Aftertreatment Models in Full System Simulations for System Integration

Innovation You Can Depend On.™

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Gary Salemme
Lars Henrichsen

13th CLEERS Workshop
22 April 2010

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Overview

- A/T models
- Analysis Lead Design
- Vehicle System Simulation
- Hardware in the Loop
- Develop Controls and Calibrations

Lean Exhaust Aftertreatment

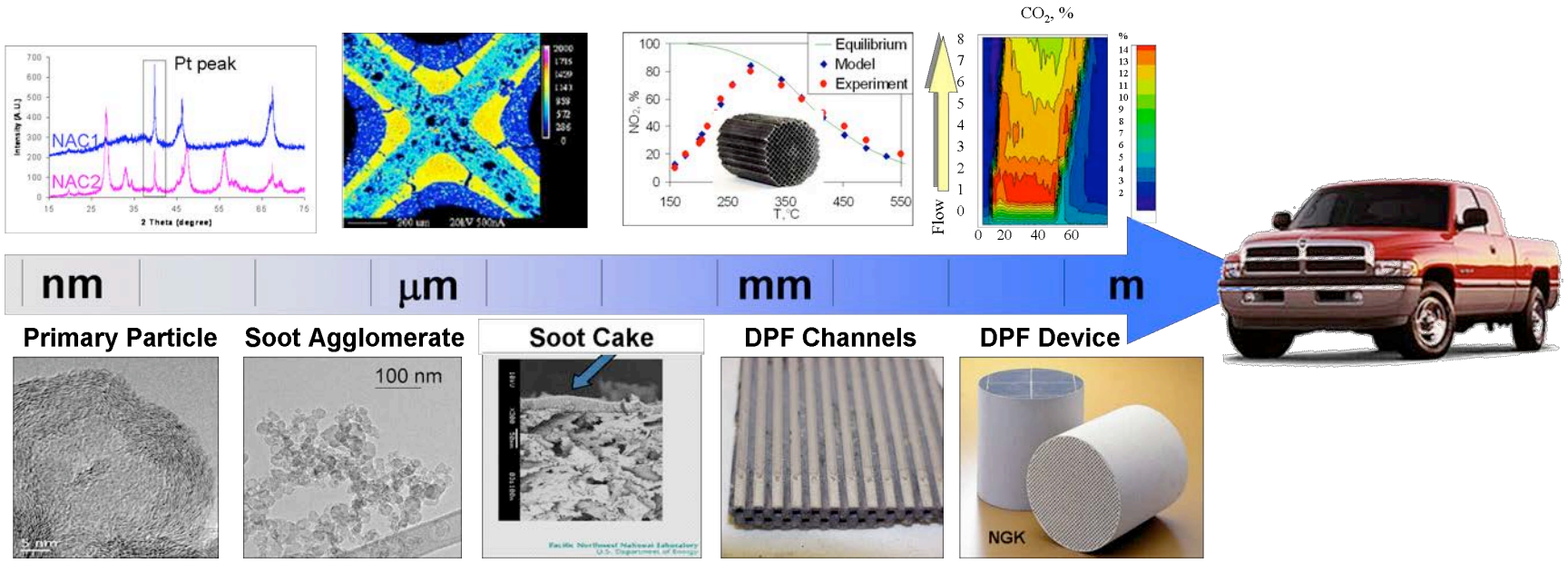
Inherent chemical challenges are

- Broad range of conditions and applications
  - Including off-road applications (marine, locomotive, mining, etc.)
- Transient and *unpredictable* driving cycles
- Actively controlled devices
- On-board diagnostics

Mobile applications of such “chemical plants”, with high *efficiency*, *durability* and *diagnostic transparency*, require detailed, ***quantitative*** understanding of their chemistry, reaction engineering:

- Models-assisted system/application design and controls (*kinetics in the “brains” of the trucks!*)

A/T Catalyst Fundamentals

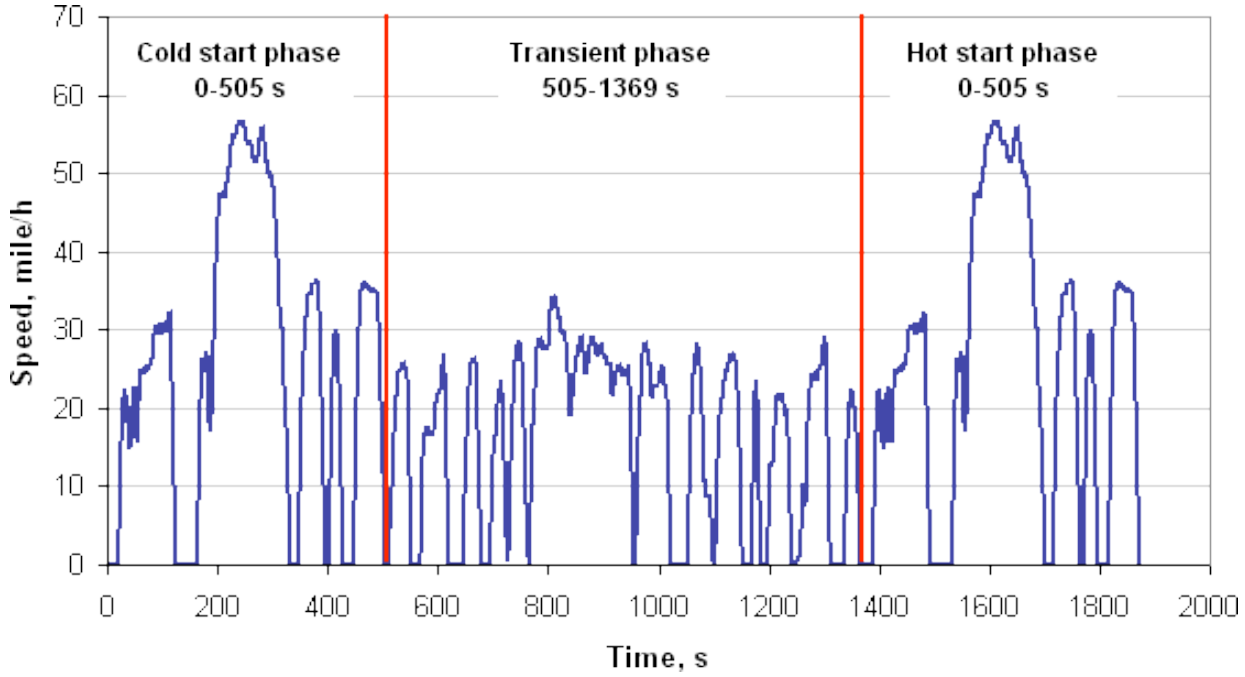


- Collect performance data
  - Do performance and properties roughly fit the application?
  - New control strategy not new catalyst
- Develop understanding of catalyst chemistry and kinetics
  - Precursor to control strategies
  - Physical limit maps
- Collect data for model development

Active Catalytic Devices With a "*Memory*"

Catalyst Performance = F(T, P, [A_i], S.V., *History*)

- Short-term History: e.g., trapping efficiency=f(amount trapped)
- Mid-term History: reversible morphological and chemical changes
- Long-term History: catalyst "aging"

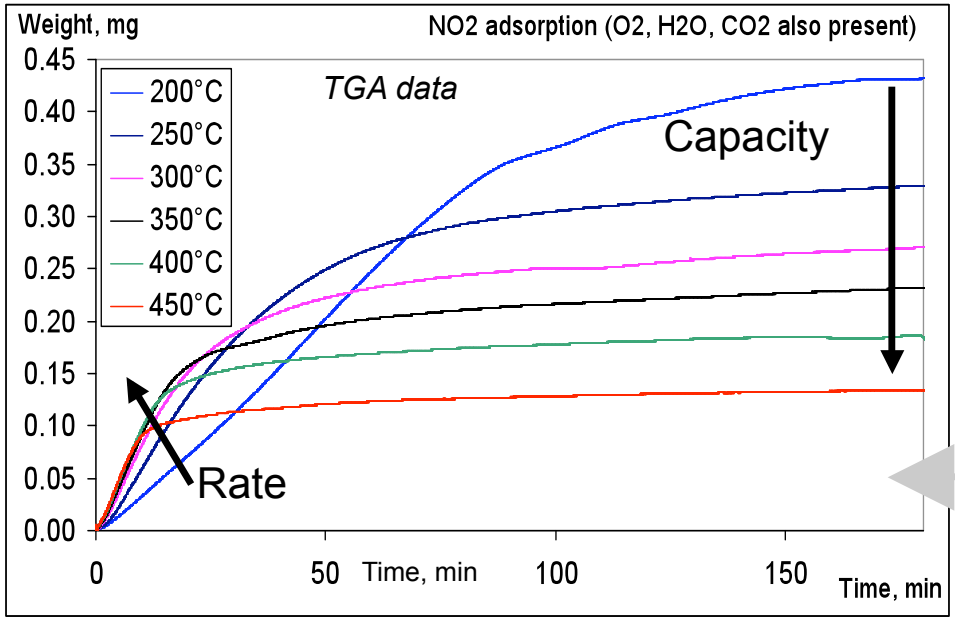


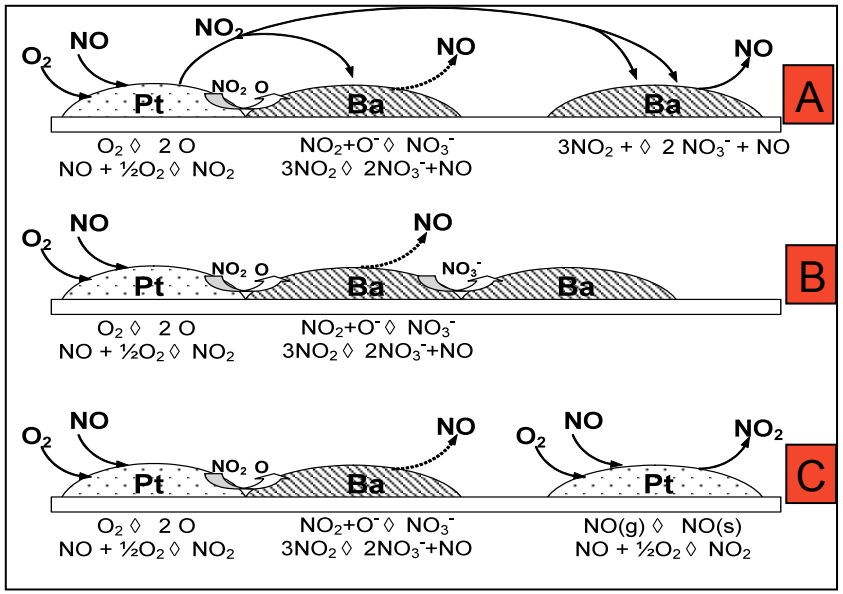
LNT NO_x **Storage** Process

Overall Reaction Equations:

- $NO + 1/2O_2 <=> NO_2$ $\qquad$ $2\overset{+4}{N}O_2 + BaO + \overset{?}{[O]} <=> Ba(\overset{+5}{N}O_3)_2$

- NO_2 adsorption includes both *acid-base* and *redox* chemistry [1]



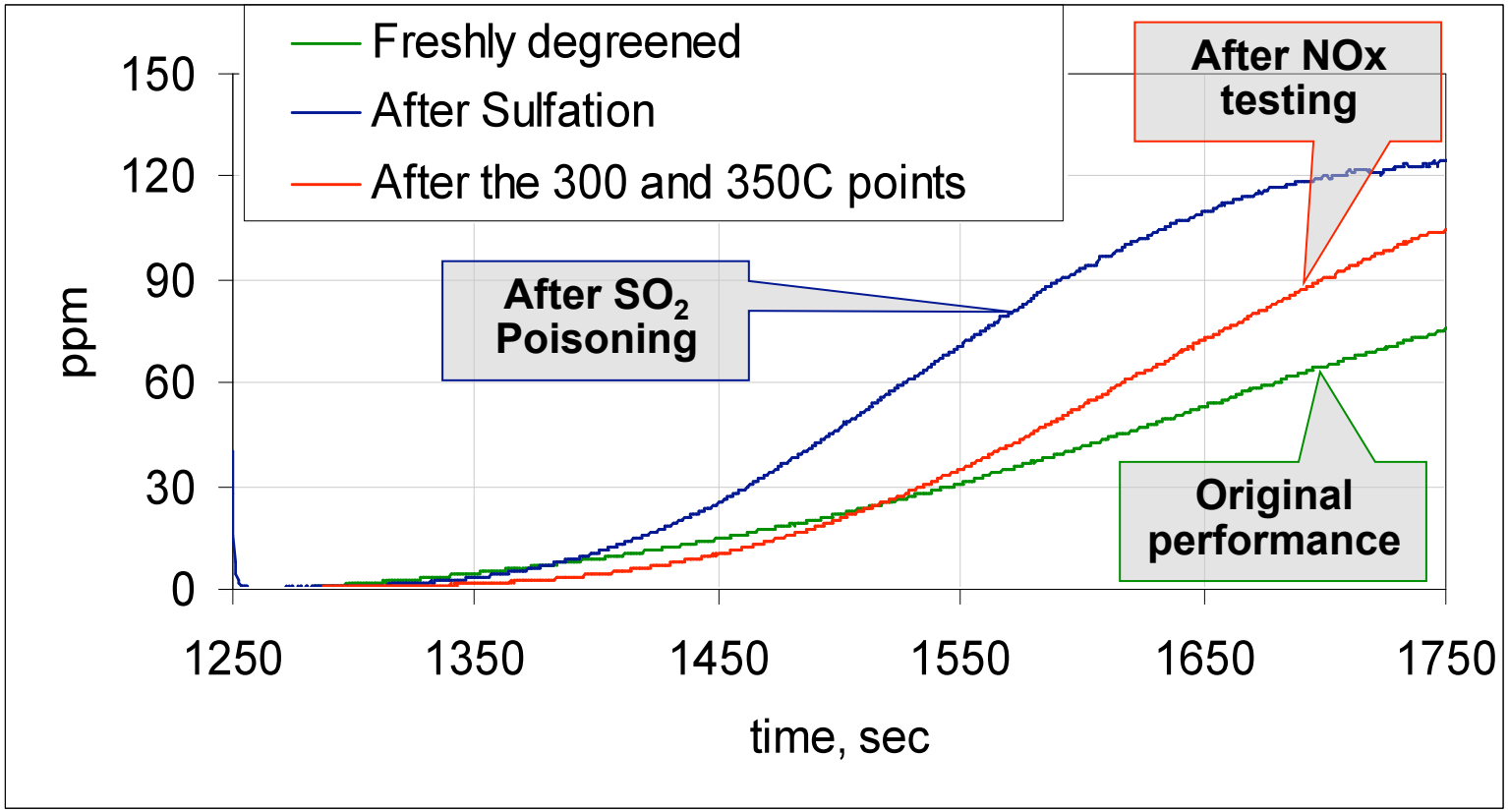


Kinetics, mass-transport and thermodynamics all play a role, depending on operation regime

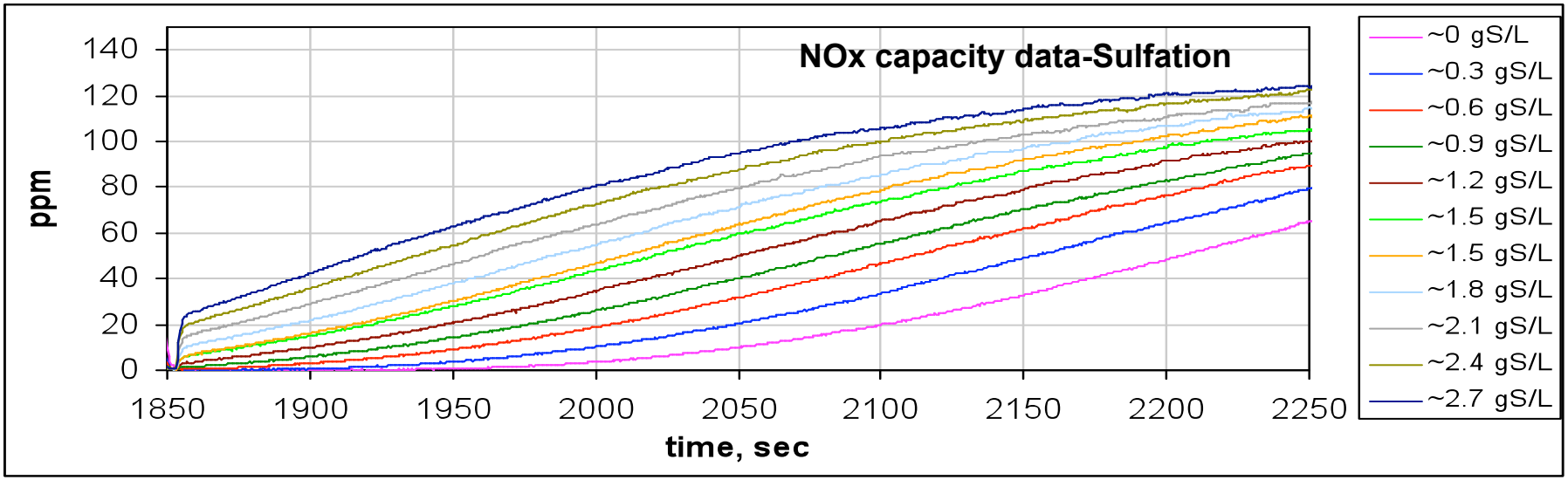
[1] Epling, Yezerets, Currier et al. "*Overview of the Fundamental Reactions and Degradation Mechanisms of NOx Storage/ Reduction Catalysts*". **Catalysis Reviews**; V46(2004), p.163-245

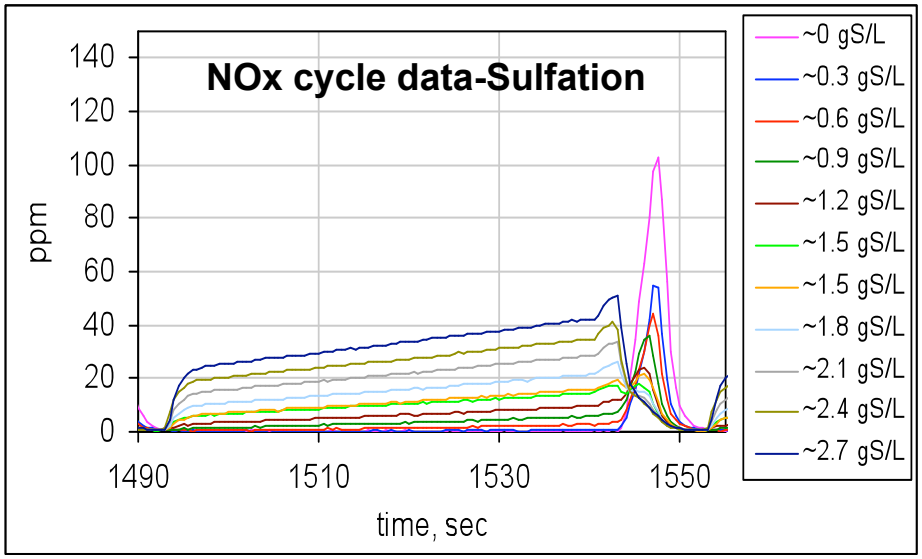
Re-arrangements via “nitrate melting”

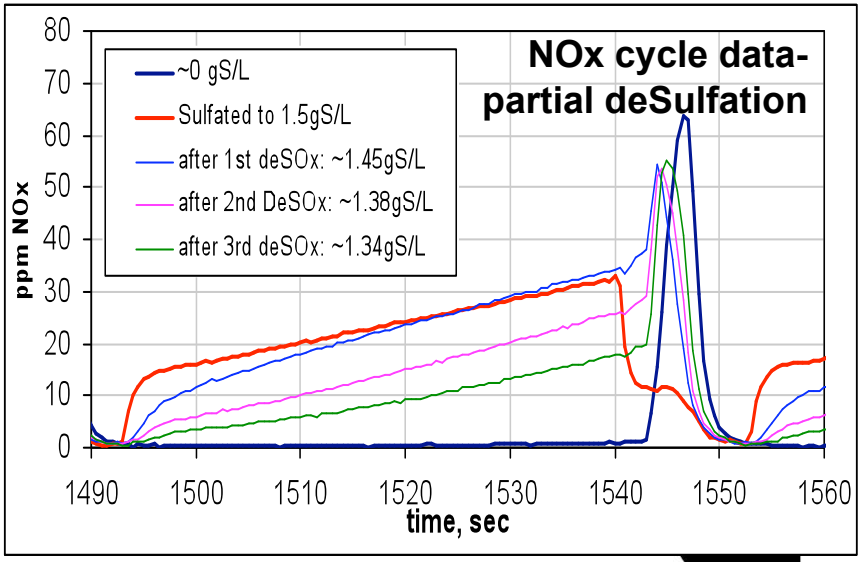
- Sulfated a “Degreened” LNT,
  - Lost ~1/3 of NOx capacity
- 300-400C NOx operation
- Subsequent Temperature-Programmed Reduction (TPR): no change in [S] amount or nature



Sulfur poisoning

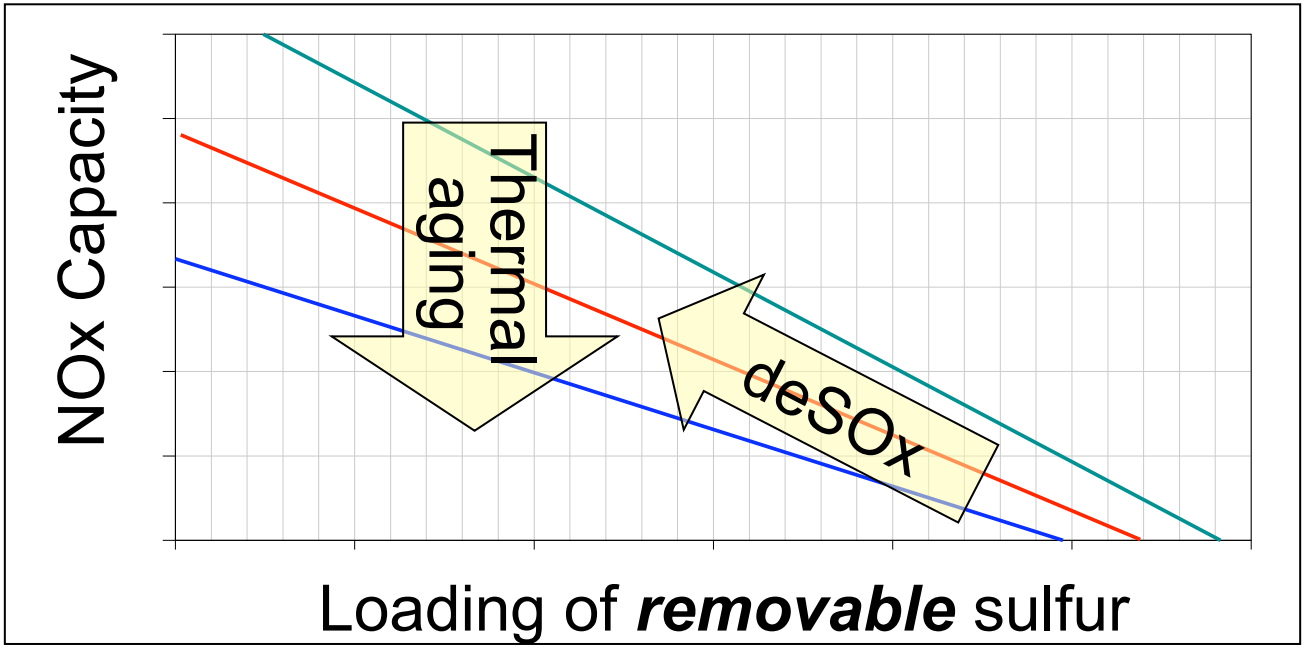






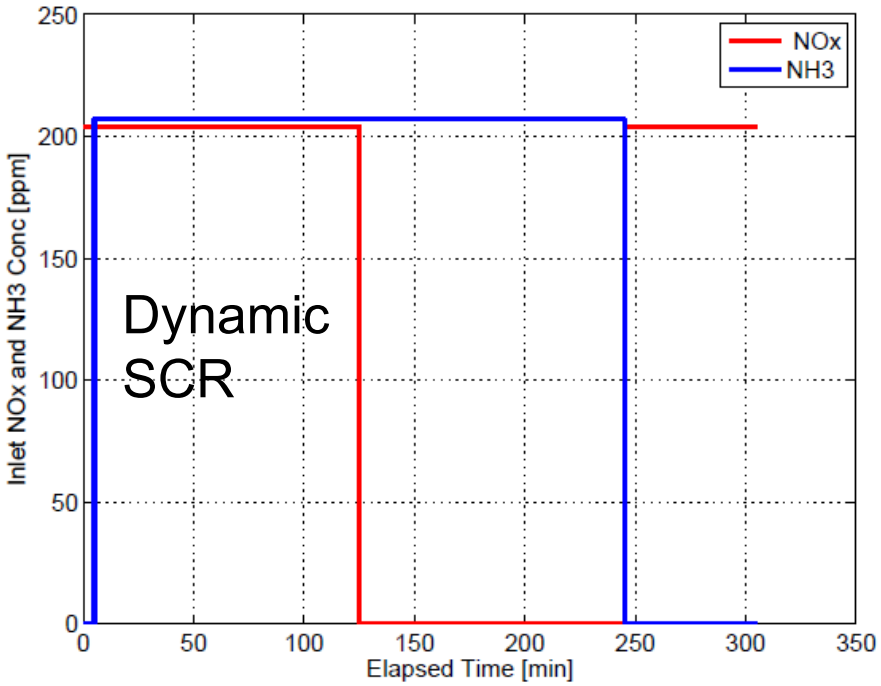
Sulfur Removal vs. Thermal Deactivation

- Minimize excessive temperature exposure
  - Accurate control of deSOx temperature
  - Minimize temperature gradients across the NAC
  - Optimize reductant quality
  - Target only relevant forms of sulfur
  - Capable laboratory diagnostic tools

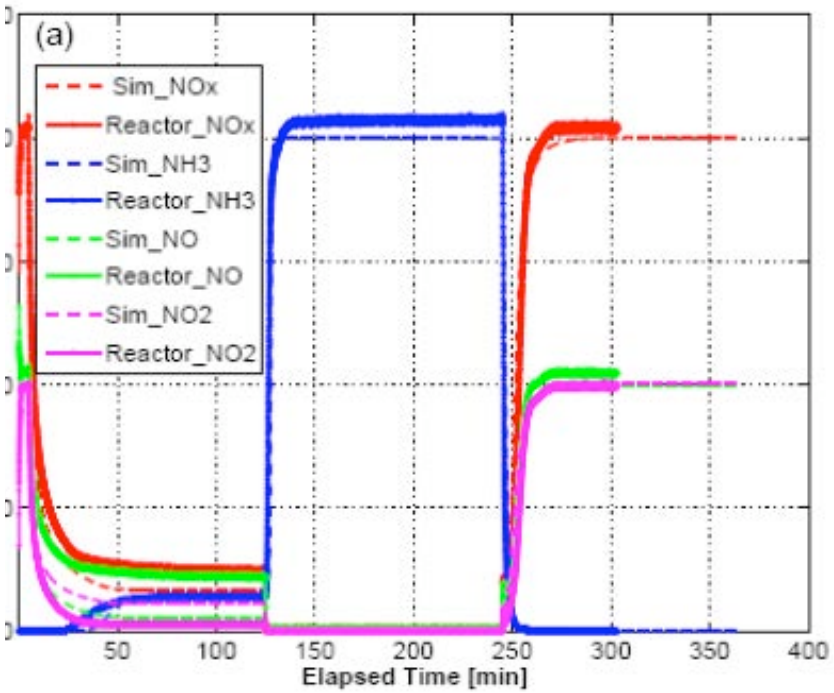


Model Validation – How good is good?

SCR Inlet NOx, NH3



SCR Outlet NOx, NH3

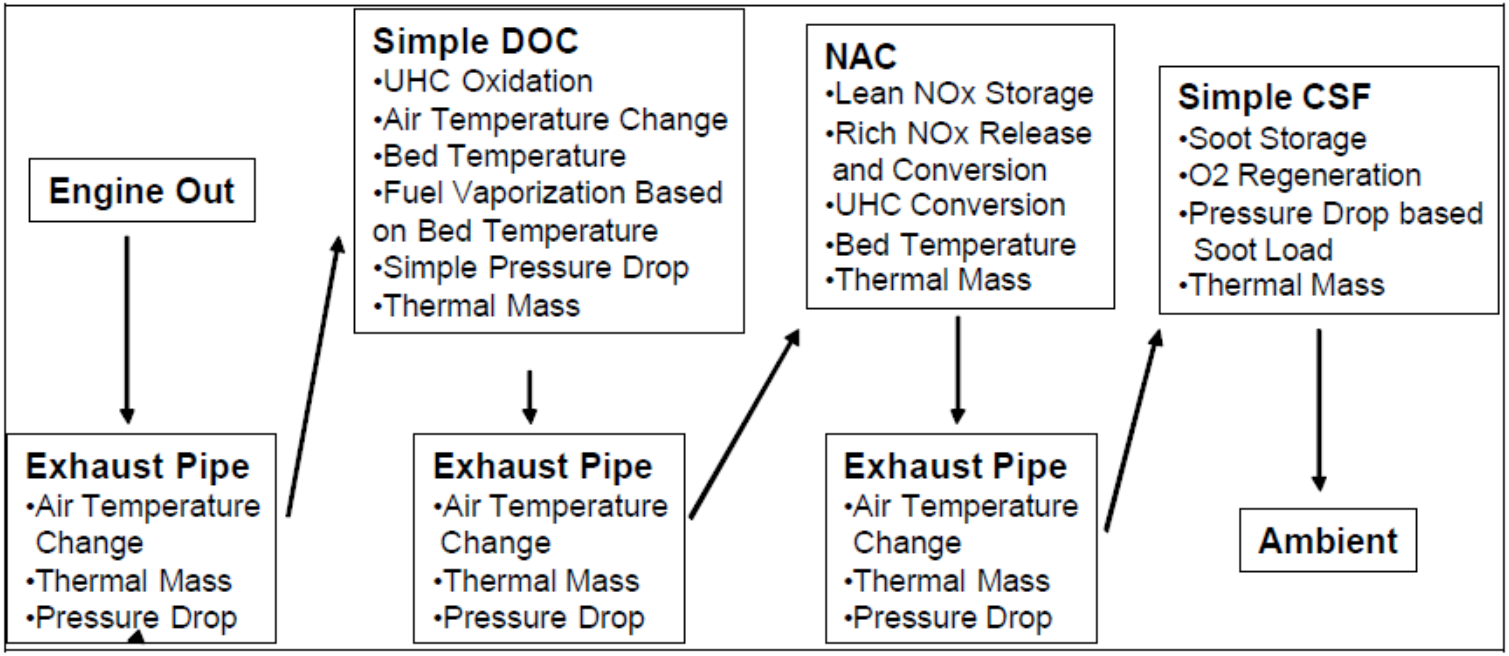


Space Velocity: 40 [k/hour];

Temperature: 200 [C]

NOx Split: 0.5

From the components, an A/T System is Built



- The level of model is appropriate to
  - the element modeled
  - the use of the model
  - The existing understanding of the component

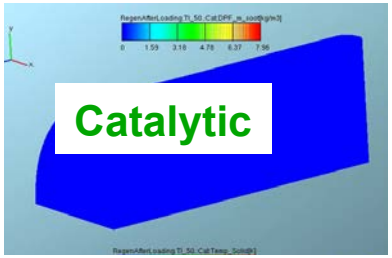
What level of A/T Model Detail is needed?

- Map-based Models
  - Adequate for less complex catalysts in some simple applications
- Simple 0D Models
  - Where spatial effects are minimal – either because of simple cycles (SS) or simple applications (heat generation)
- 1D Models
  - Where temperatures and other gradients exist
- 1D by 1D Models
  - Where catalyst is coating changes formulation with depth in the coating
  - Wall flow devices
- 2D Models
  - Where radial temperature gradients are significant
- 3D CFD
  - Where flow distributions or compositional gradients exist

Systems Performance Analysis Tools

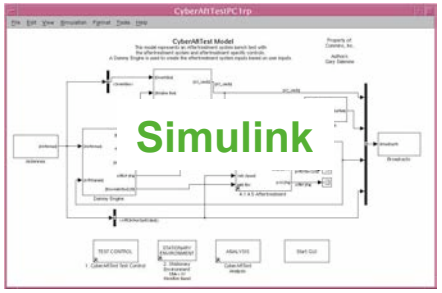
All models are wrong, some are useful – George Box

Engine CFD & Combustion



3D CFD

1D A/T Simulation



Engine Cycle Simulation

System Simulation

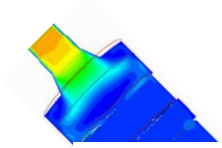
Design Calculation Spreadsheet

Matlab

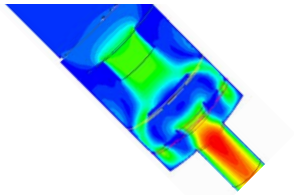
Slower — Execution Speed/Real Time — Faster

0.0001 | 0.001 | 0.01 | 0.1 | 1 | 100

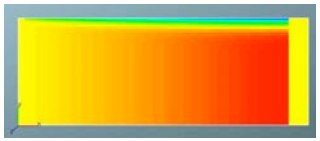
More Detail — Less Detail



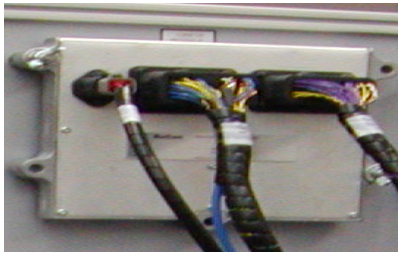
Flow CFD



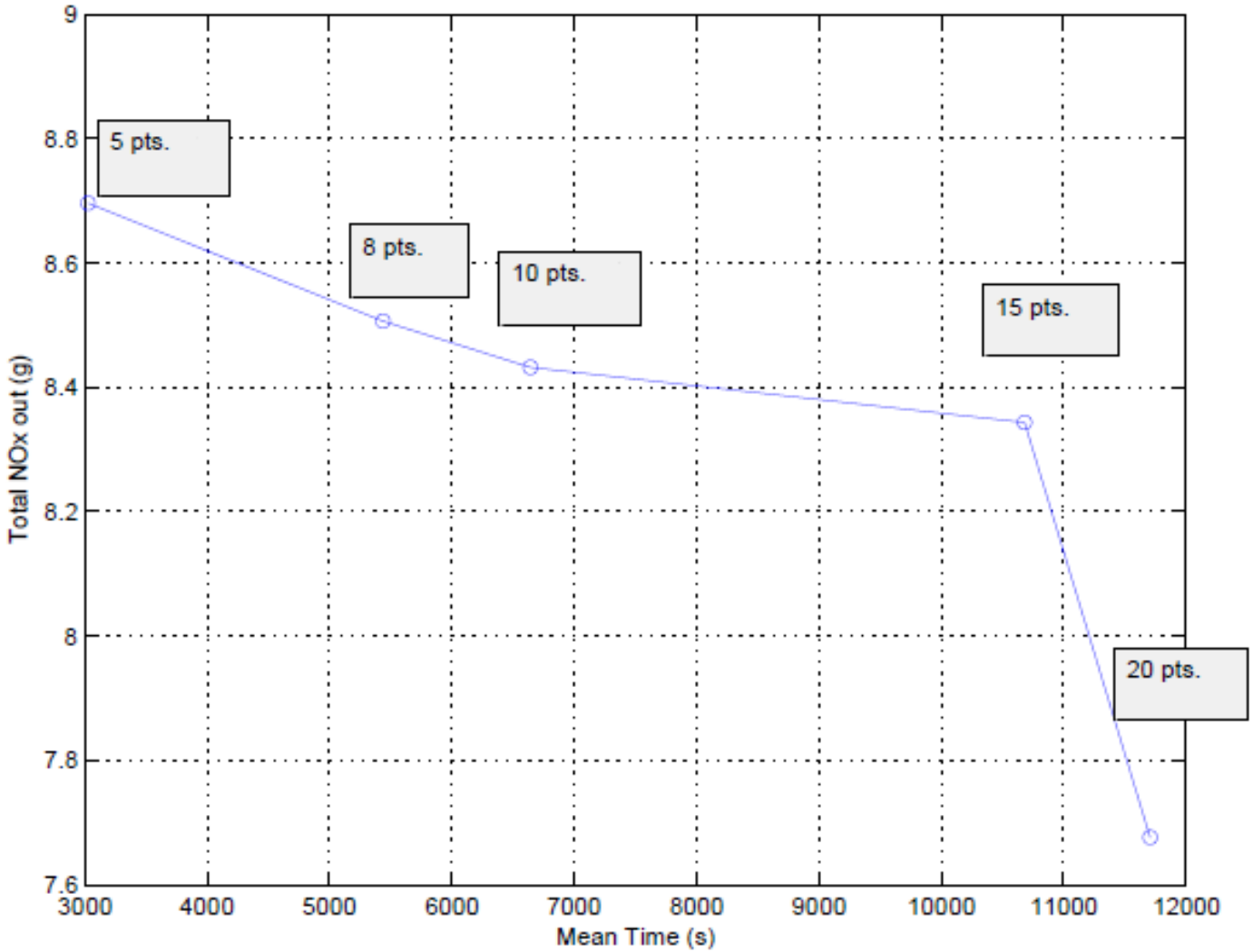
2D CFD



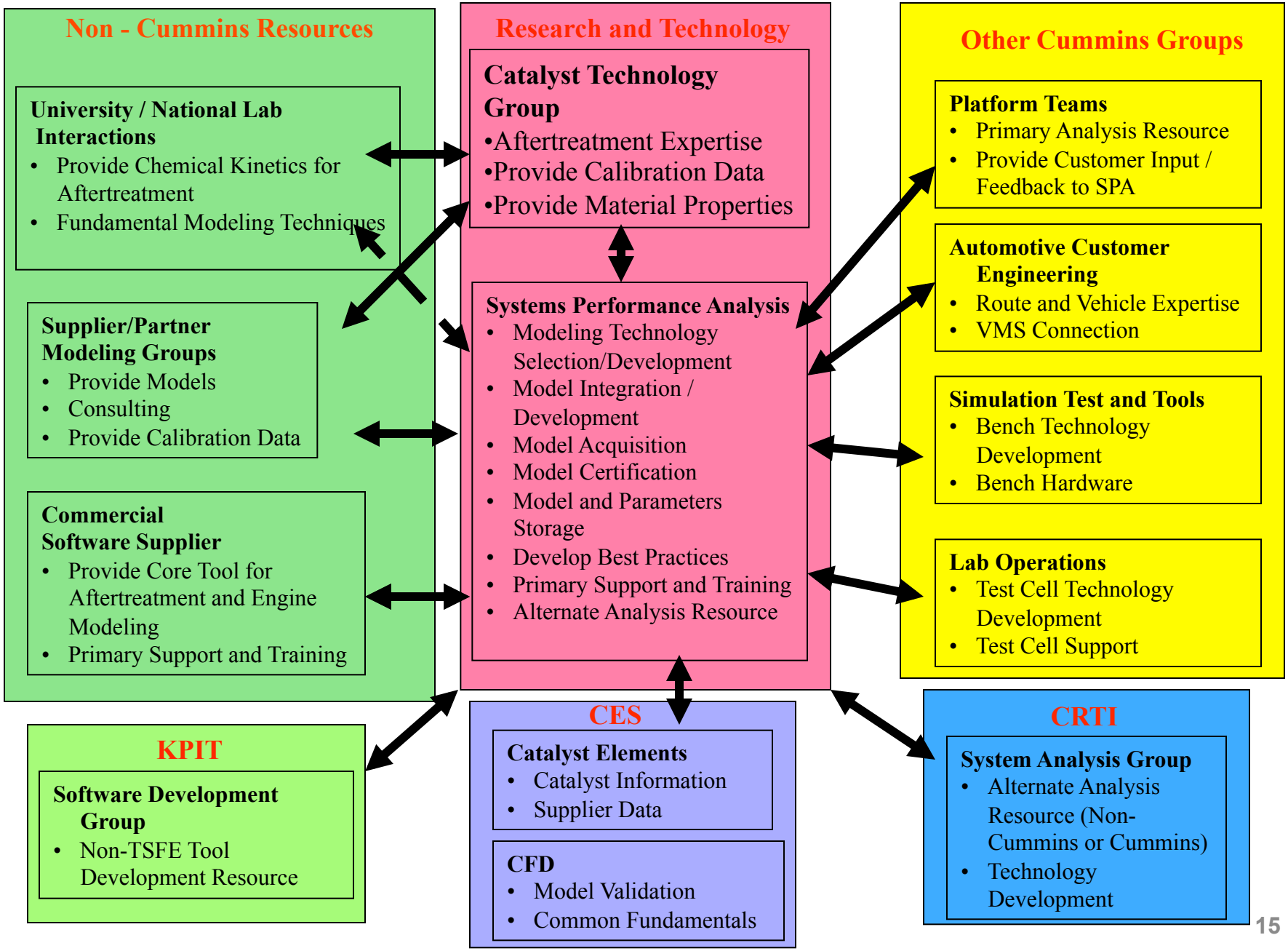
Embedded Models



FTP: Accuracy/Speed Trade-off

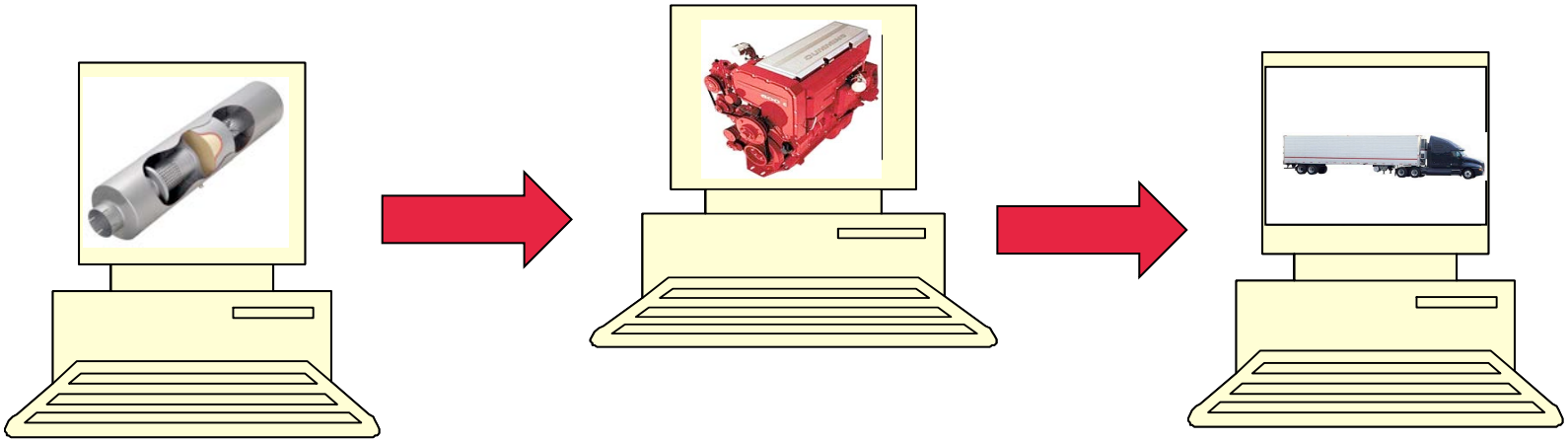


Systems Performance Analysis Roles



Analysis Led Design Engine Development

Pure Simulation



•Aftertreatment Parameter Studies
•Uncoupled Flow, Temperature, Emissions
•Aftertreatment Controls
•Steady State and Transient

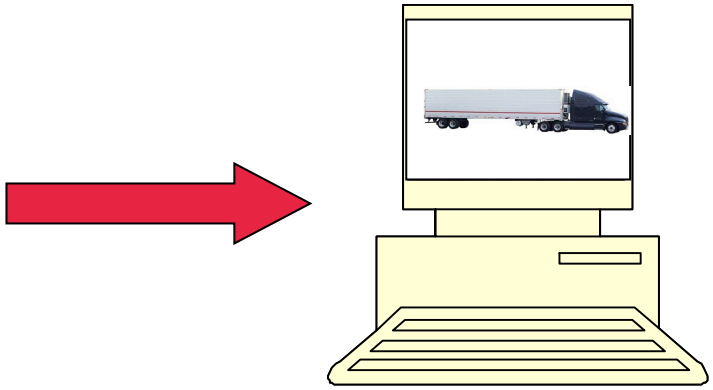
•Engine Parameter Studies
•Coupled Torque, Flow, Temperature, Emissions
•Engine and Aftertreatment Controls Interactions
•Steady State and Transient

•Vehicle Parameter Studies
•Engine and Aftertreatment Controls Interactions
•Drive Cycle Transients

Vehicle System Simulation Concept

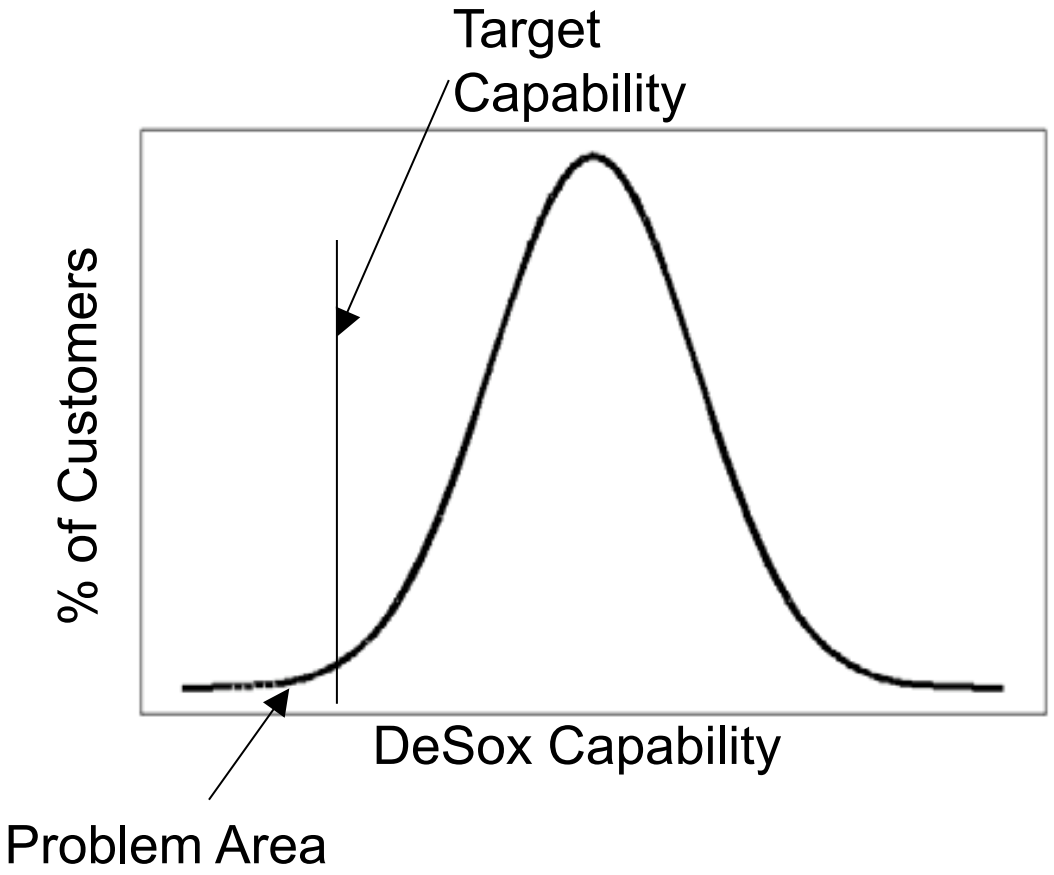
Move truck testing to computers and test cells

- Easier Data Acquisition
- Repeatable and Realistic Testing
- Off nominal and “out of season” tests
- Automated Testing
- Engine Controls development and testing
- Fuel Economy Studies
- Transient Emissions Testing



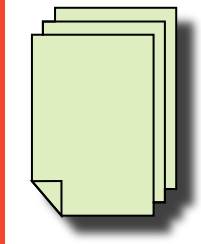
Population Evaluation

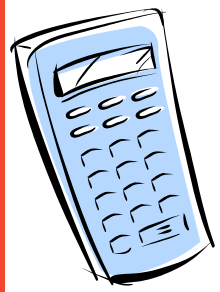
Need a way to characterize the population of vehicles

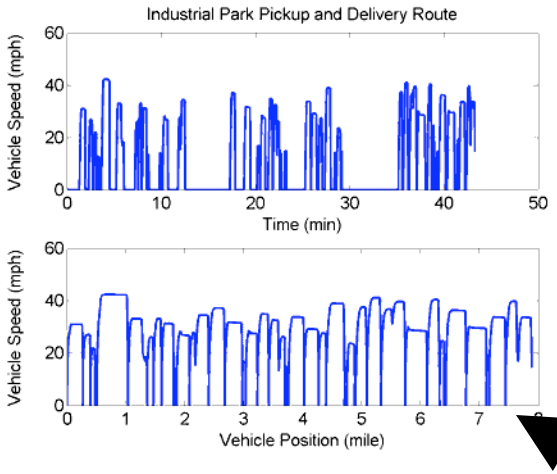


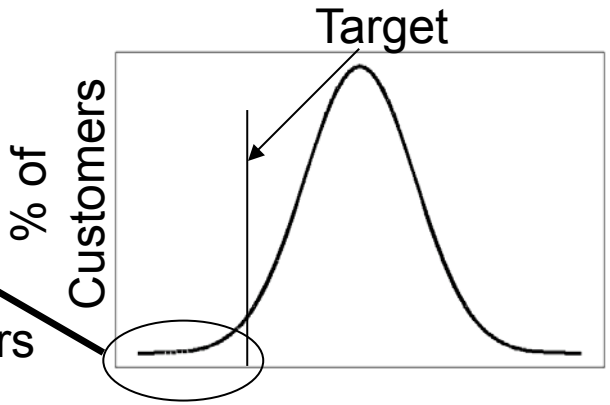
Plan to Evaluate Population

Customer Survey

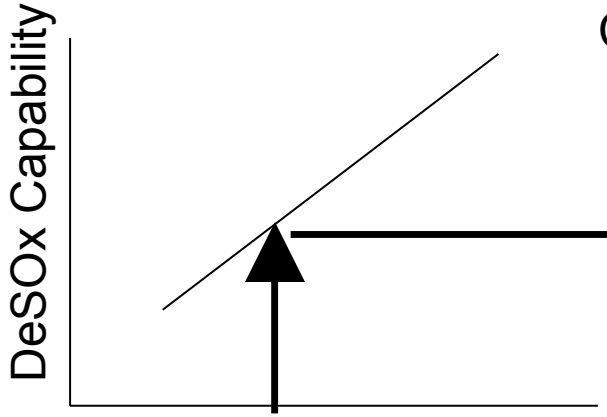






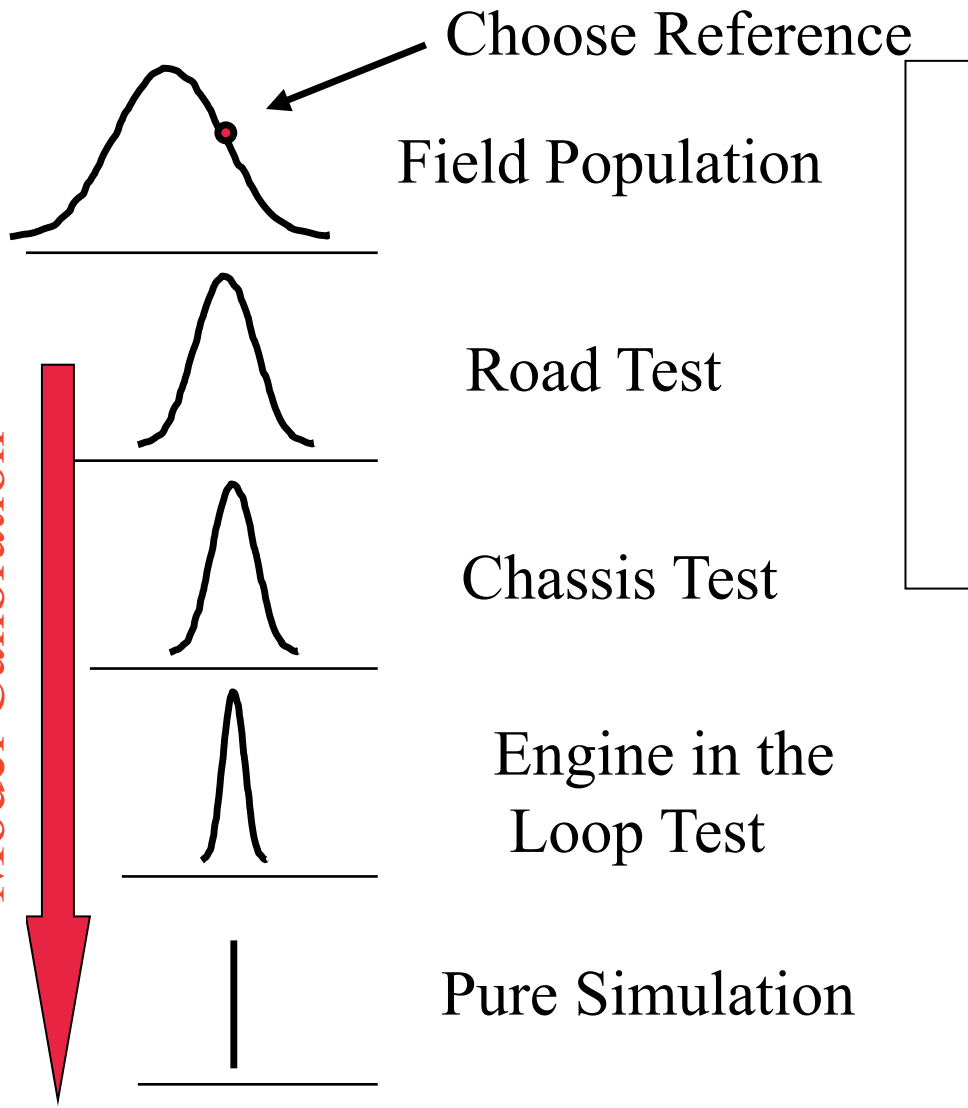


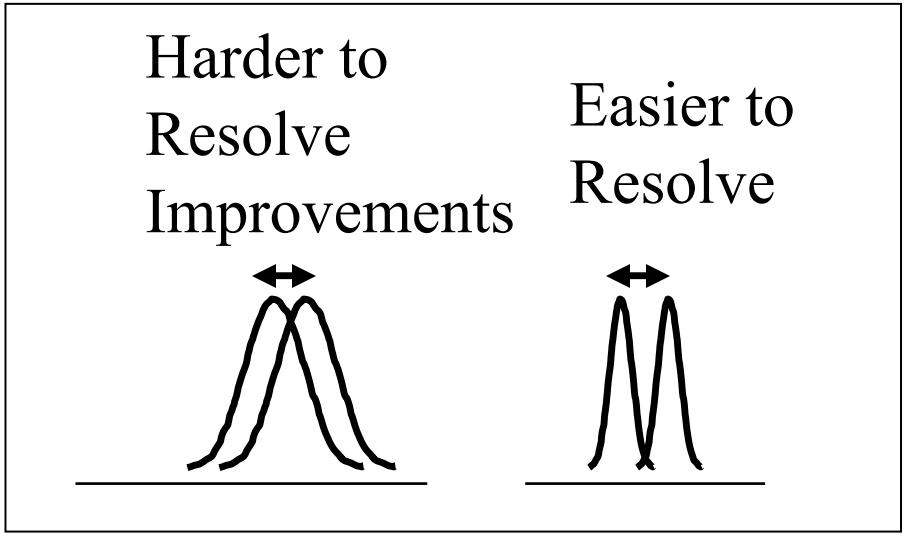
At Risk Customers



"Duty Cycle Parameter"

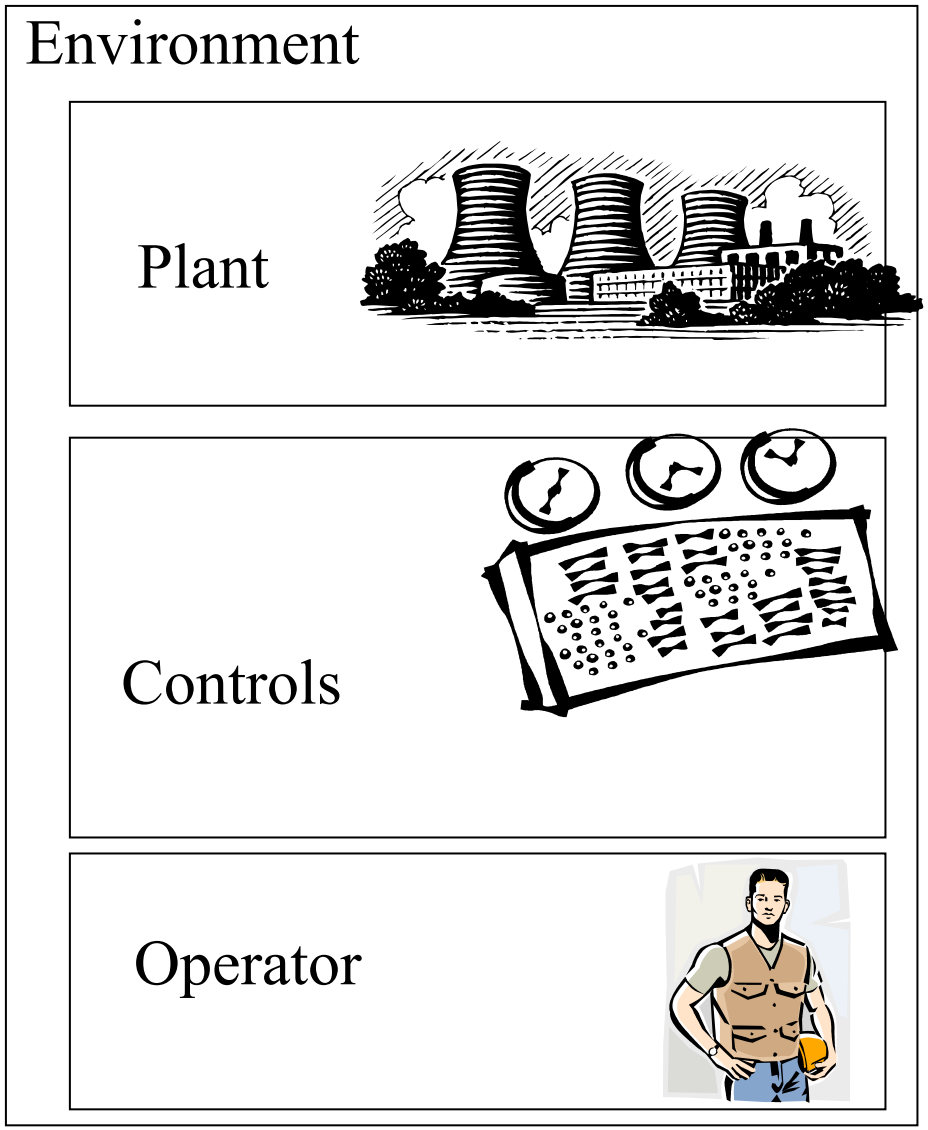
Case for high repeatability evaluation

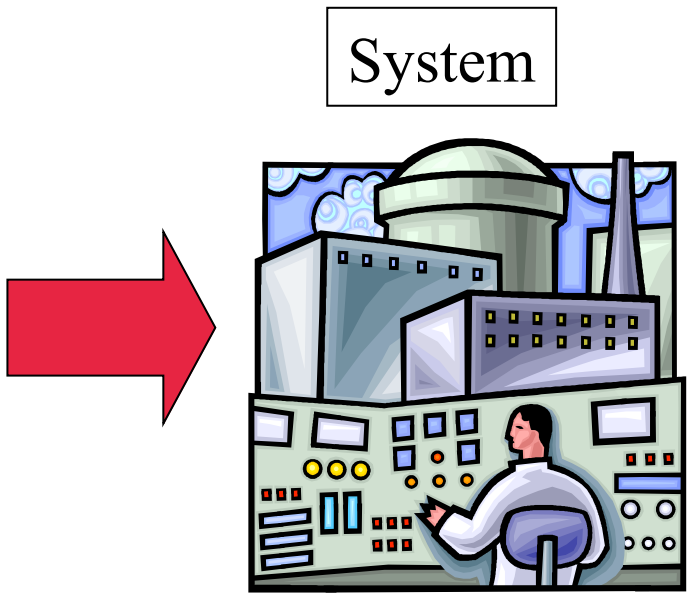




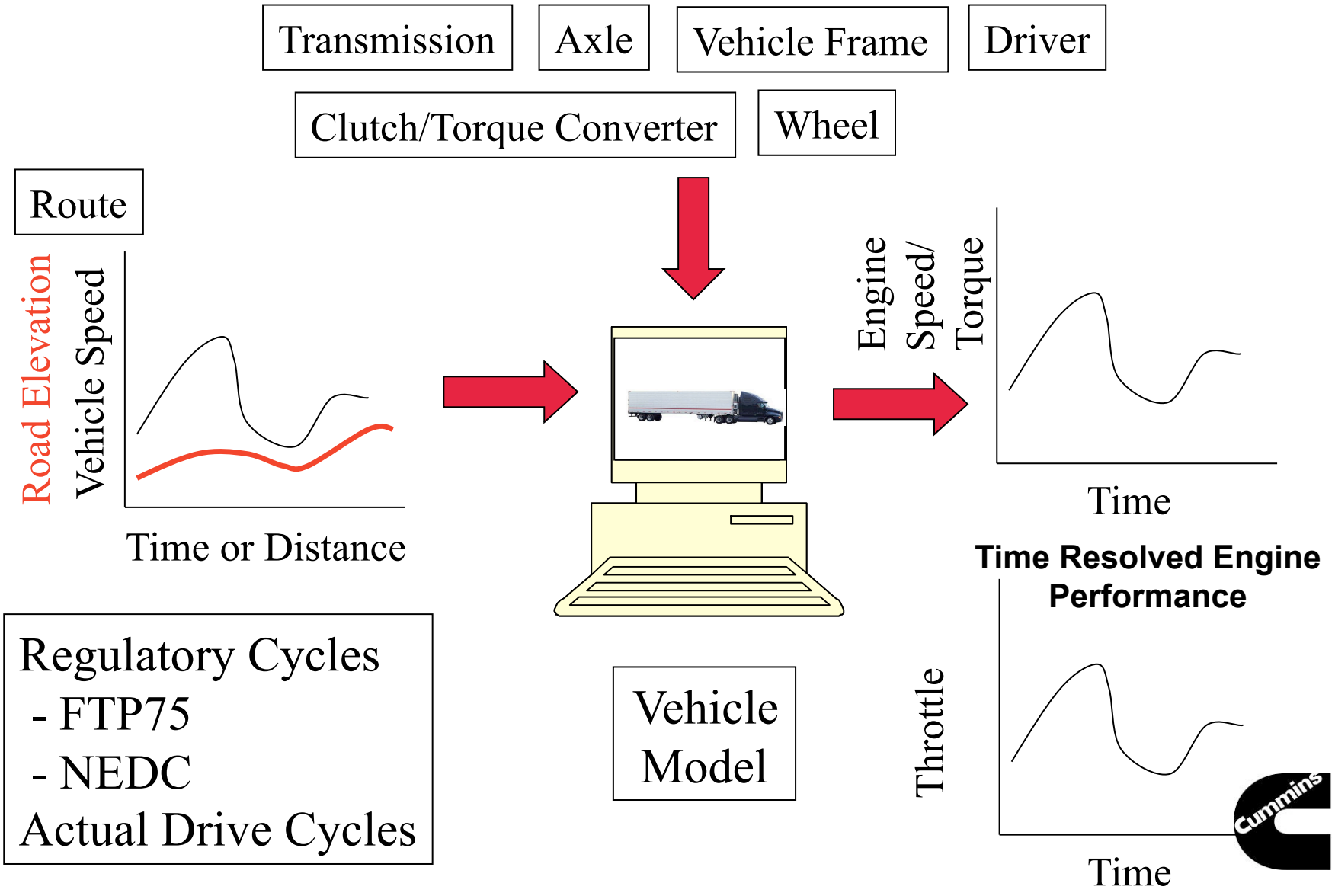
Relative Comparisons Best Handled Here

Dynamic System Overview

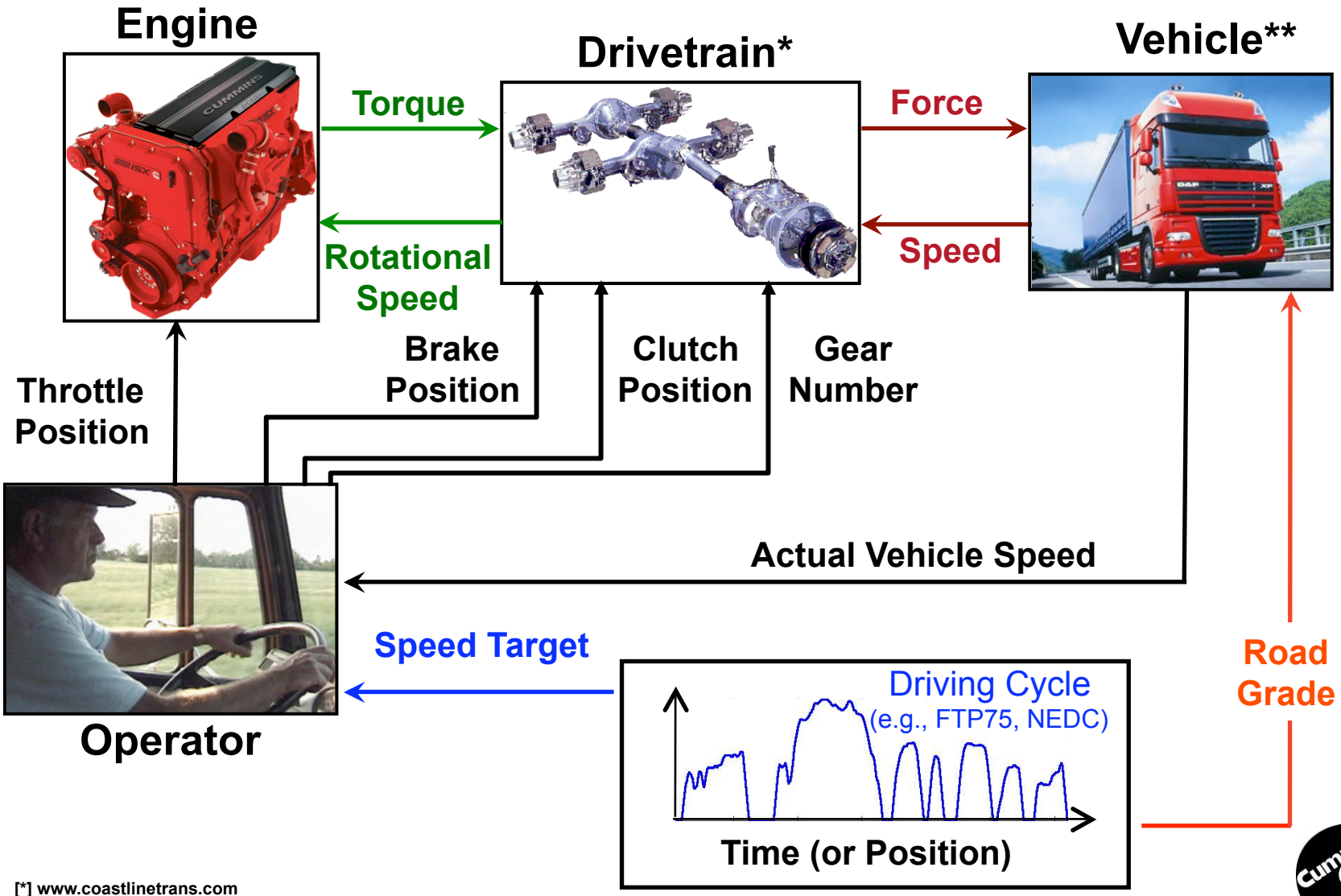




Vehicle System Performance Simulation

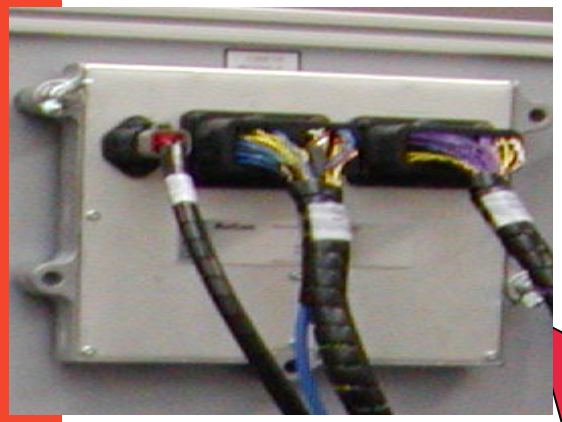


Signal Flows in Vehicle Simulation



[*] www.coastlinetrans.com

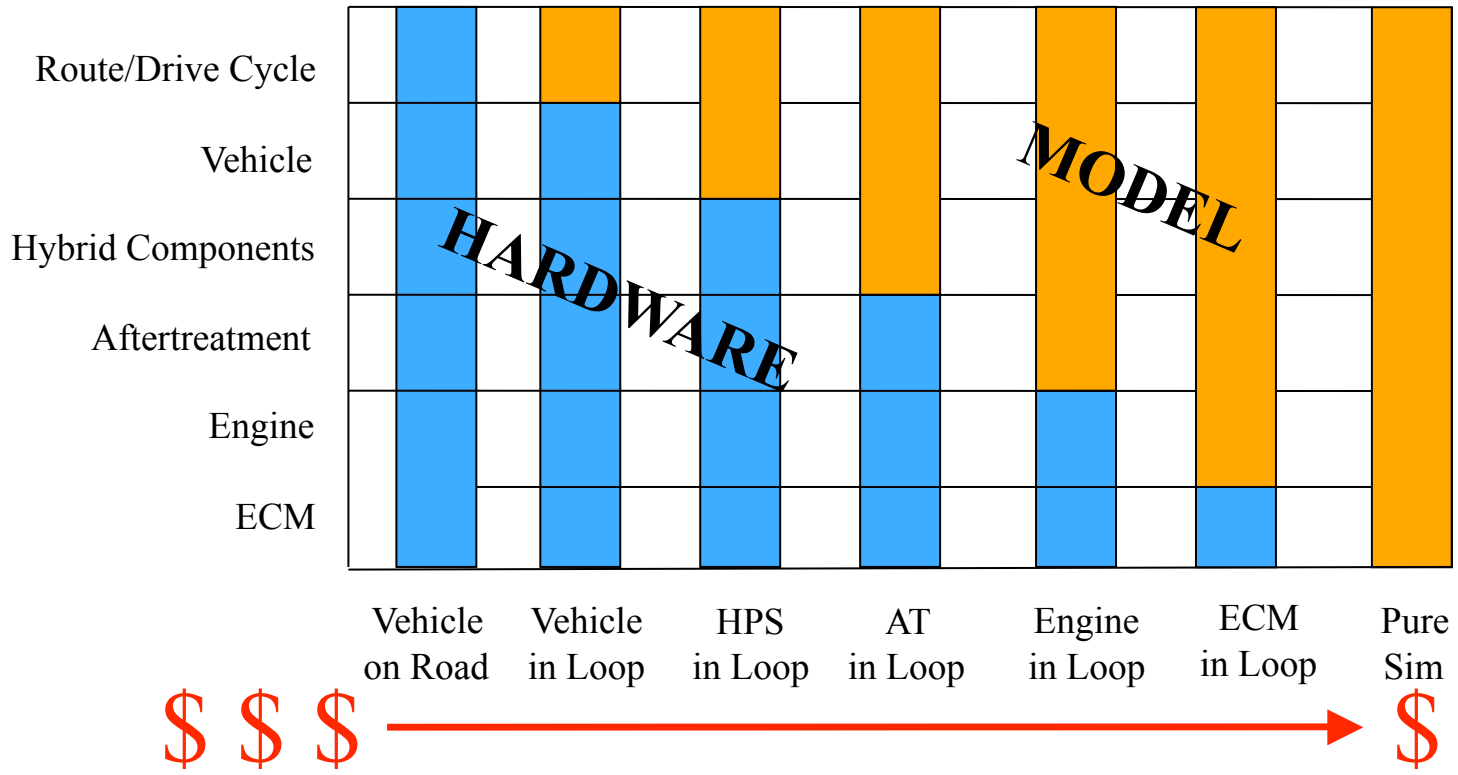
[**] www.leylandtrucksltd.co.uk



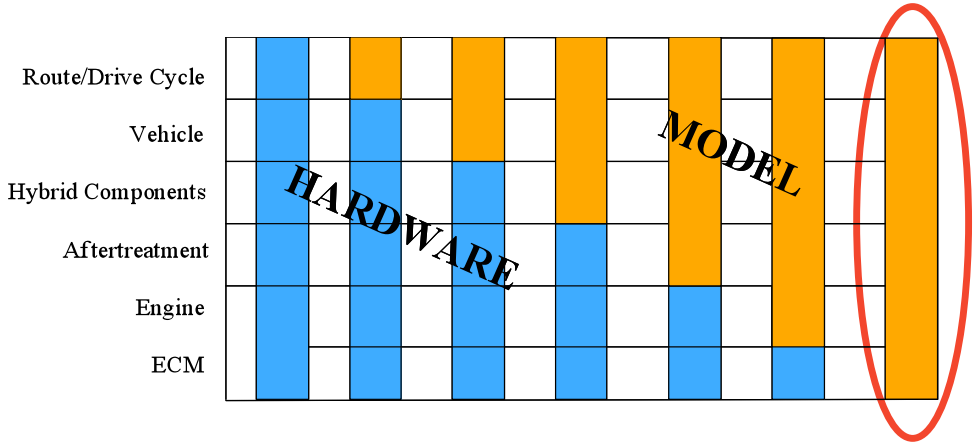
But CyberApps is more than just vehicle simulation

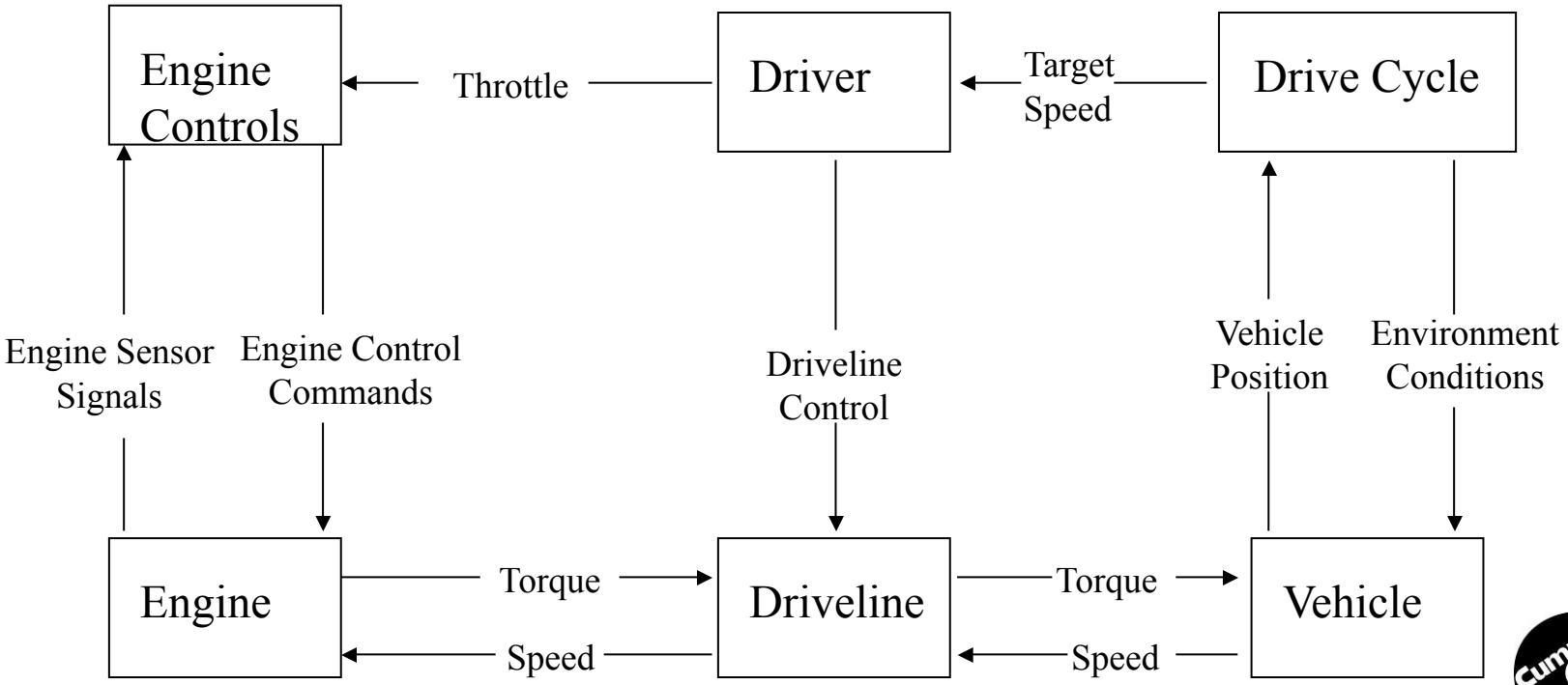
CyberApps© Sim → Sim + Hardware

Systems Performance Simulation



Pure Simulation Application



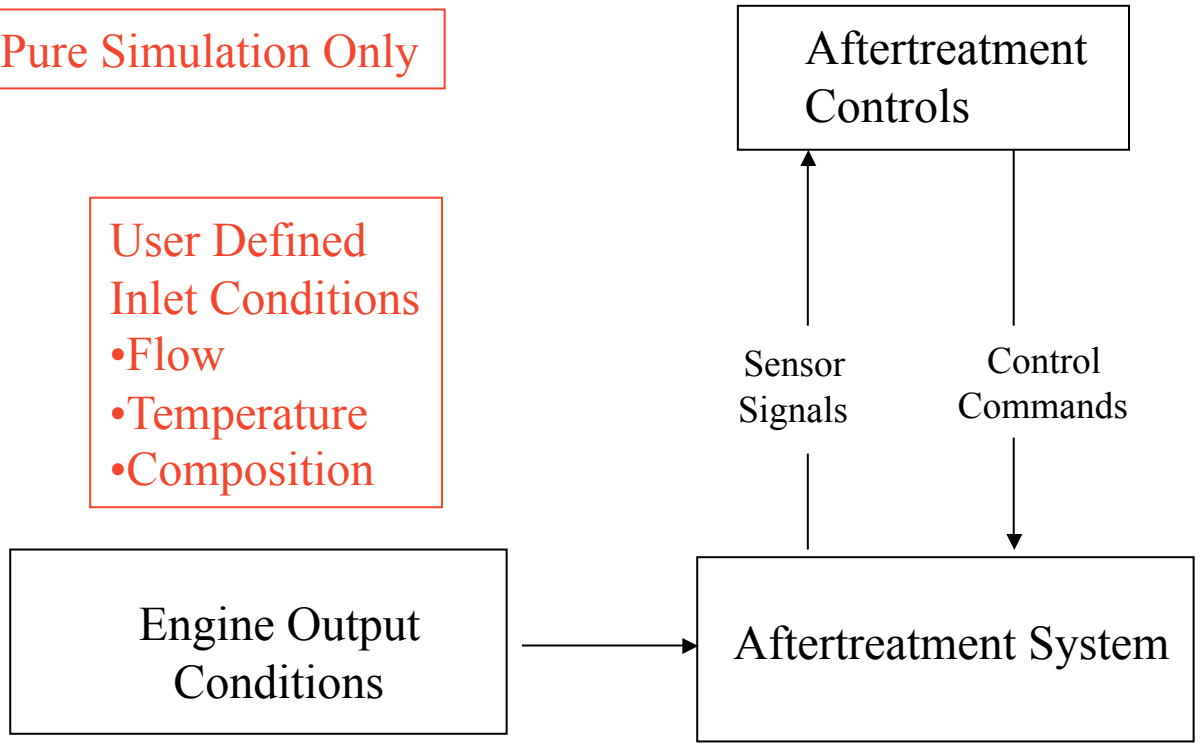


CyberAftTest Application

Aftertreatment System Bench Test

Pure Simulation Only

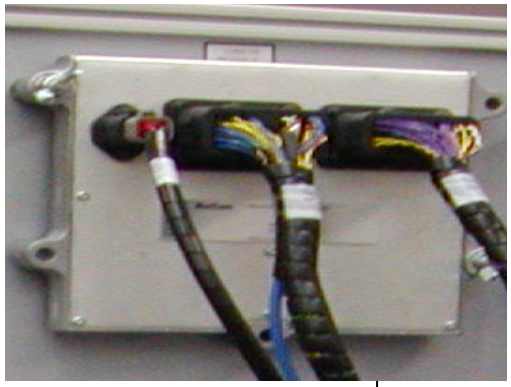
User Defined Inlet Conditions
- Flow
- Temperature
- Composition

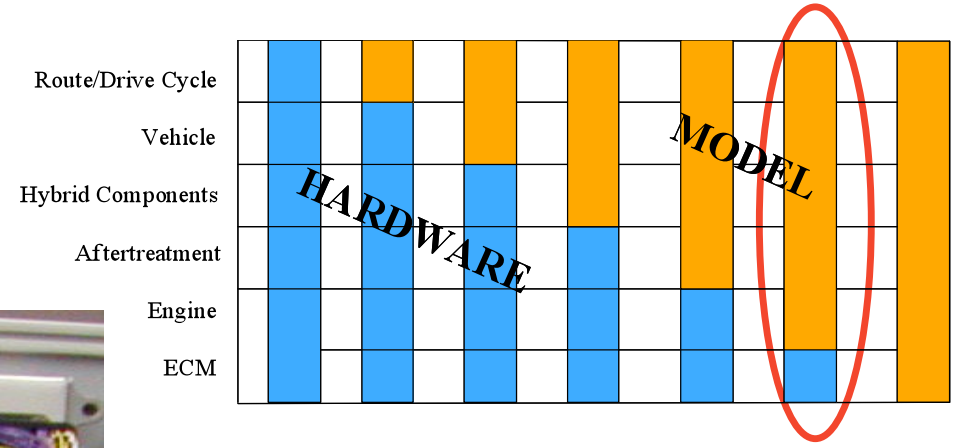


- Automated Tests
- Steady State Tests
- Transient Tests

Configurable Catalyst Elements

Controller in the Loop (CIL) Application Simulation





Throttle

Driver

Target Speed

Drive Cycle

Engine Sensor Signals

Engine Control Commands

Driveline Control

Vehicle Position

Environment Conditions

Engine

Torque

Speed

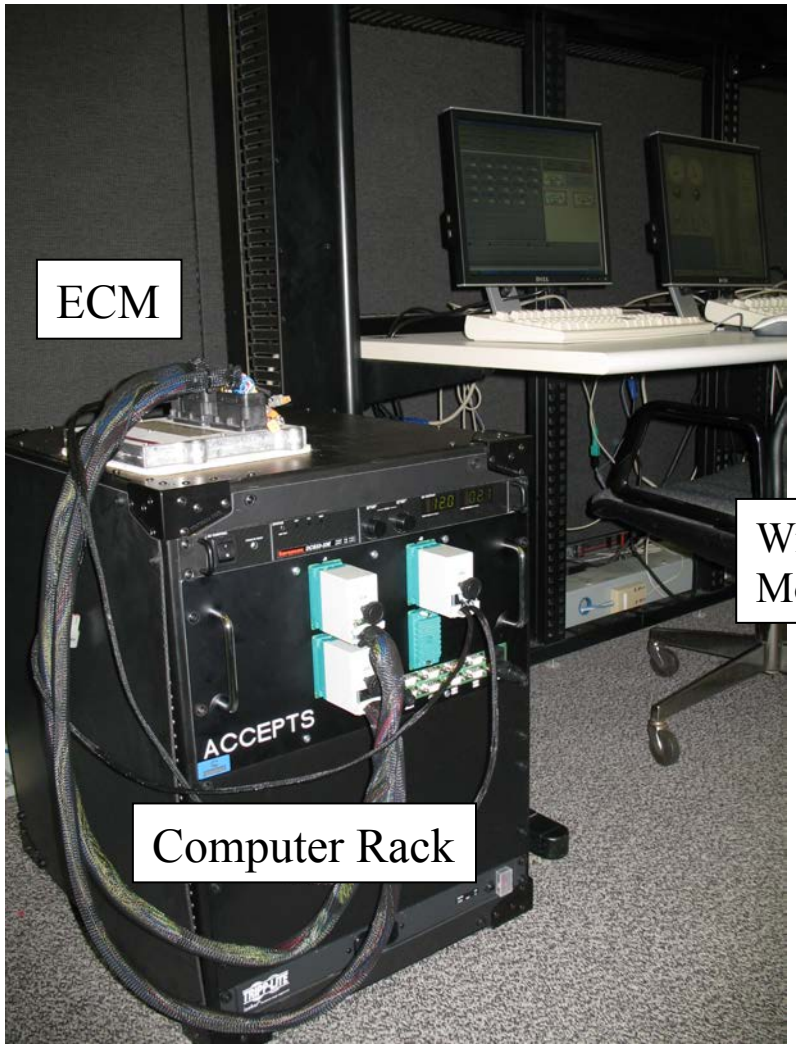
Driveline

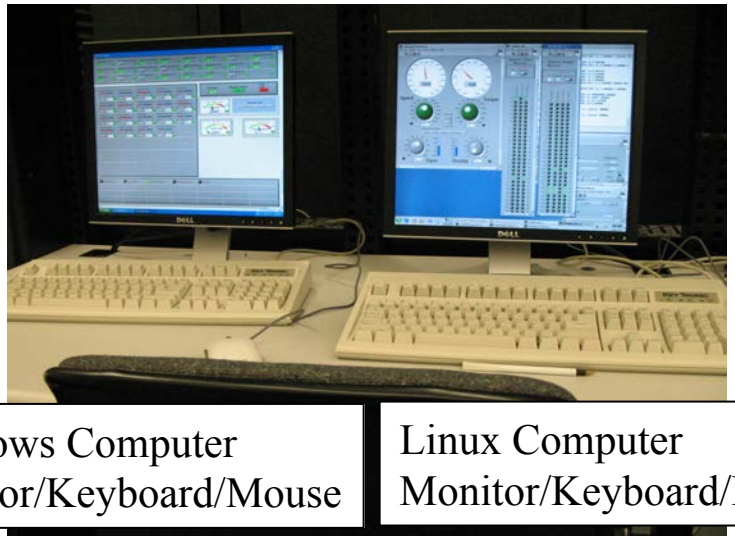
Torque

Speed

Vehicle

CyberBench Example - Computers

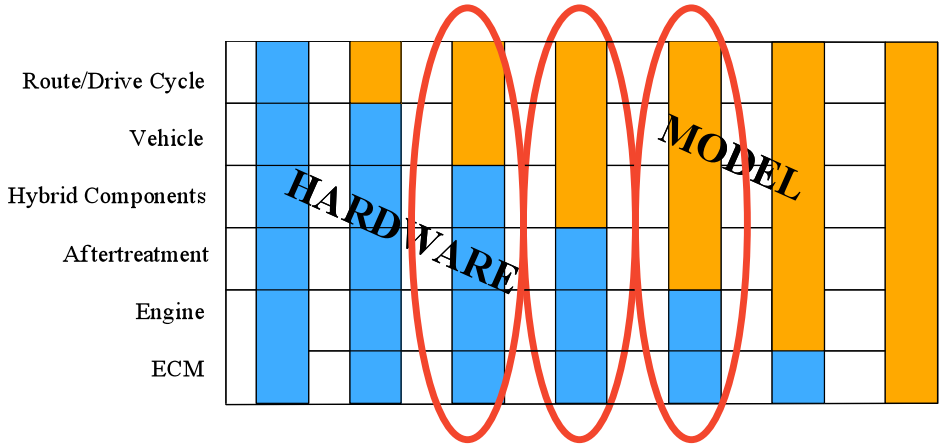


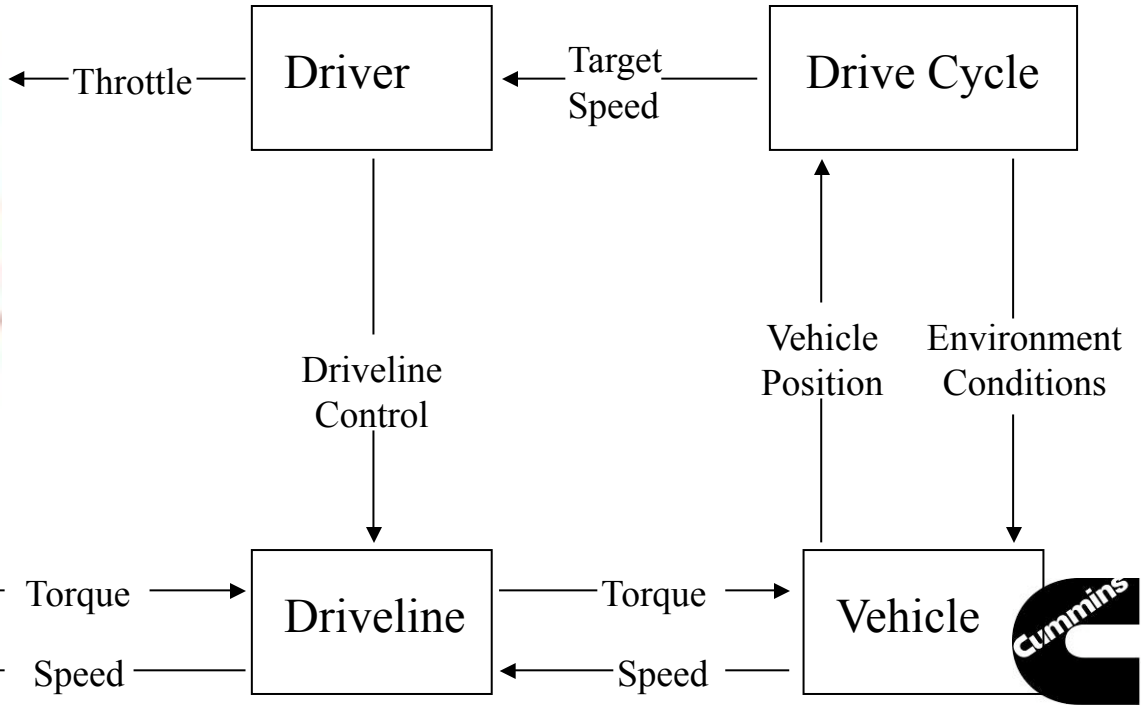


Windows Computer Monitor/Keyboard/Mouse

Linux Computer Monitor/Keyboard/Mouse

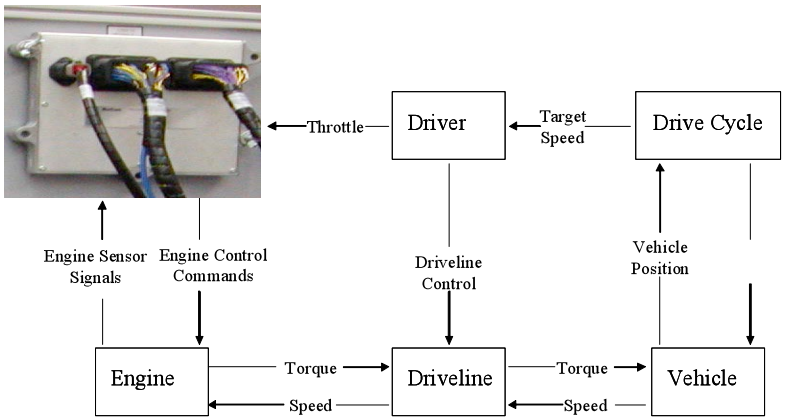
Engine in the Loop (EIL) Application Simulation

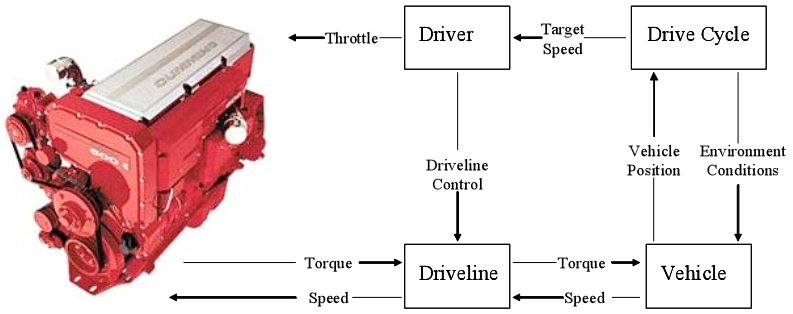




Analysis Led Design Engine Development

Hardware In the Loop

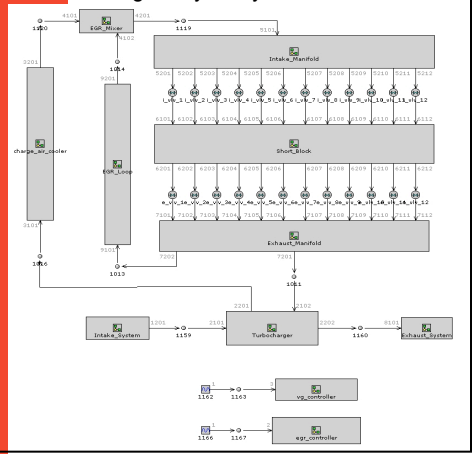




- Engine Parameter Studies
- Coupled Torque, Flow, Temperature, Emissions
- Real Engine and Aftertreatment Controls Interactions
- Steady State and Transient

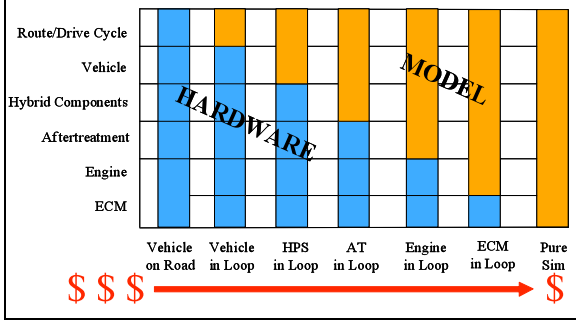
- Vehicle Parameter Studies
- Real Engine and Aftertreatment Controls Interactions
- Real Engine Performance and Emissions
- Drive Cycle Transients
- Vehicle speed based regulatory cycles

Engine Cycle/System Simulation

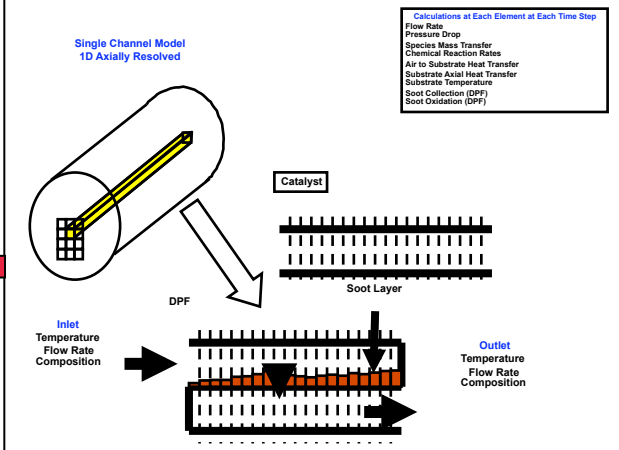


Integrated Engine/Aftertreatment/Vehicle System Simulation

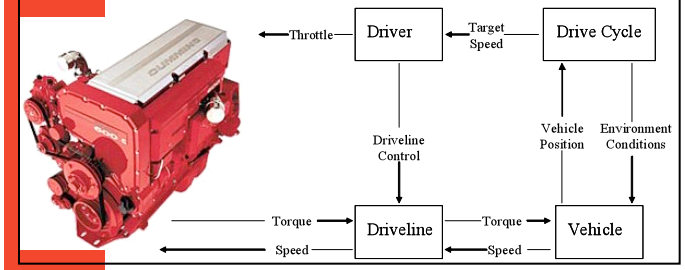
Modeling is Key to Successful Controls Development and System Integration



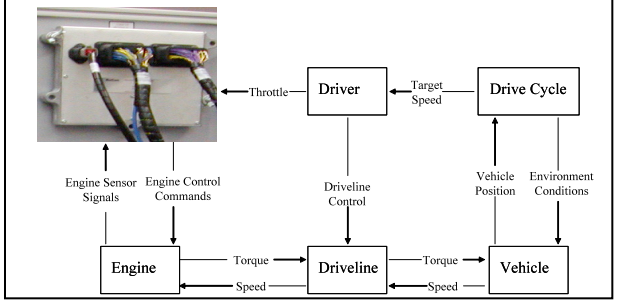
Aftertreatment System Simulation



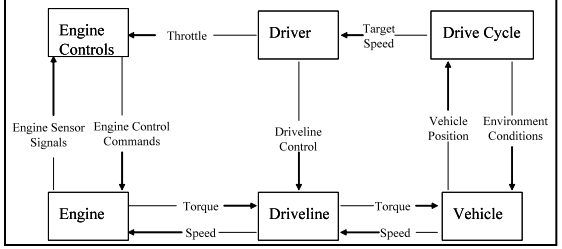
Engine in the Loop (EIL) Application Simulation



Controller in the Loop (CIL) Application Simulation



Pure Simulation Application



Component Models

Component	Features
Operator	▪Input: Target vehicle speed. ▪PIF controller with adaptive gains ▪Outputs: Operator throttle and brake command (automatic), throttle, brake, clutch position, gear number (manual). Manual operator has a sophisticated shifting model. ▪Target accel and decel rates can be changed to study variability
Routes	▪ Time based / position based. ▪ Grade input. ▪ Stop / idle time vs. time / position. ▪VehMass vs. time / position.
Engine – Map Based	▪Inputs: Throttle, speed and switch. ▪Output: Torque ▪ Allows input of fuel map collected from test cell. ▪ Allows to perform quick engine sizing exercise.
Engine – Reduced GTPower	▪ Mean Value Cylinder ▪Simplified air handling subsystems ▪Trends with air handling and fuel system commands

Component Models

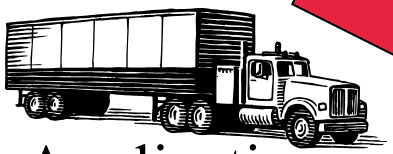
Component	Features
Aftertreatment - Simple	▪Map based models for real time ▪Thermal response
Aftertreatment – 1 D	▪Axially resolved single channel models ▪Global kinetics of reactions ▪Thermal response
Engine/Aftertreatment Controls - Simple	▪Simple map based controls for engine and aftertreatment commands
Engine/Aftertreatment Controls – Detailed (COMET)	▪Parts of actual production code running in simulation ▪Import of actual calibration
Torque Converter	▪ Map based model; Maps of Torque ratio vs. speed ratio and K factor vs. speed ratio

Component Models

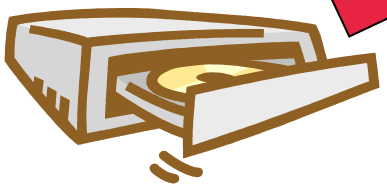
Component	Features
Transmission	▪Allows input of gear ratios Automatic ▪Shift schedule map as a function of throttle angle and trans out speed. ▪ Gear loss: polynomial equation for speed based and a constant torque based for each mesh. Manual ▪Gear loss: polynomial equation for speed based and a constant torque based for each mesh.
Axle	▪ Efficiency model similar to transmission
Wheel	▪ Allows input of wheel size. ▪ Wheel rolling loss model is a function of vehicle speed and mass ▪ Calculates brake force
Vehicle	▪ Allows input of Cd, vehicle height and width ▪ Allows input of A, B, C coefficients ▪ Calculates aerodynamic drag, grade force and vehicle acceleration (F=ma)

Example Simulation Capability

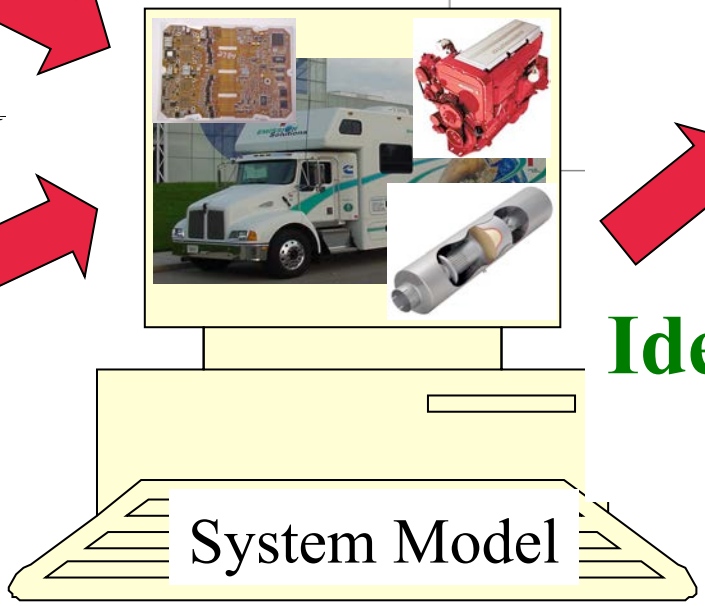
What is sensitivity of aftertreatment performance to drive route, engine calibration change, and regeneration temperature?



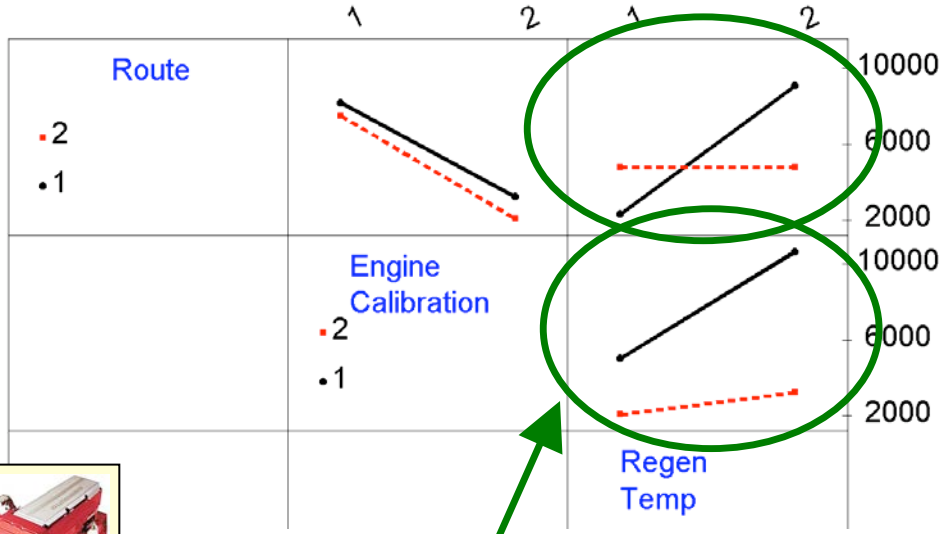
Application



Calibration



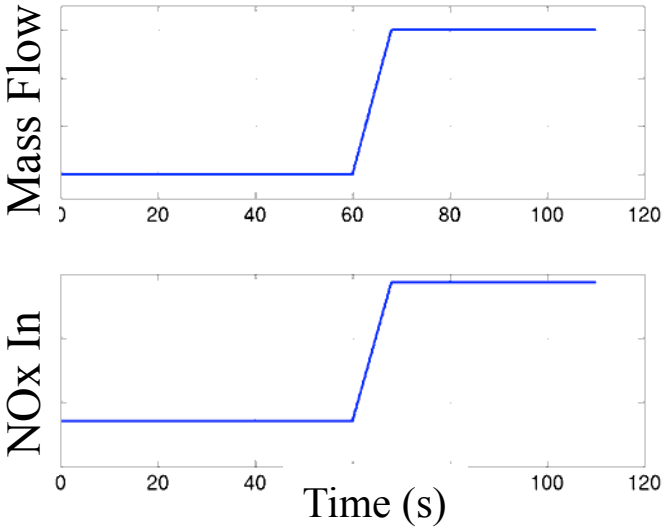
Peak Oxidation Catalyst Outlet Hydrocarbons (ppm)

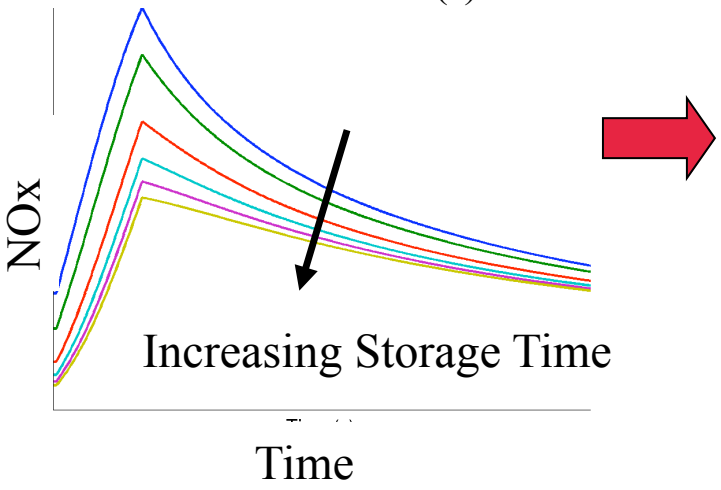


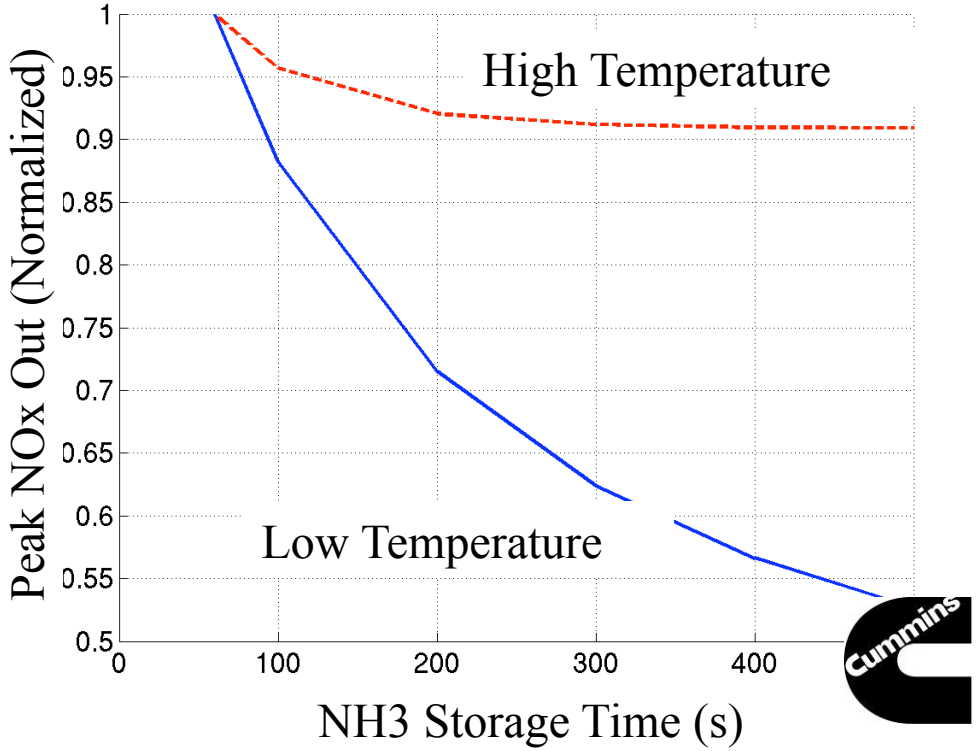
Significant Interactions Identified with *System* Model

Aftertreatment Controls Development Using Models

Aftertreatment Only Simulation

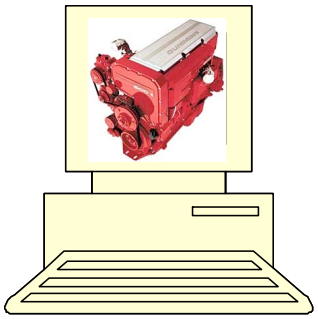


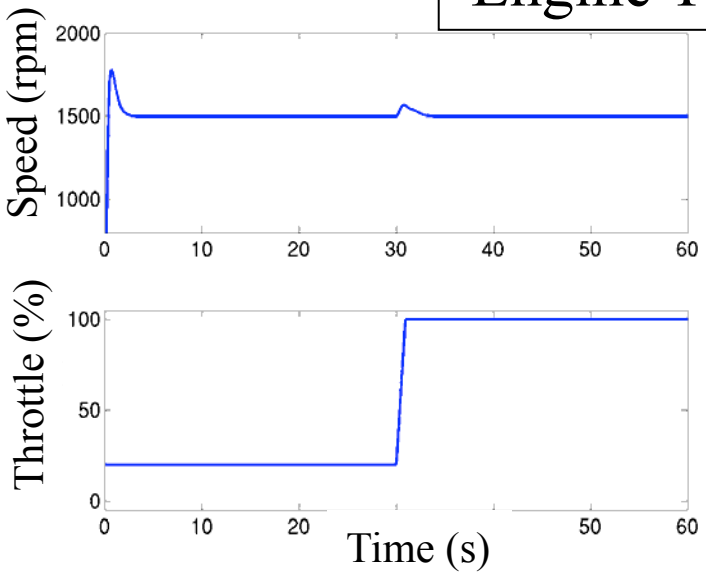


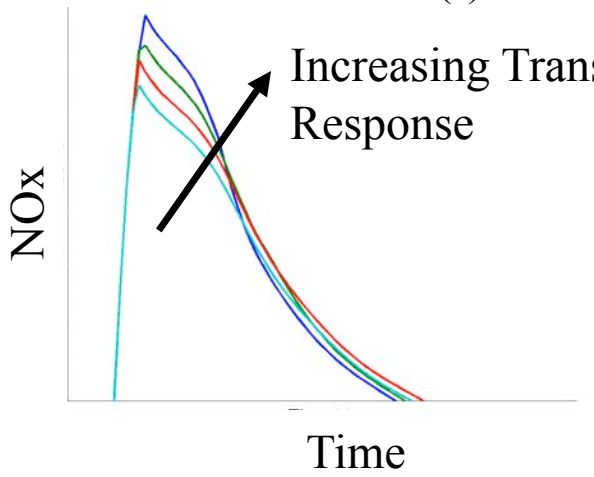


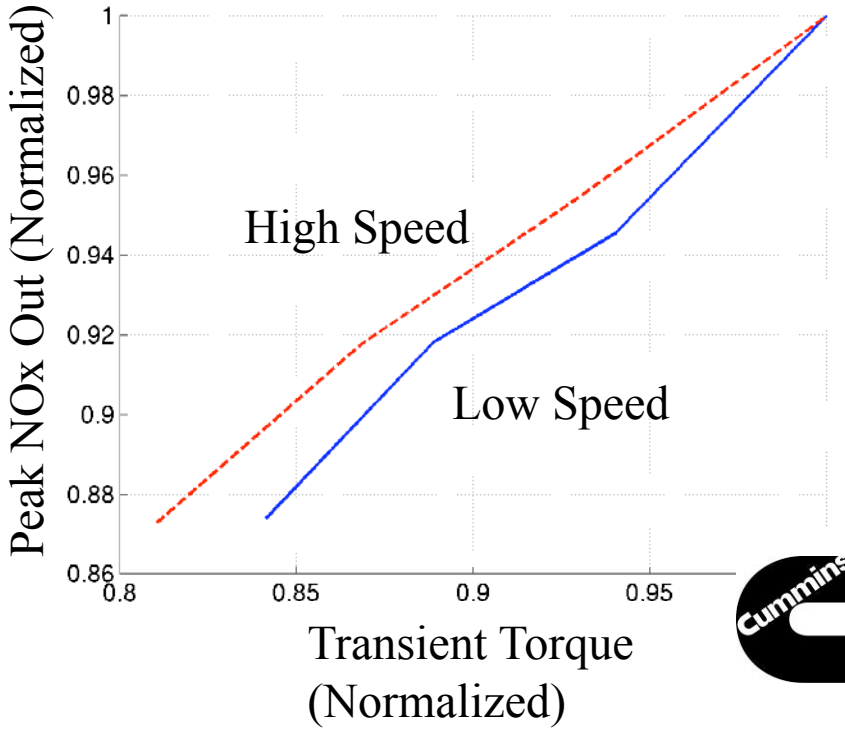
Aftertreatment Controls Development Using Models

Engine Test Cell Simulation



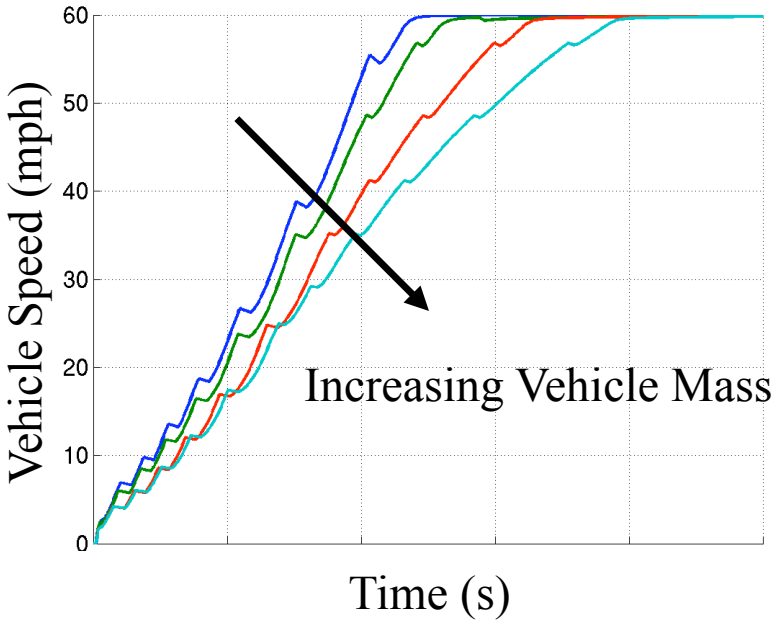


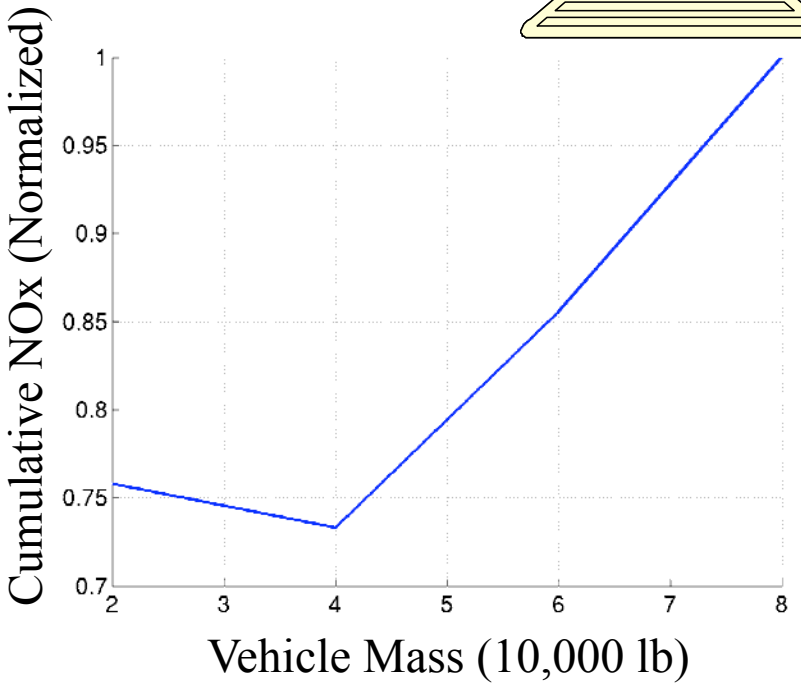




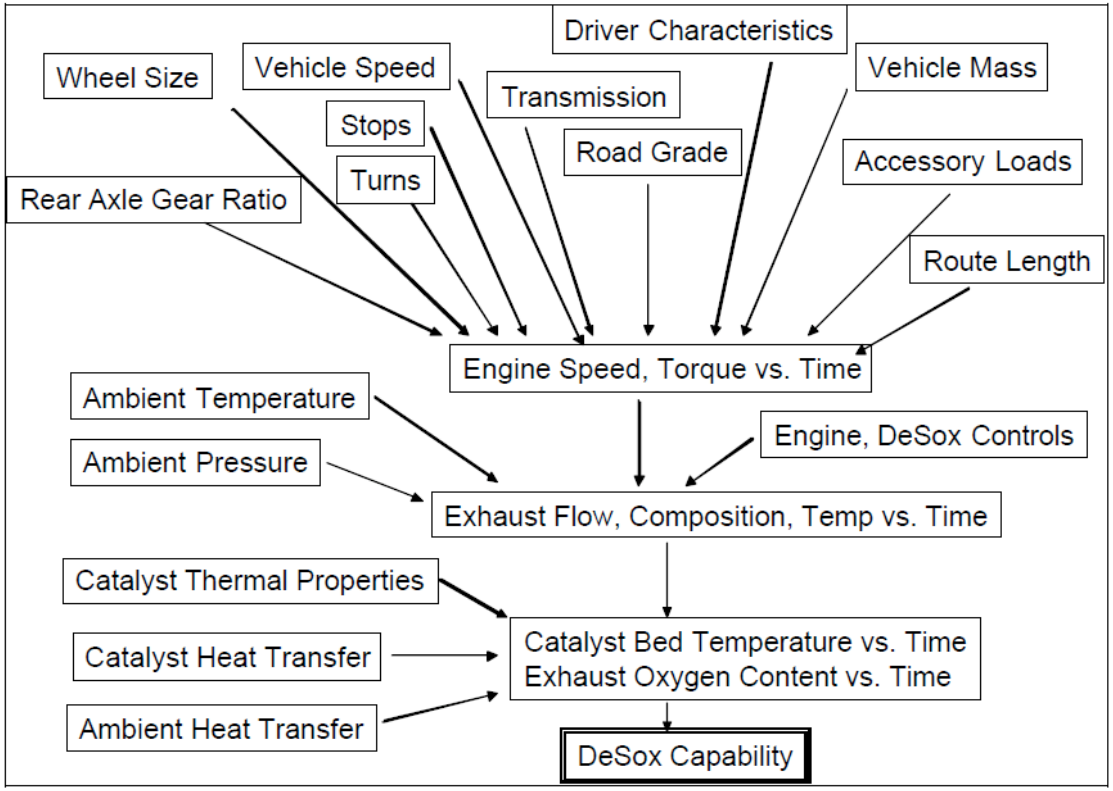
Aftertreatment Controls Development Using Models

Vehicle Simulation





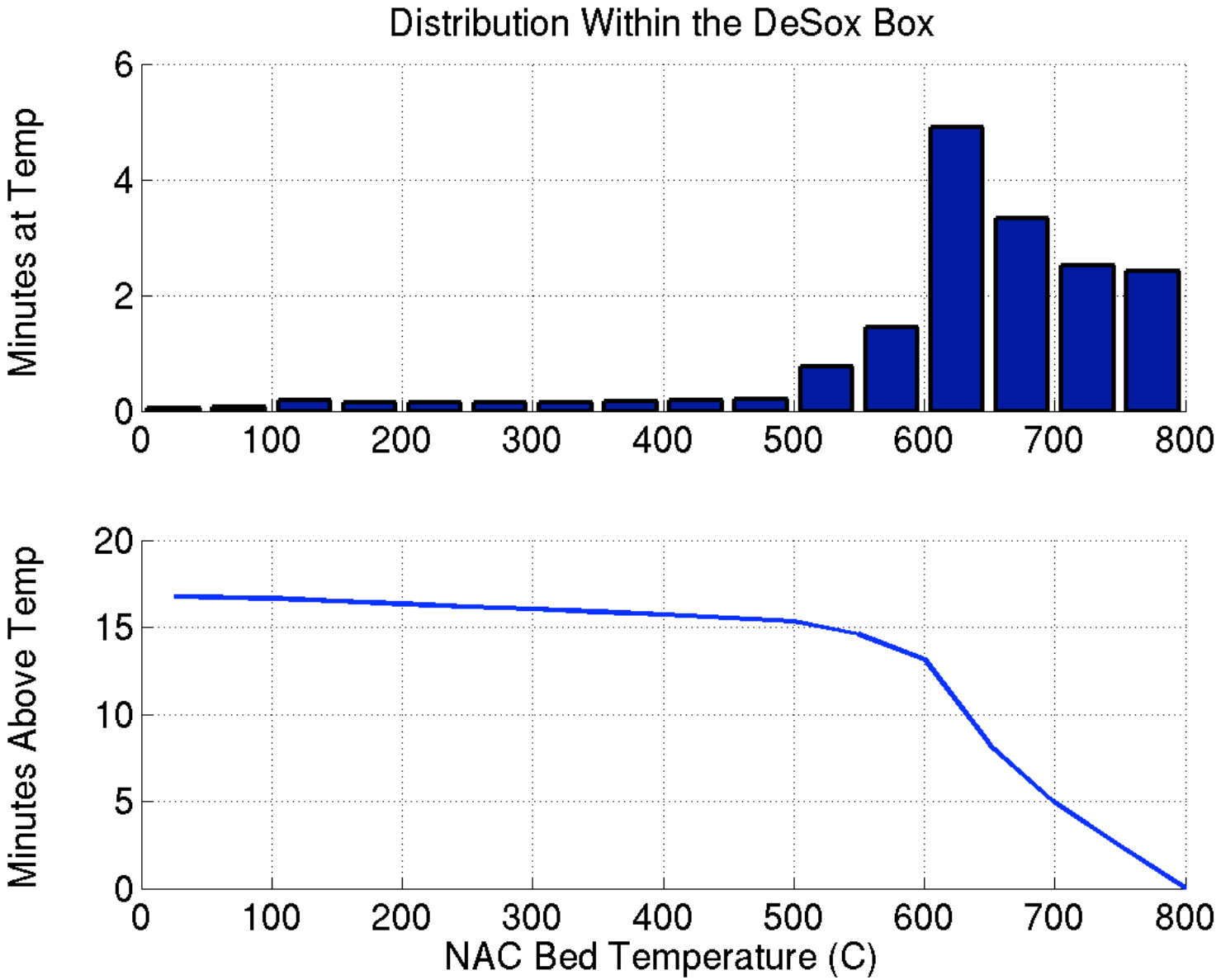
Simulation of deSOx Opportunities



- Run vehicle simulations over various duty cycles to determine deSOx opportunities

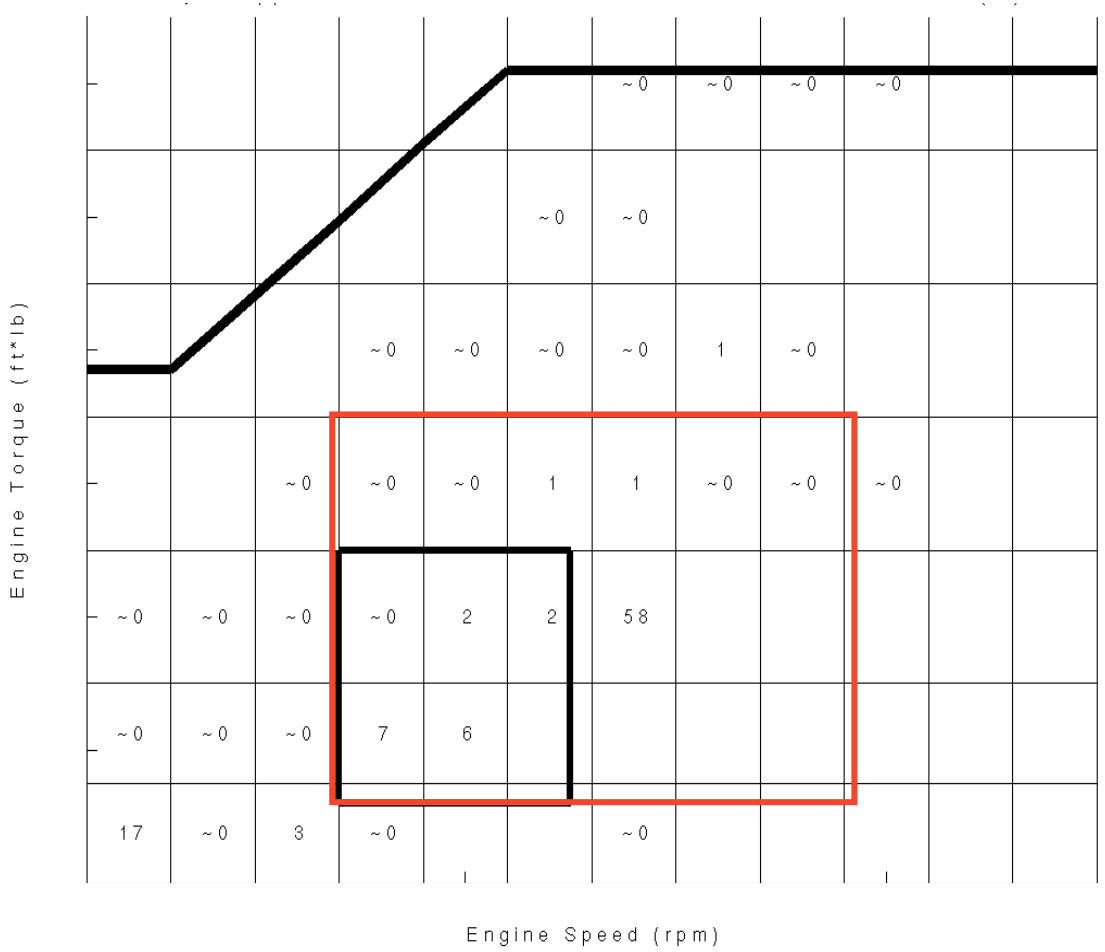
- LNTs require periodic regeneration to remove sulfur
- Using engine managed measures, deSOx can only happen in limited areas of the engine operating map

Time at Temperature

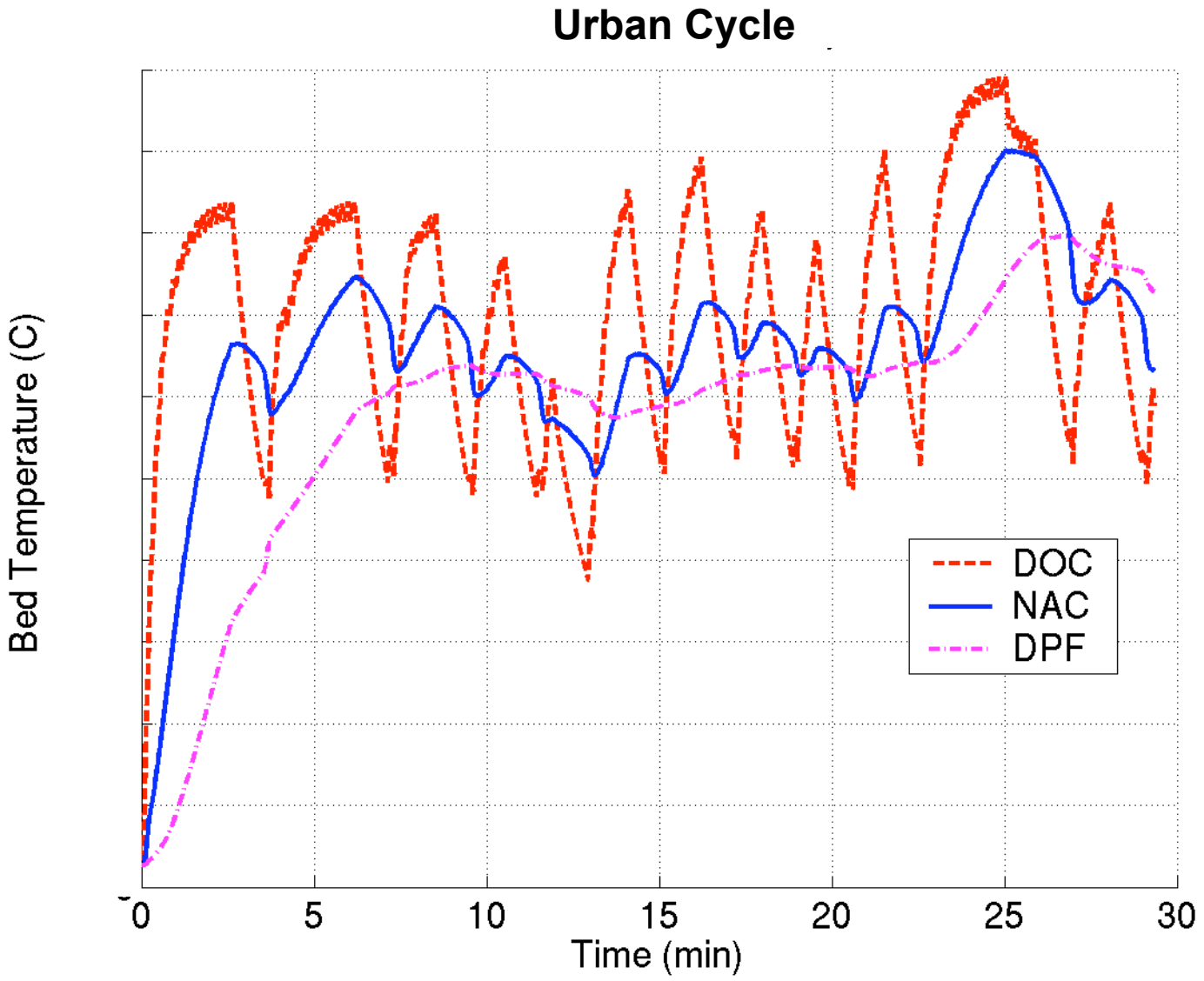


What if?

- We can now visualize where on the engine map adequate opportunities exist for desulfation



Detailed Evaluation



Summary

- Vehicle simulation is an important part of the development of engine systems
- Combinations of simulation and hardware are a critical part of that process
  - Controls
  - Engine
  - Vehicle
- Model sophistication required may vary depending on the intent of the simulation and the available simulation resources
- Vehicle simulations are not the only uses of A/T models