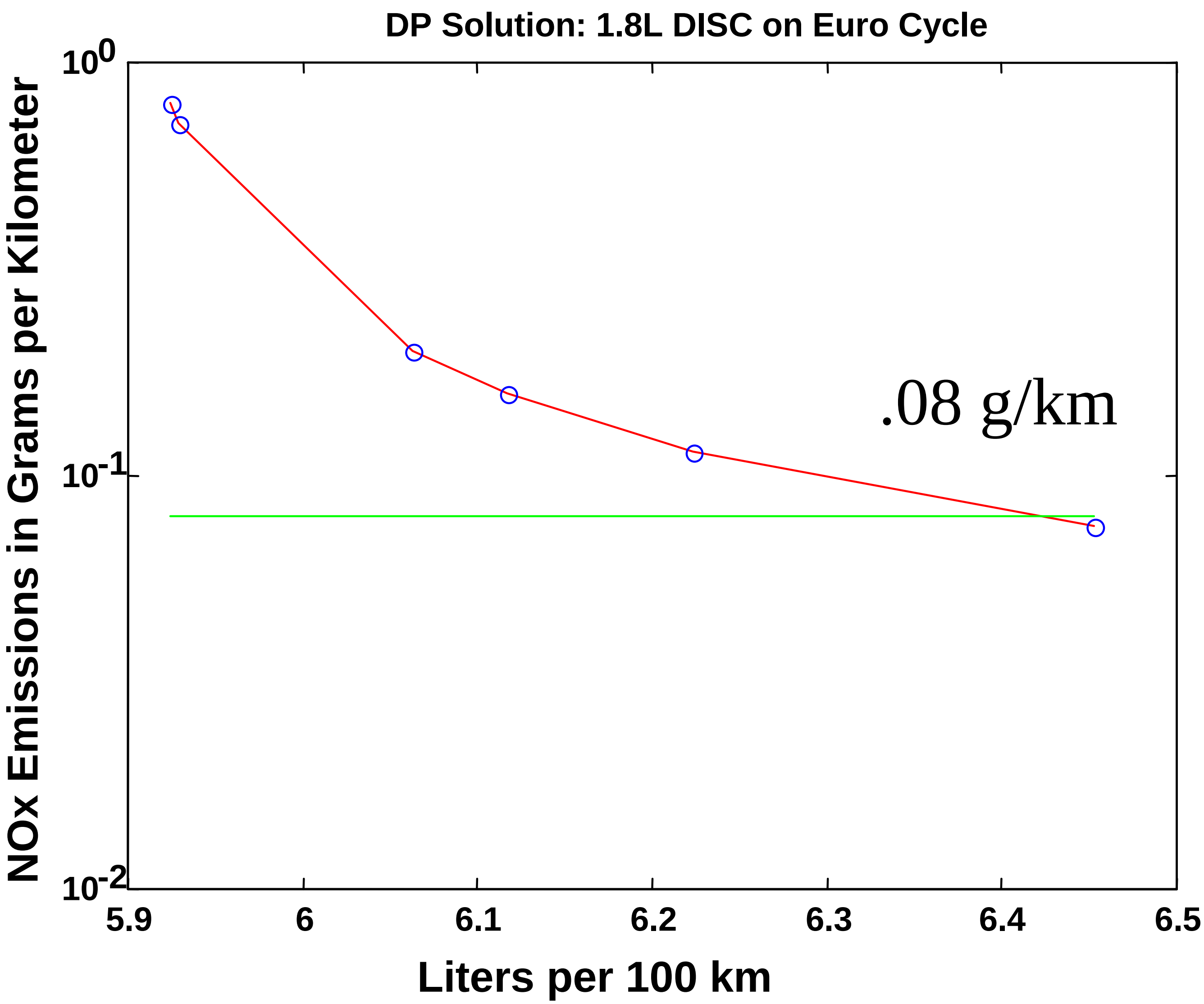


Temperature Dependence in LNT Performance



- Trap capacity and storage rate depend on temperature
- Will assess impact on performance

Trade-off Curve w/ Temp. Model



TWC Cap = 0.5 g

LNT Cap = 0.15 g

FE = 6.41 l/100 km

= **36.7 mpg**

Nominal = **37.3** mpg

Remarks

- Capacity of trap becomes low in many sections of the Euro-cycle due to temperature variations
  - idles
  - high torque output
- This cannot be easily off-set through feedgas temperature management via spark, for example
- Loss of trap capacity due to temperature is very significant over the Euro-cycle
- Purge control will probably require LNT temperature sensing.

Conclusions

- Rapid development process requires technology assessment prior to full hardware build-ups
- A model based performance assessment of a lean burn system was undertaken here
  - models were developed separately and in parallel
  - exhaust system models were a key component
  - optimization based methods allows one to systematically sort through dynamic performance issues …
  - … if you can determine a low dimensional set of dominant dynamics