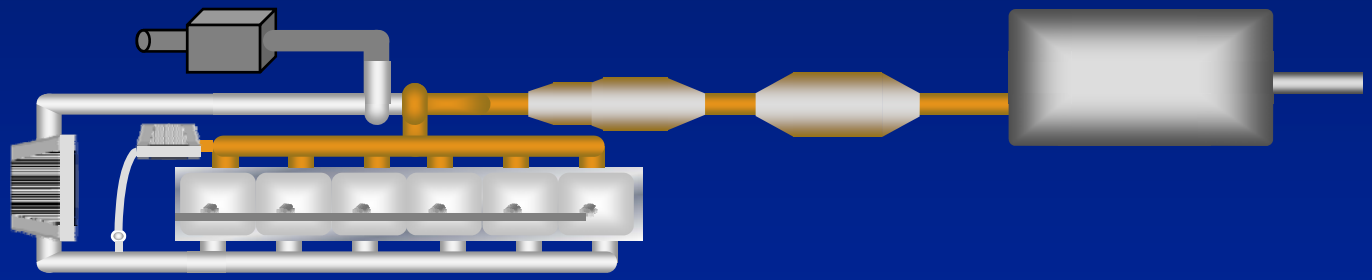
Development of Real Time Catalyst Model for Engine & Powertrain Control Design

S. Wenzel, B. Despujols, S. Wahiduzzaman, I. Papadimitriou
Gamma Technologies Inc., Westmont, IL, USA



12th DOE Crosscut Workshop
on Lean Emissions Reduction Simulation
April 28th - 30th, 2009
University of Michigan - Dearborn, 4901 Evergreen Road, Dearborn, Michigan 48128

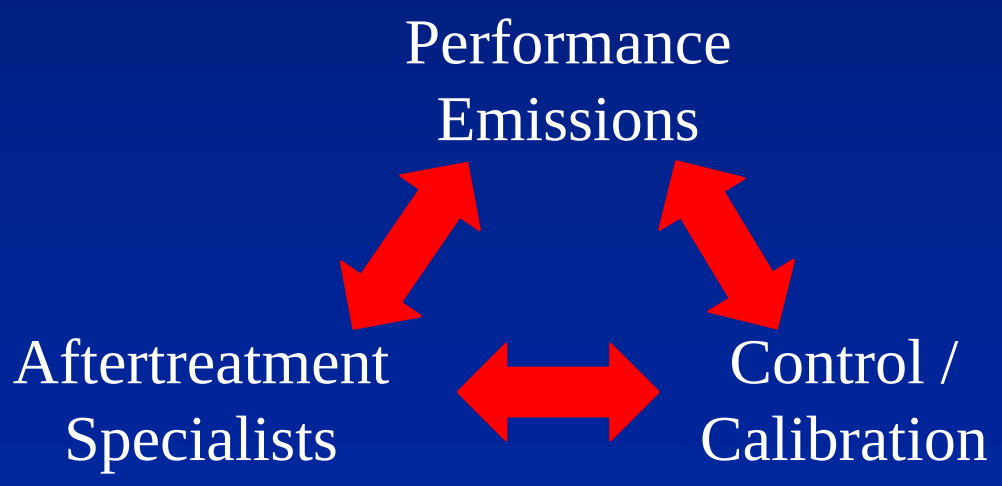
Motivation

- **Exhaust aftertreatment modeling must be *Collaborative Effort* among:**

  Performance engineers: Detailed cycle simulation tools

  Aftertreatment domain experts/chemists: Standalone models

  Control/Calibration engineers: Real time capable tools

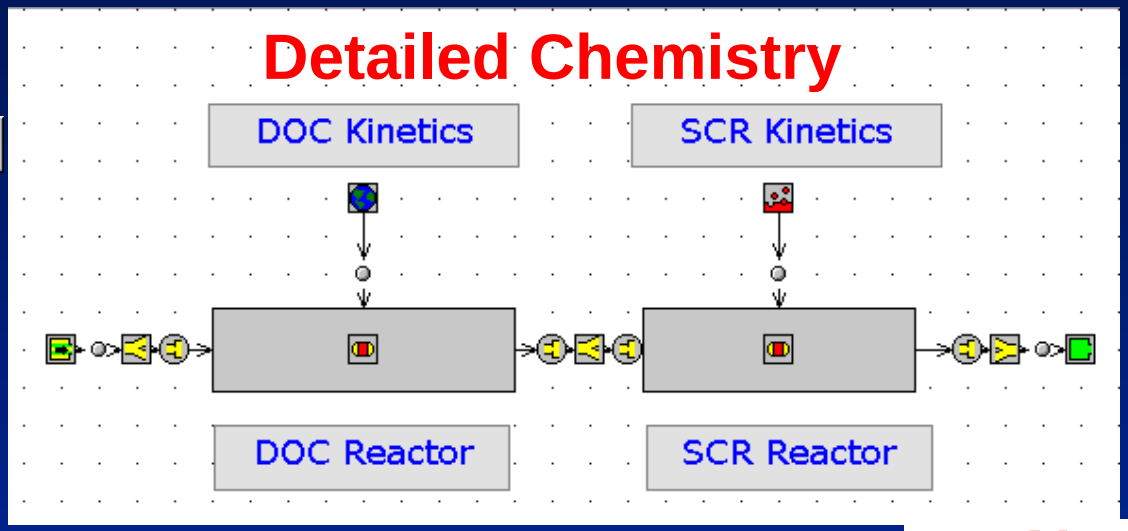


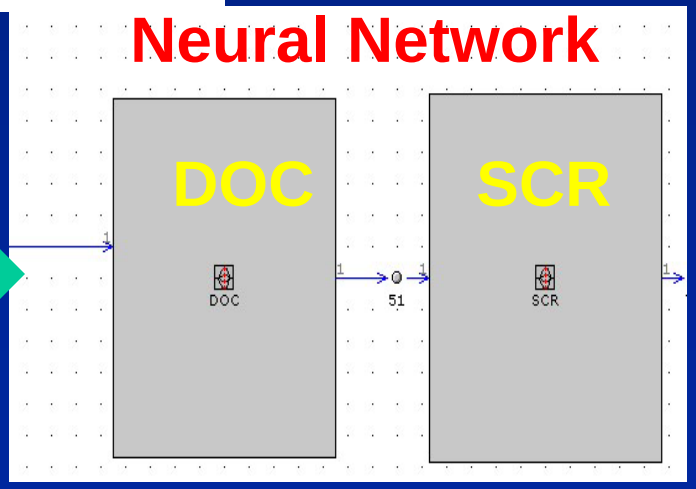
Motivation

- Standalone aftertreatement solutions can be "faster than real time"
  - Example: Quasi-Steady Solution
- "faster than real time" does not necessarily indicate suitable for HIL (Hardware in the Loop)
- Constrained by stiff ODE and DAE numerical solutions resulting in one of the following:
  - Adaptive time step sizing,
  - Faulty/Unstable results, prone to numerical failure
  - Becomes numerically inefficient when linked to hi-fidelity engine model
- True HIL systems require fixed timesteps

Methodology

- Create fast running hybrid neural network models derived from detailed chemistry





- Not constrained by stiff ODE and DAE systems

Simulation Workflow
Experiment => calibration => Prediction

Initial parameters Values

Start

GT-POWER model

Altered parameters

Customized objective function

GT-POWER solver

Online sensors/controls evaluating objective

Yes/no

Built-in DoE or Direct Optimizer

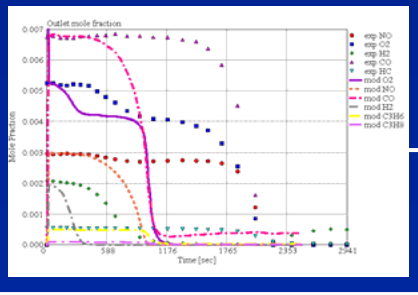
End

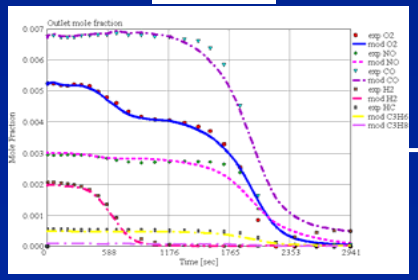
Applied to TWC Light-off Data

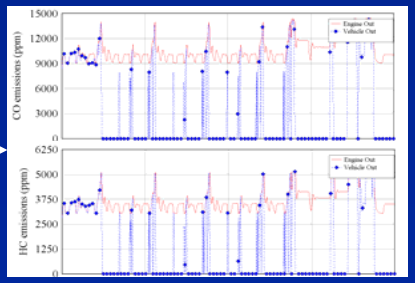
before

after

cycle emissions prediction



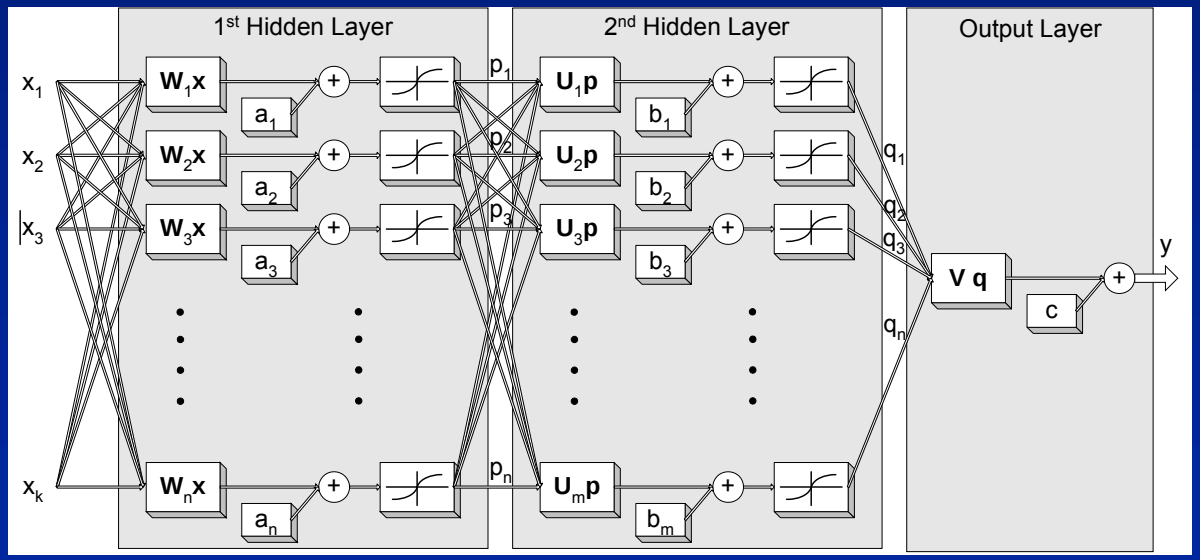




All in a one integrated environment

Neural Network Training

- Three-Layer Feedforward Neural Network
  - ✓ 2 hidden layers with tan-sigmoid activation functions
  - ✓ 1 output layer with linear activation function
- Levenberg-Marquardt algorithm for training
- Excellent Neural Network generalization capability
  - ✓ Fixed balanced penalties
  - ✓ Adjustable penalties ("Bayesian Regularization")



Detailed DOC Model

- **DOC Reaction Set:**

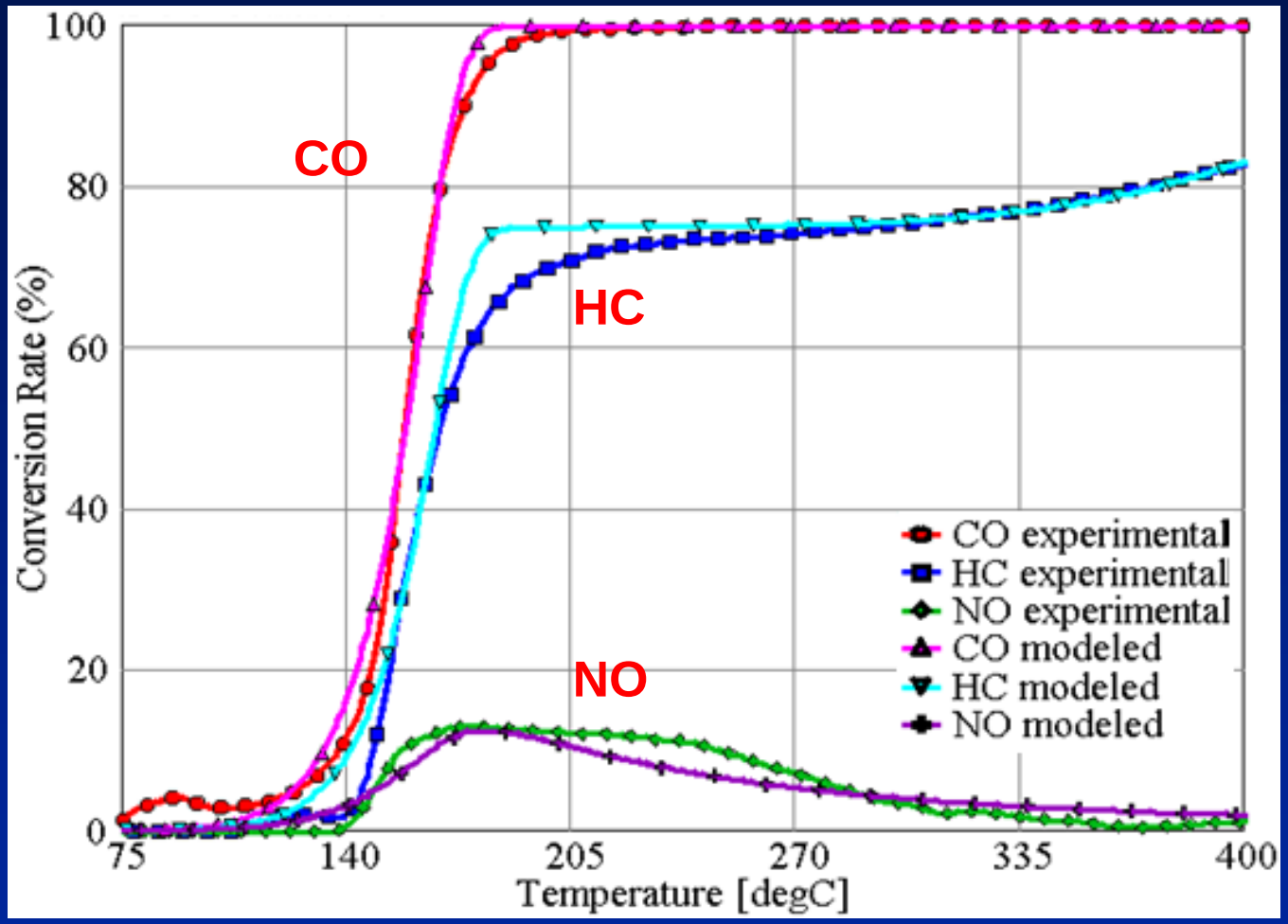
R1: $CO + 0.5O_2 \rightarrow CO_2$
R2: $C_3H_6 + 4.5O_2 \rightarrow 3CO_2 + 3H_2O$
R3: $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$
R4: $CO + NO \rightarrow CO_2 + 0.5N_2$
R5: $H_2 + 0.5O_2 \rightarrow H_2O$
R6: $NO + 0.5O_2 \rightarrow NO_2$
R7: $NO_2 \rightarrow NO + 0.5O_2$

- **Inputs to DOE of DOC model:**

Inlet condition	Min	Max
Catalyst Wall Temp. (K)	280	800
Inlet mass flow rate (kg/s)	0.001	0.15
NO mole fraction	0.0	4.0e-4
NO_2 mole fraction	0.0	4.0e-4
CO mole fraction	0.0	0.002
Total HC mole fraction	0.0	1.5e-4

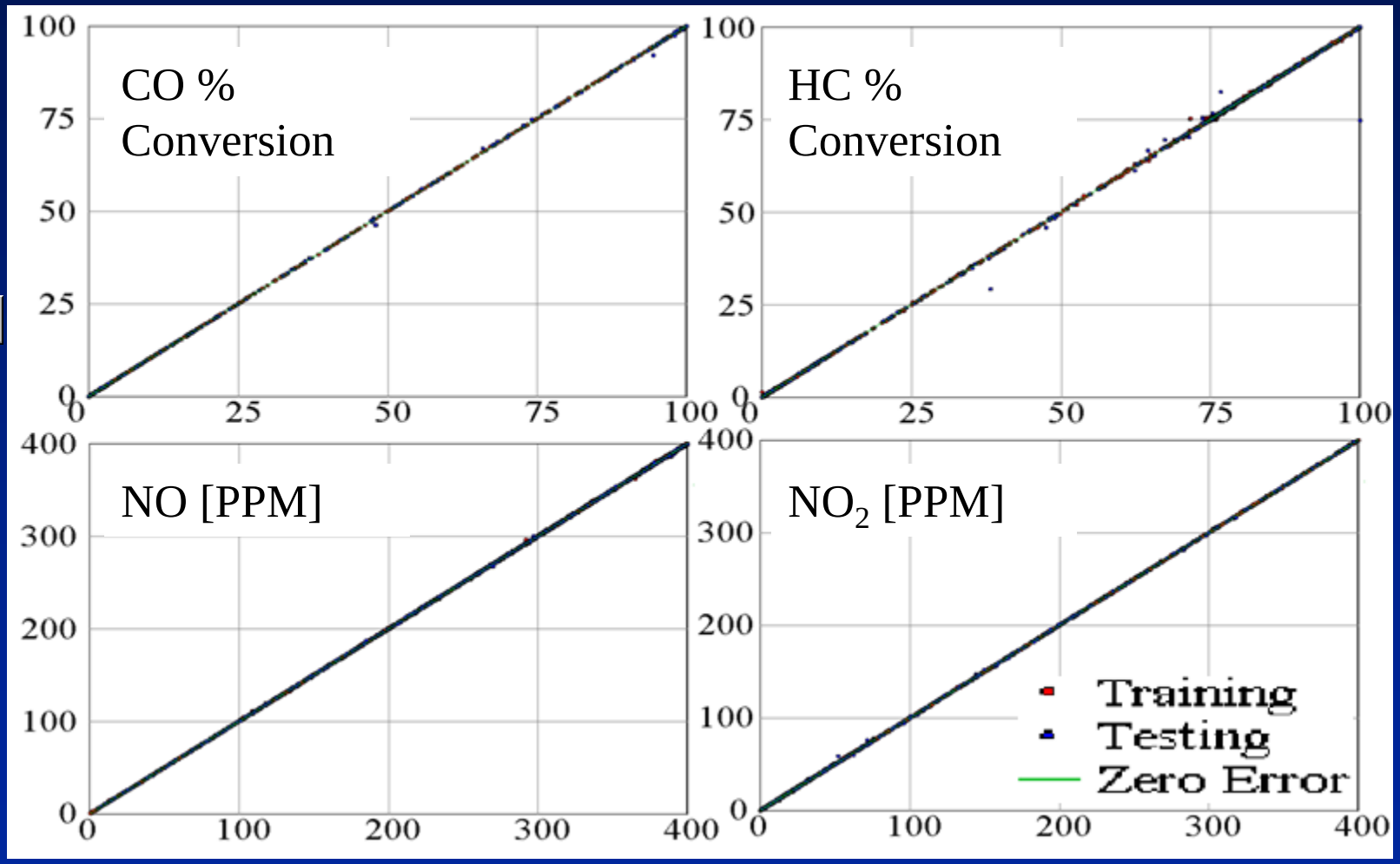
- **DOE of 5000 cases using Latin Hypercube**

Detailed DOC Model



Full model development described in SAE 2008-01-0866

DOC NN Training Results



Detailed SCR Model

- **SCR Reaction Set:**

R8:	$NH_3 + S$	=> $NH_3(S)$
R9:	$NH_3(S)$	=> $NH_3 + S$
R10:	$4NH_3 + 3O_2$	=> $2N_2 + 6H_2O$
R11:	$4NH_3 + 4NO + O_2$	=> $4N_2 + 6H_2O$
R12:	$8NH_3(S) + 6NO_2$	=> $7N_2 + 12H_2O + 8S$
R13:	$4NH_3(S) + 2NO + 2NO_2$	=> $4N_2 + 6H_2O + 4S$

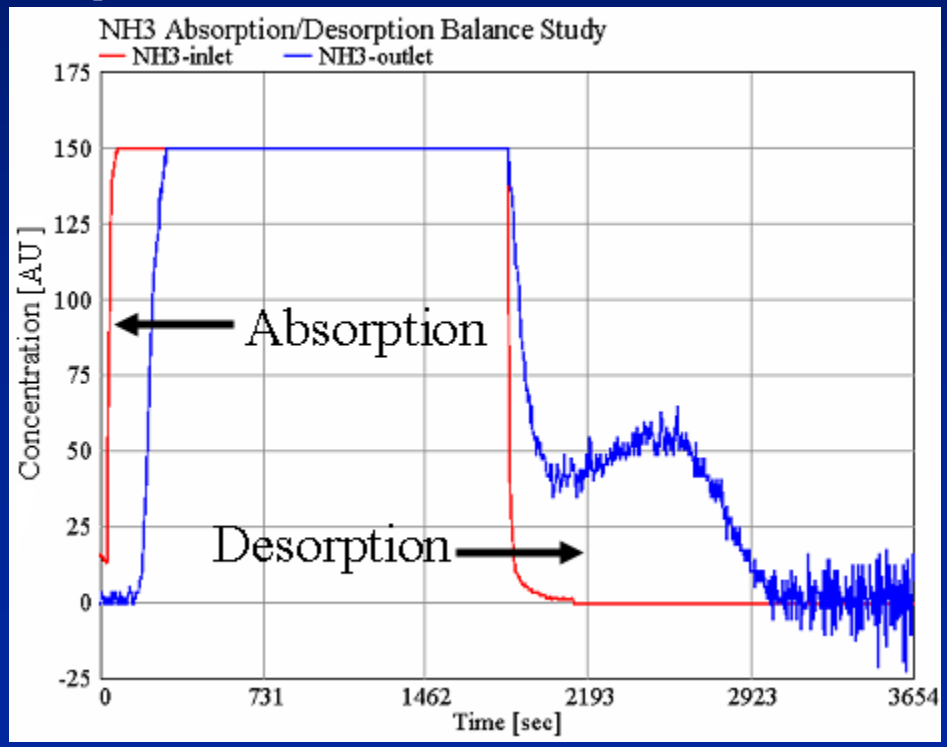
- **Inputs to DOE of SCR model:**

Inlet condition	Min	Max
Catalyst Wall Temp. (K)	280	800
Inlet mass flow rate (kg/s)	0.001	0.15
NO mole fraction	0.0	4.0e-4
NO_2 mole fraction	0.0	4.0e-4
NH_3 mole fraction	0.0	6.0e-4
Coverage	0.0	1.0

- **DOE of 5000 cases using Latin Hypercube**

Calculation of Storage Capacity

- Experimental results suggest more NH_3 desorbed than could be accounted for by absorption
- Two possibilities exist:
  1. experimental error in one or both NH_3 sensors
  2. NH_3 is pre-stored

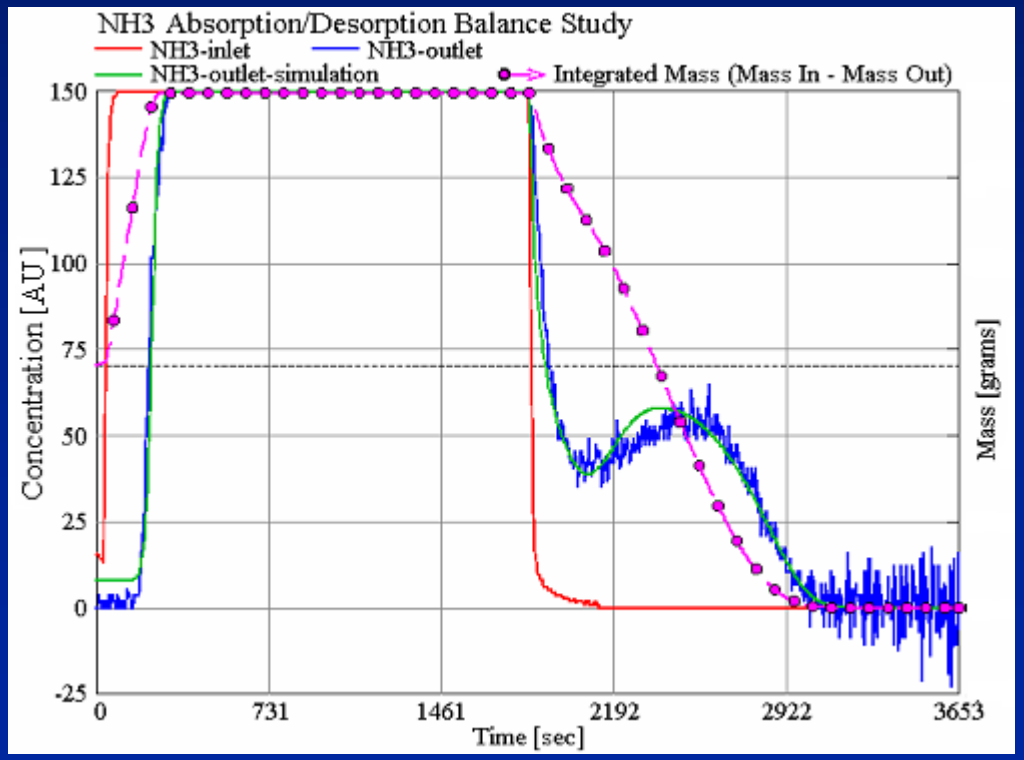


Storage Capacity (cont.)

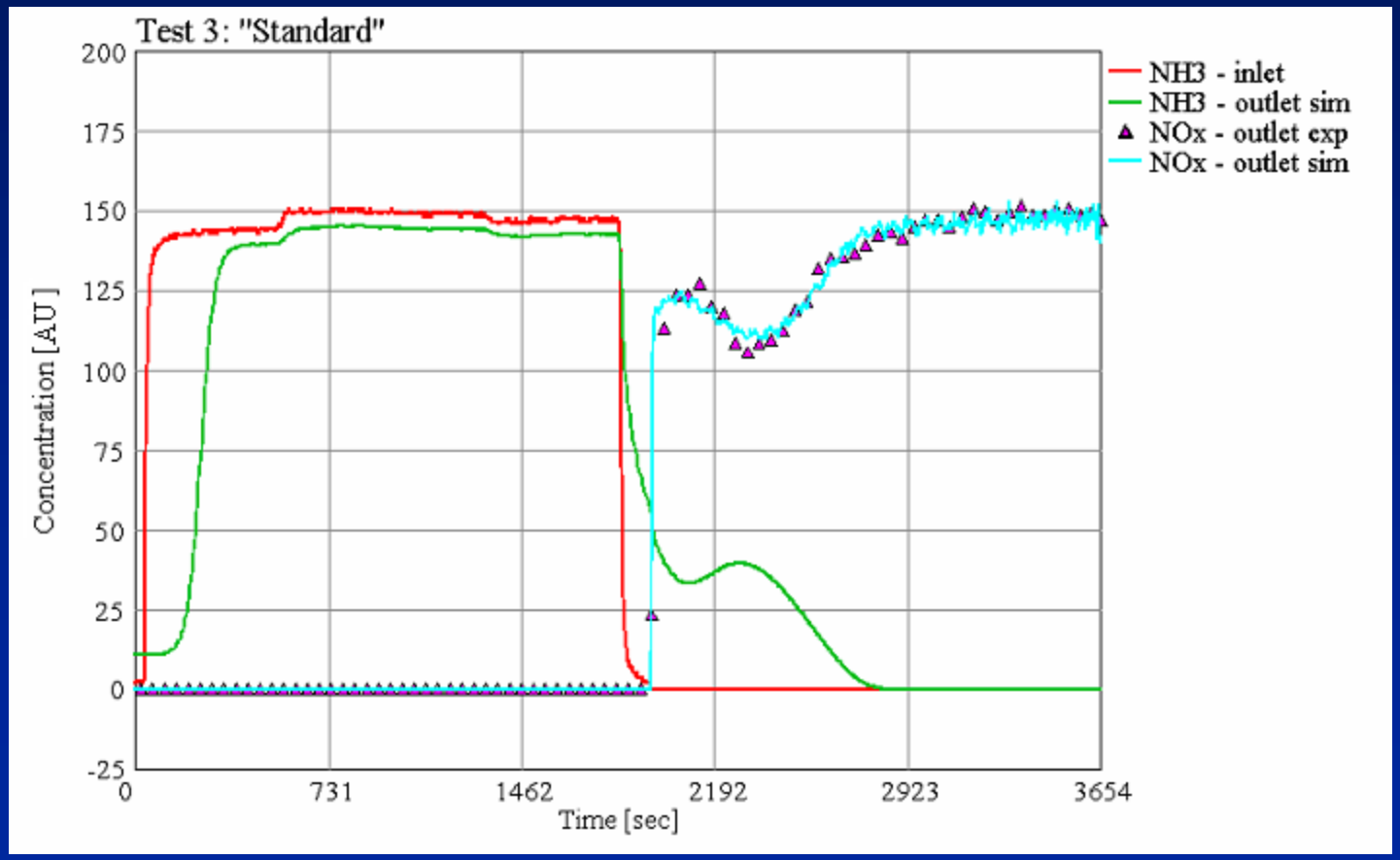
- The onset of saturation and shape of saturation curve indicated by the exit NH_3 sensor seemed to be consistent
- Optimization was performed to determine:
  - storage capacity
  - pre-stored NH_3 (if any)
- Optimization goal:
  - conserve NH_3 mass
  - conserve onset/shape of NH_3 saturation curve
- Built-in Brent direct optimizer was used

Storage Capacity (cont.)

- A pre-storage corresponding to 45% coverage and a storage capacity of 4.9E-3gmole/m^2 were determined
- These generally agree with all experiments

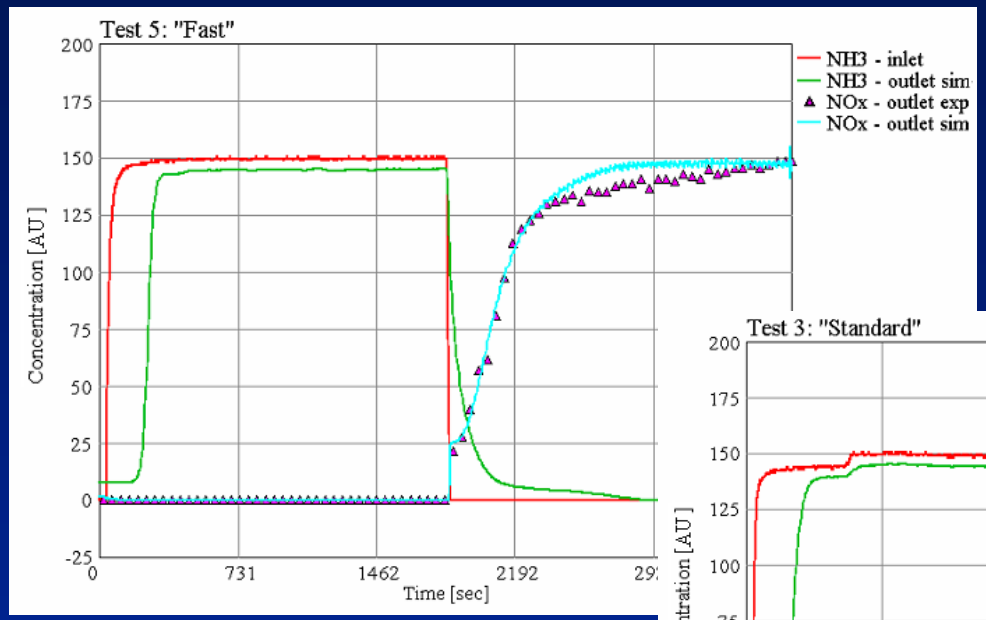


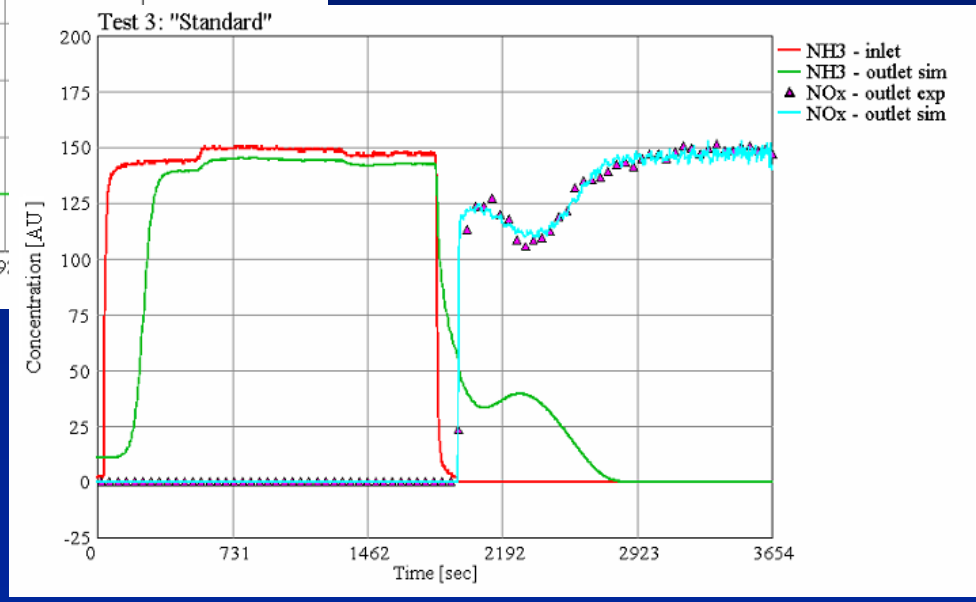
Standard Reaction



Validations

Fast: $4NH_3 + 2NO + 2NO_2 \Rightarrow 4N_2 + 6H_2O$

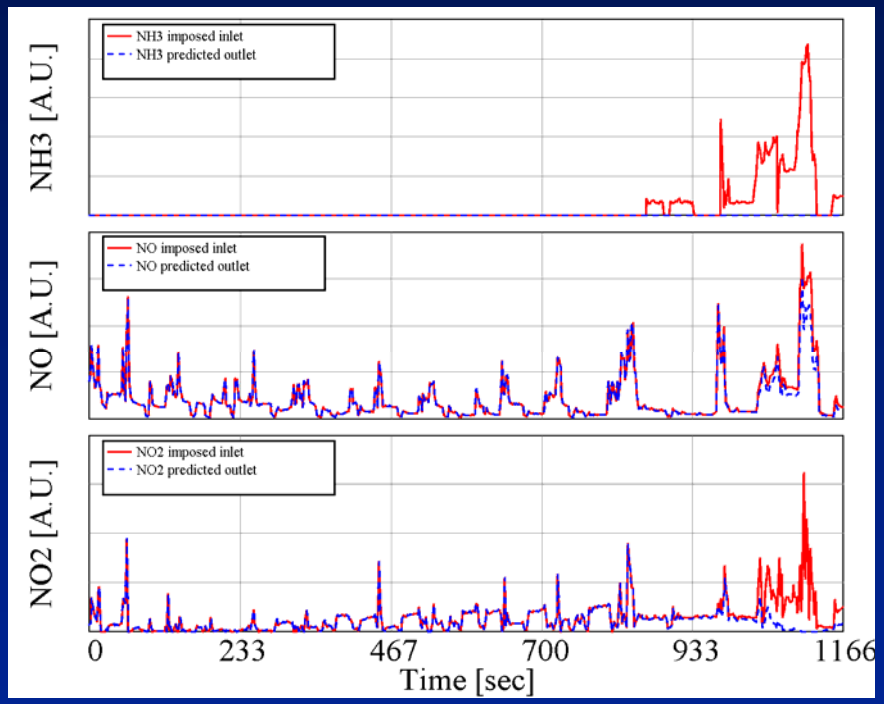




Standard: $4NH_3 + 4NO + O_2 \Rightarrow 4N_2 + 6H_2O$

Emission Predictions (cont.)

- All sites "open" (no NH_3 prestored)

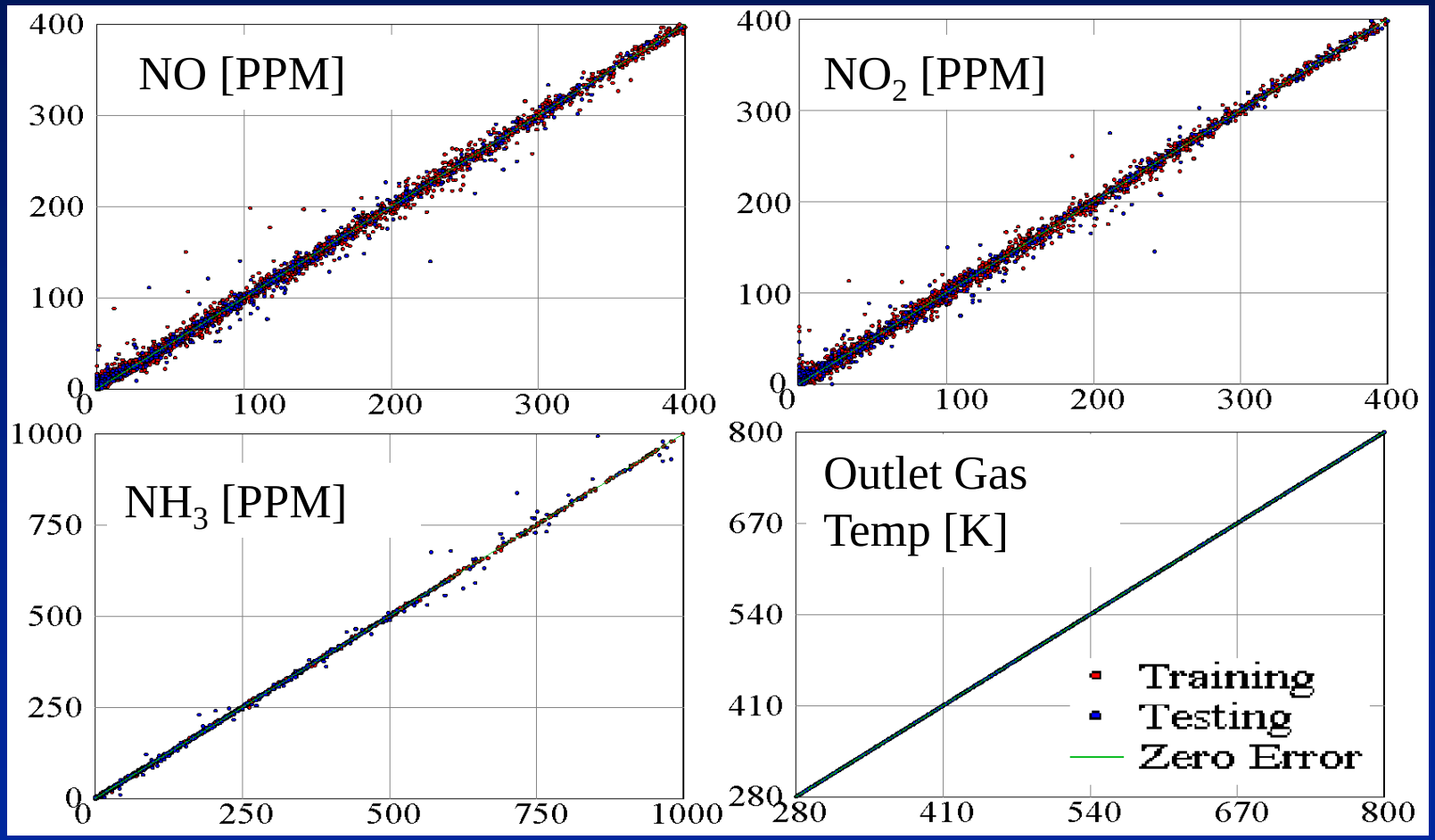


- Cumulative Mass Changes:

$NO = -28\%$ $NO_X = -37\%$

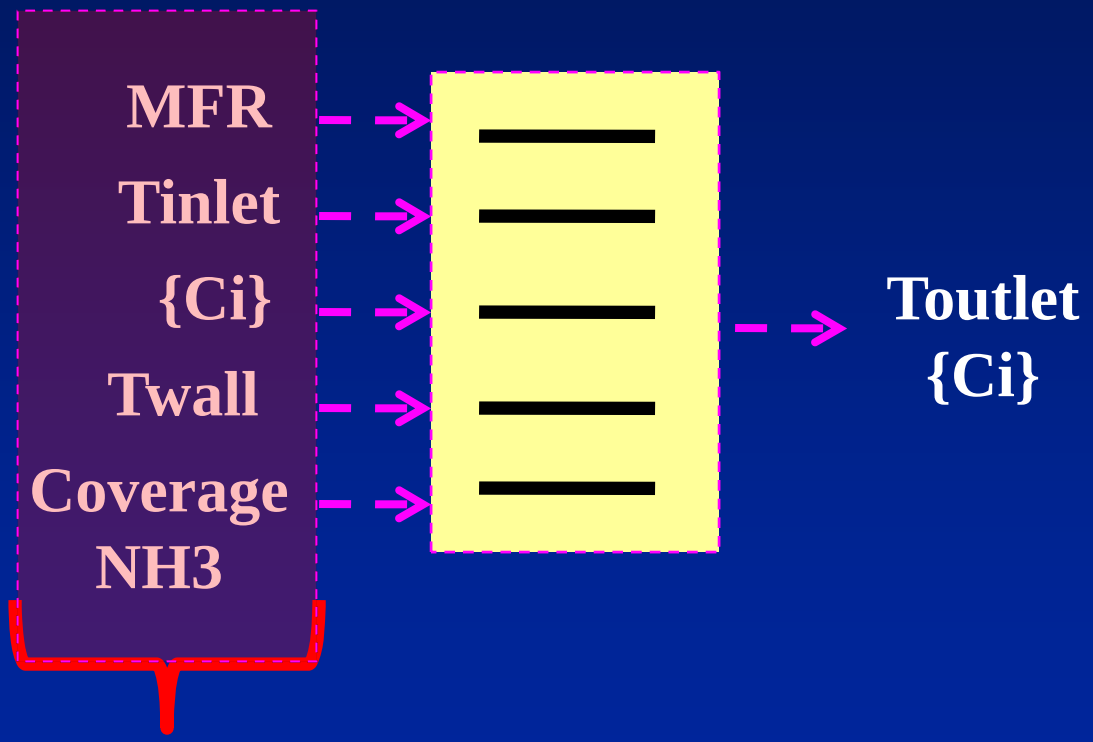
$NO_2 = -49\%$ $NH_3 = -100\%$

SCR NN Training Results



SCR NN Training data

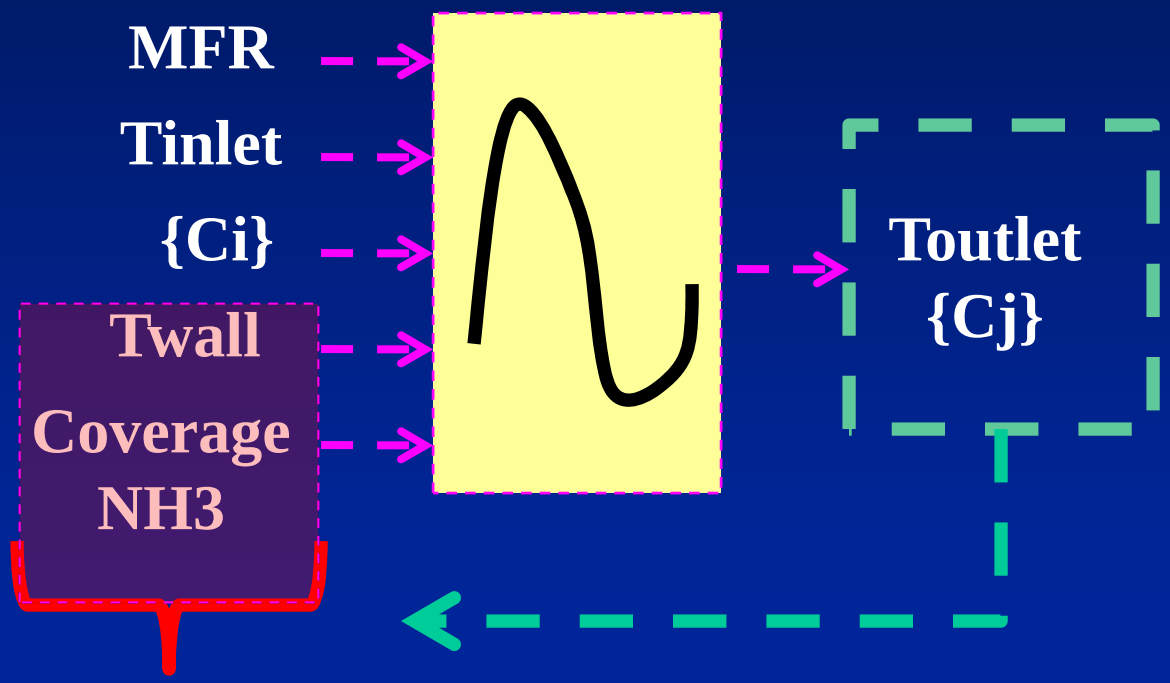
Duration =10-100*residence time



Imposed in the Steady State DOE used to train NN

SCR NN Training data

Transient/NEDEC

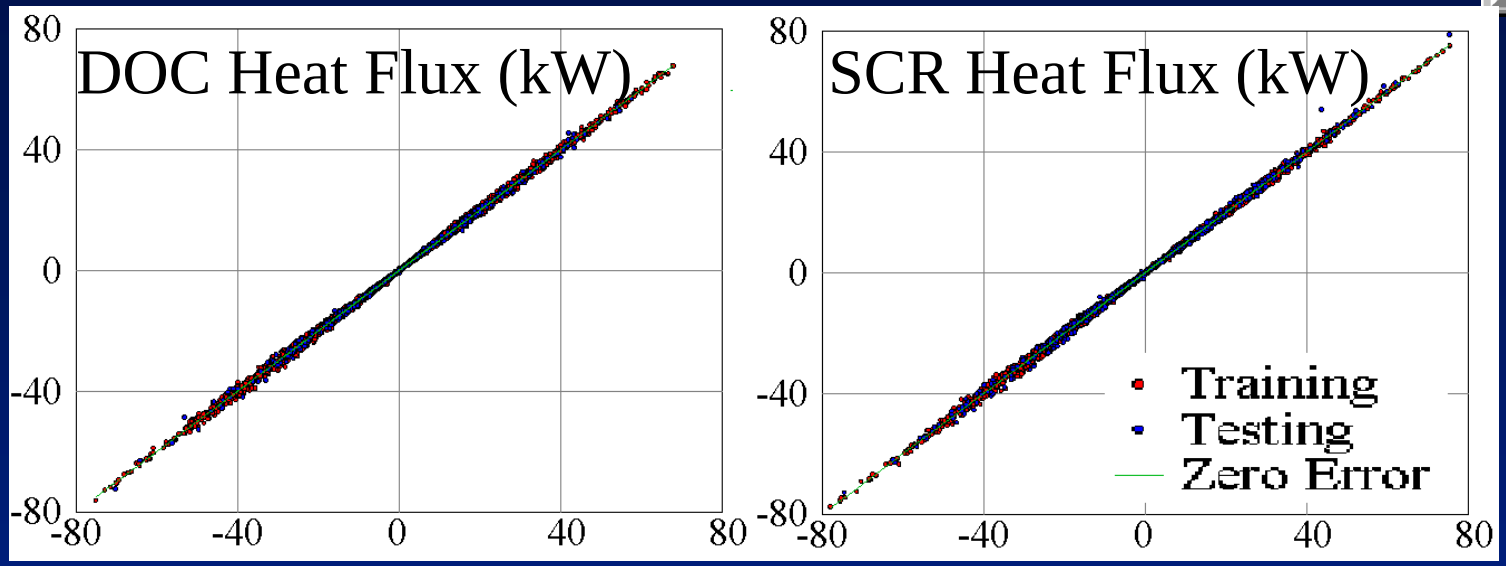


Cannot be imposed in transient, depends on previous state

Dynamics Modeling

- GT-POWER uses “static” neural networks
- Static Neural Networks
  - Can model “transients” based on successive steady states (quasi-steady) – ideal for IMEP, Vol Eff, etc.
  - Does NOT account for dynamics modeling (history of events)
- For exhaust aftertreatment modeling there is additional dynamic phenomena
  - Catalyst wall temperatures
  - Storage affects

Catalysts Wall Temperature



(1) Static Neural Networks Accounts for:

- **internal heat transfer**
- **catalytic heat release**

$$Q_{Flux} = Q_{convection} + Q_{chemistry}$$

(2) Transient Physical Model Accounts for:

- **wall temperature solution**

$$Q_{Flux} = m \cdot C_p \cdot \frac{dT}{dt}$$

SCR NH_3 Coverage Models

- NH_3 absorption/desorption is a "dynamic" phenomenon

- Detailed models calculates "coverage" of stored NH_3 (amount of NH_3 stored on the surface)

SCR NH_3 Coverage Models

(1) NH_3 conservation

$$NH_{3IN} = NH_{3OUT} + NH_{3REDUCE} + NH_{3STORE}$$

(2) NH_3 In

$$NH_{3IN} = \int_0^t NH_3 Inlet(\text{mole/s})dt$$

(3) NH_3 Out

$$NH_{3OUT} = \int_0^t NH_3 Outlet(\text{moles/s})dt$$

(4) NH_3 Reduce

-amount needed to reduce NO_X

-assume 1 mole NH_3 required to reduce 1 mole NO_X

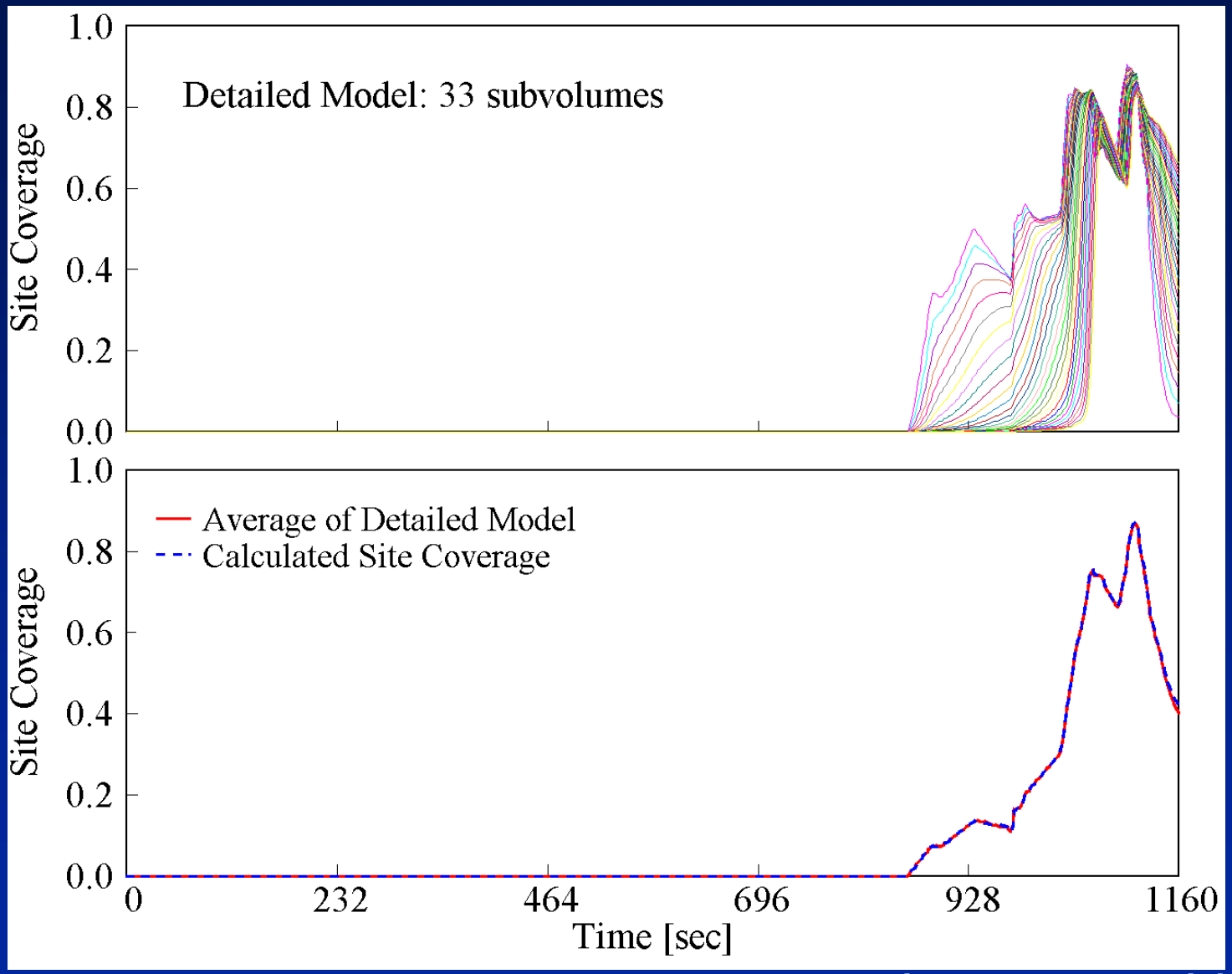
$$NH_{3REDUCE} = \int_0^1 (NO(in) + NO_2(in))dt - \int_0^1 (NO(out) + NO_2(out))dt$$

Based on Equations n 1-4, solve for NH_{3STORE}

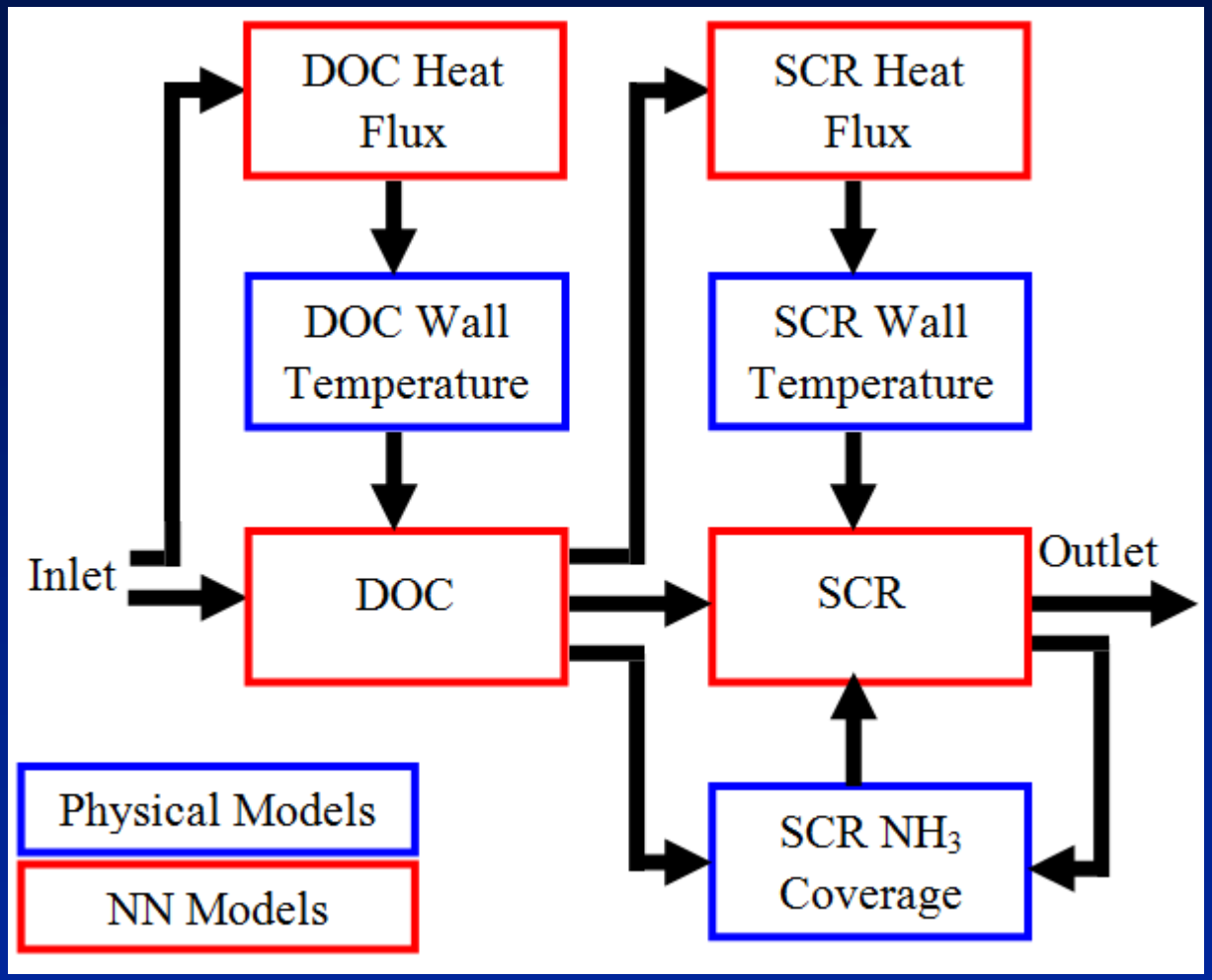
(5) Coverage

$$\text{Coverage } \Theta = \frac{NH_3(\text{STORE})}{NH_3(\text{Site Capacity})}$$

SCR NH3 Coverage Models

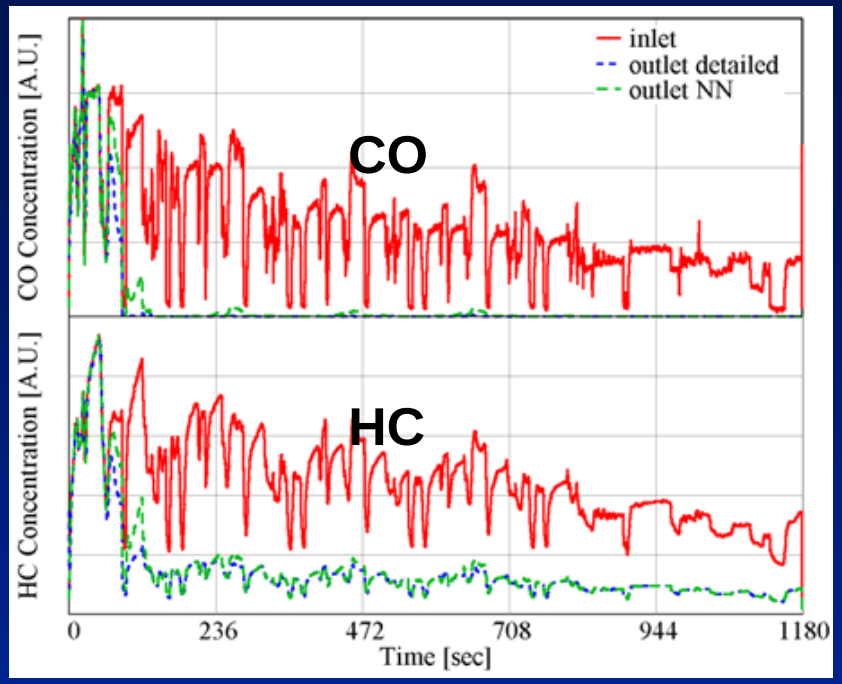


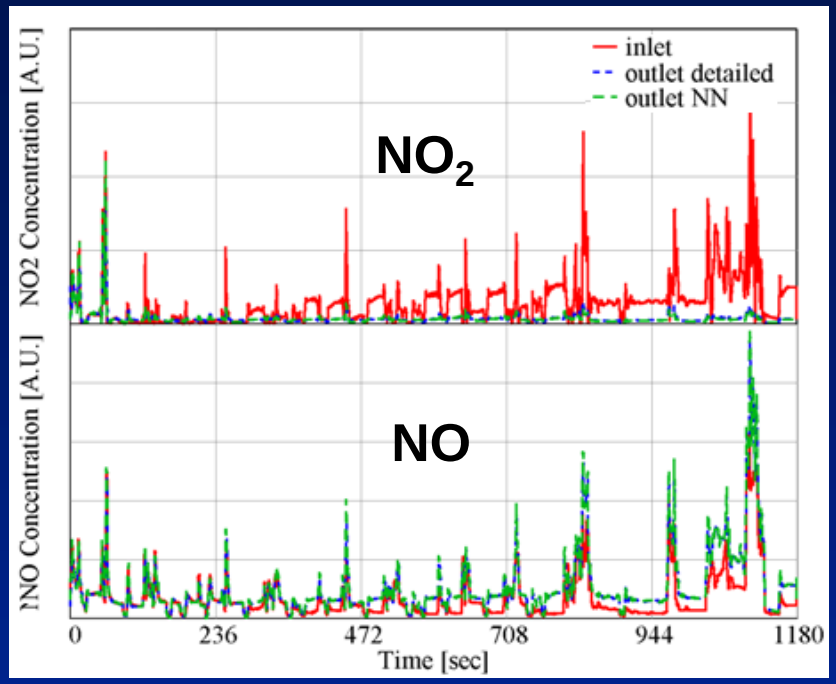
SIL/HIL Model Generation

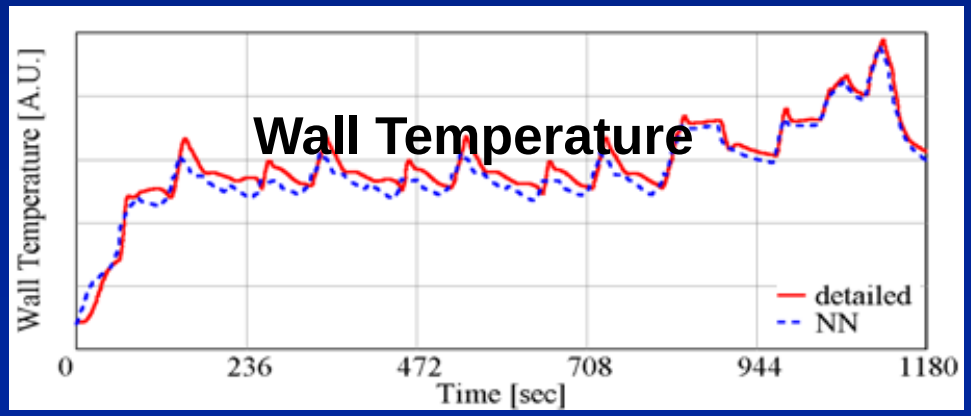


- Consist of Neural Networks or physical models
- No detailed chemistry or flow is modeled

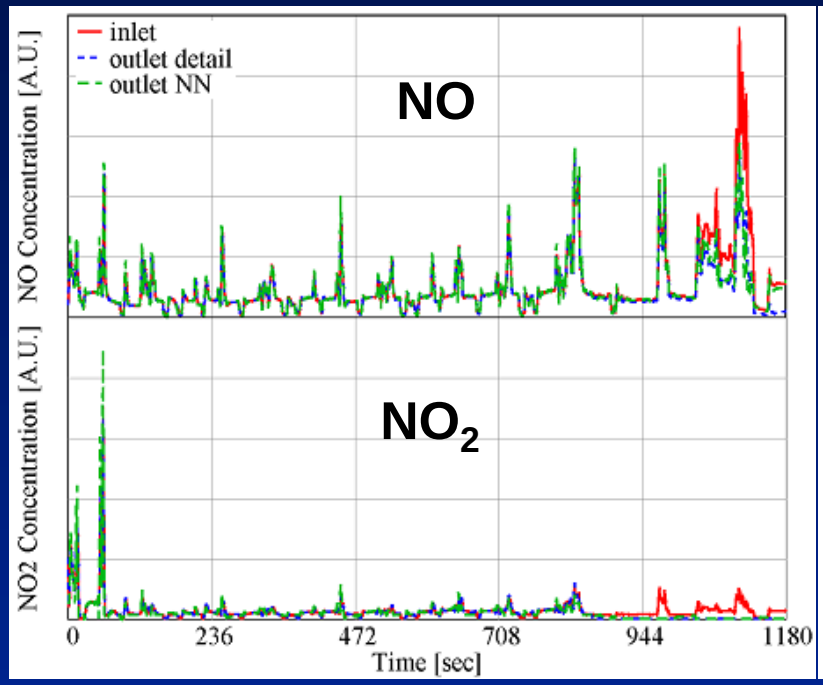
SIL/HIL Enabled NN-AT Model
DOC Results

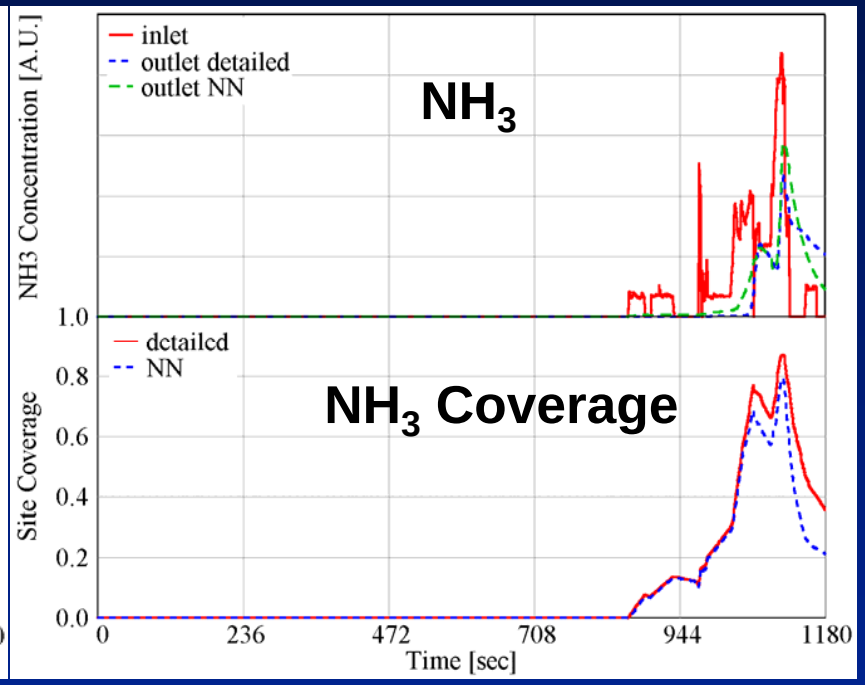


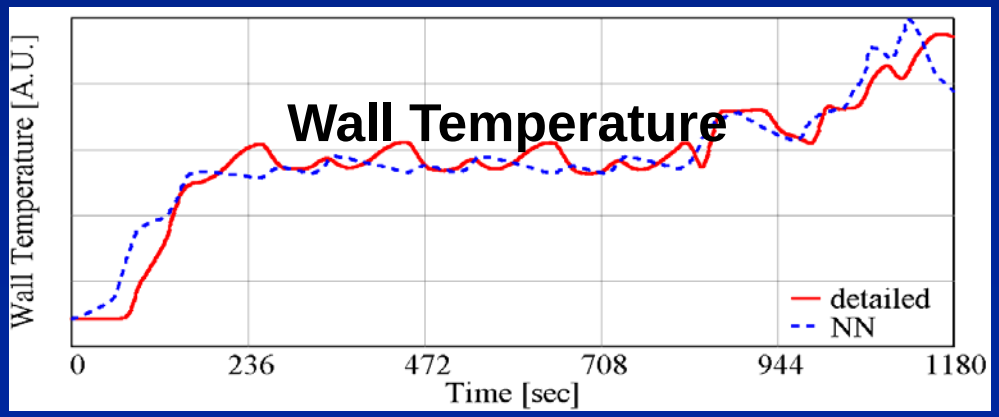




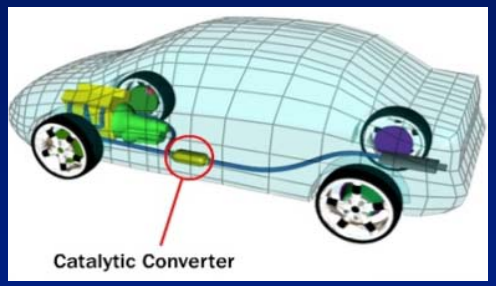
SIL/HIL Enabled NN-AT Model
SCR Results

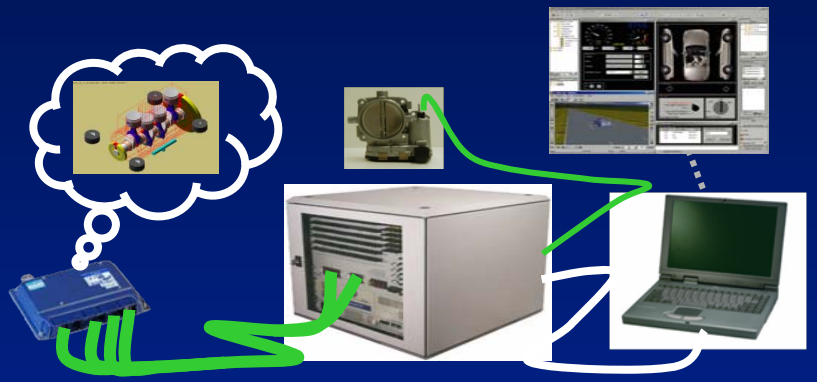


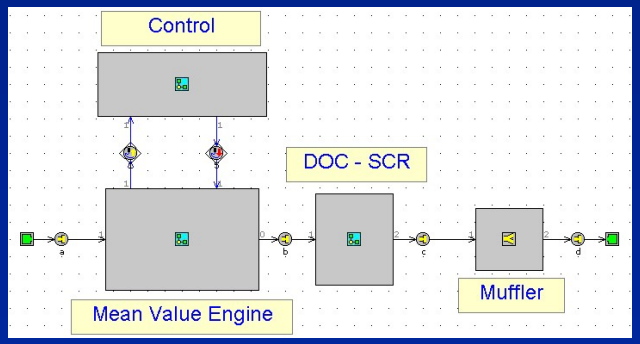




SIL/HIL Enabled Engine/NN-AT Model







Computational Speed Comparison

(1180s NEDC)

Model Type	Solver	CPU
Standalone Kinetic AT	QS	90s
Standalone Neural Network AT	Explicit	2s
Detailed Engine + Kinetic AT	Explicit	60h
MV Engine + Kinetic AT	Explicit	39h
MV Engine (Explicit) + Kinetic AT (QS)	Mixed	635s
MV Engine + Neural Network AT	Explicit	625s
MV Engine + Neural Network AT	GT-Suite RT	331s

Conclusion

- A *Quasi-steady* (*QS*) based solver have been implemented that conserves accuracy of the computationally demanding fully explicit solver
- Calibration of global kinetics was shown to be computationally efficient using DOE direct optimizers
- Feasibility of SIL/HIL compatible NN model generation was demonstrated using detailed kinetic model
- NN model was improved using a hybrid methodology that improved the fidelity of the system model

Conclusion (cont.)

- **Hybrid methodology includes:**
  - **Static Neural Networks:**
    - (1) DOC and SCR emission modeling
    - (2) Heat Flux into catalyst walls
  - **Dynamic Models:**
    - (3) Thermal Models
    - (4) Coverage Model for NH_3 absorption
- Methodology preserves overall accuracy of detailed models