Development and Application of a Fast *Quasi*-Steady Solver for Integrated Modeling of Exhaust Aftertreatment Systems

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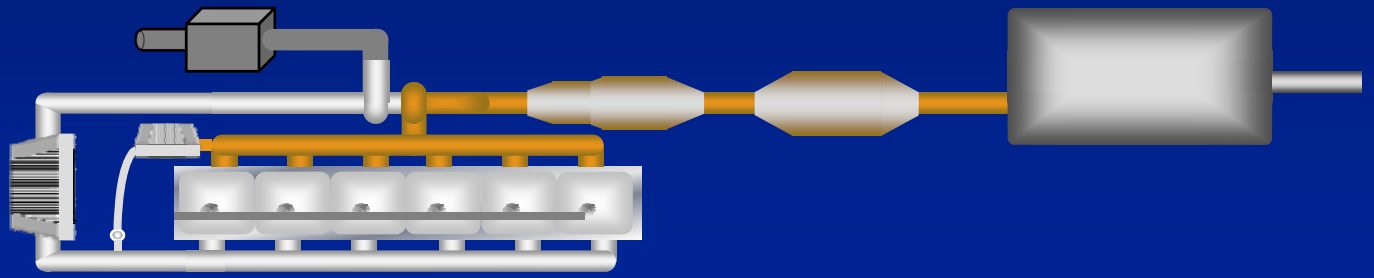


11th Cleers Workshop

May 13-14 2008, Dearborn, MI, USA

Modeling Solutions Overview

- **Flow model to coupled reactor model**
  GUI based chemistry library
  (SAE 2007-01-4127, 9-10th Cleers Workshop)

- **Computational y efficient solver**
  Quasi-Steady (QS) solver
  (SAE 2008-01-0866)

- **Kinetic parameter calibration**
  DoE (Design of Experiment) or direct optimizer
  (SAE 2007-01-4127)

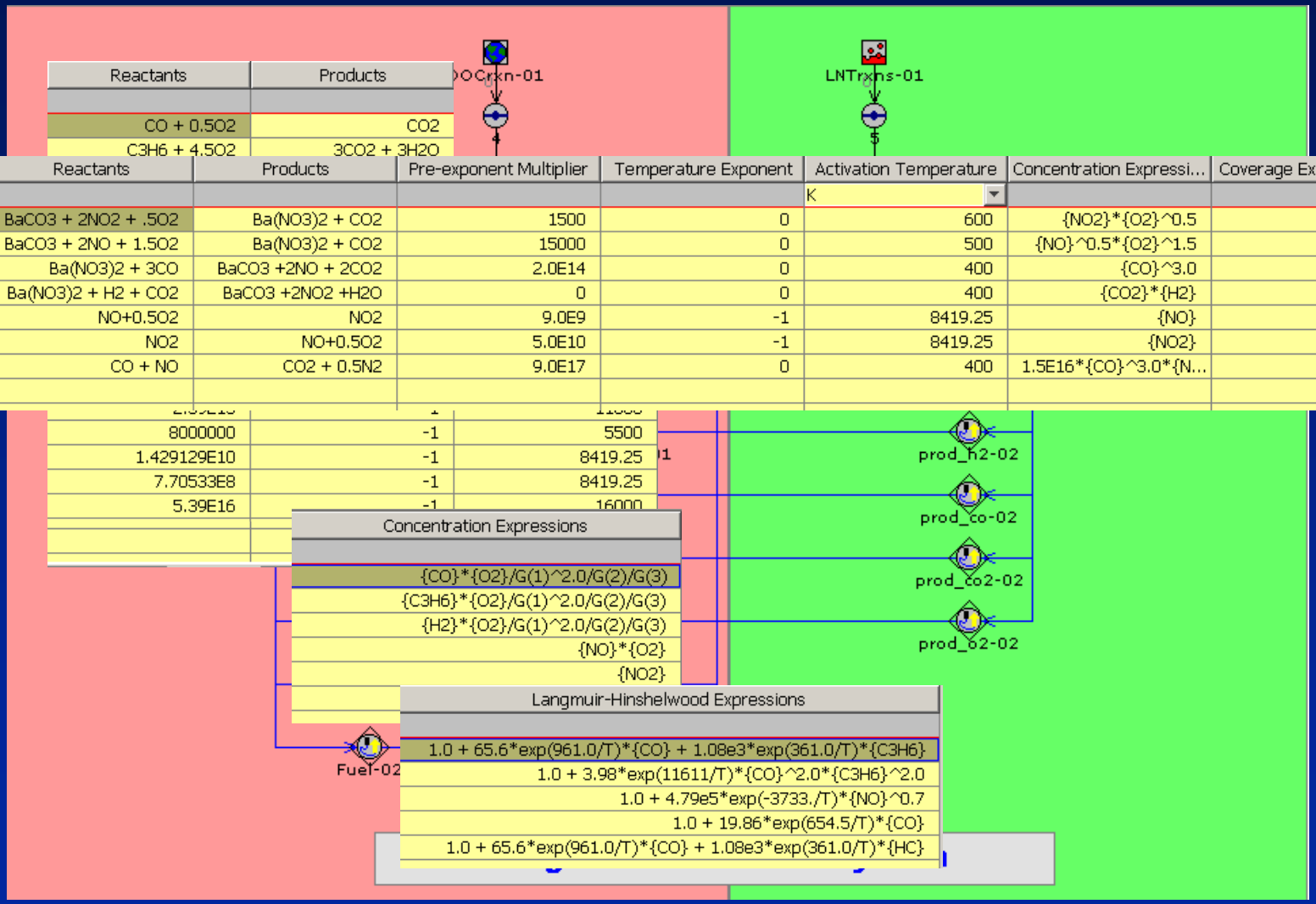
Modeling Solutions Overview (Cont.)

- *Advanced applications*
  System modeling, effect s of aging

- *Fast models for SIL and HIL applications*
  From detailed model to NN model
  (SIA, 28-29th May, 2008, INSA de Rouen, France)

- **Multi-dimensional and quasi-dimensional solution**
  QS based 2D/3D modeling

Flow Model to Reactor Model



Simulation Workflow
Experiment => calibration => Prediction

Start

Initial parameters Values

GT-POWER model

Altered parameters

GT-POWER solver

objective function

Online sensors/controls evaluating objective

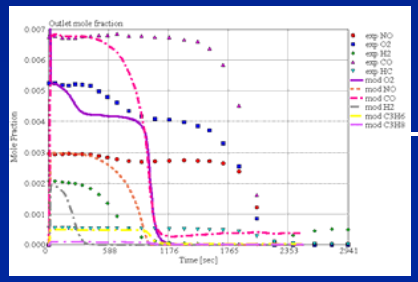
Yes/no

Built-in DoE or Direct Optimizer

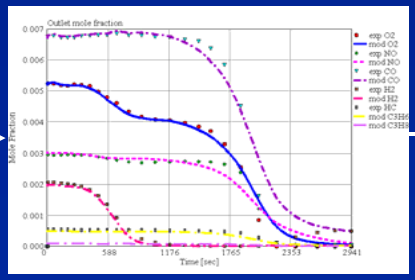
End

Applied to TWC Light-off Data

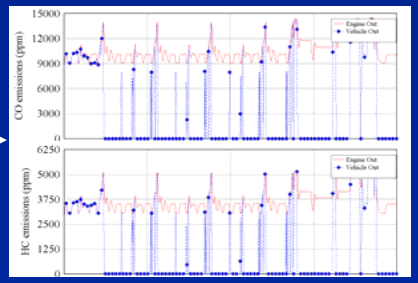
before



after



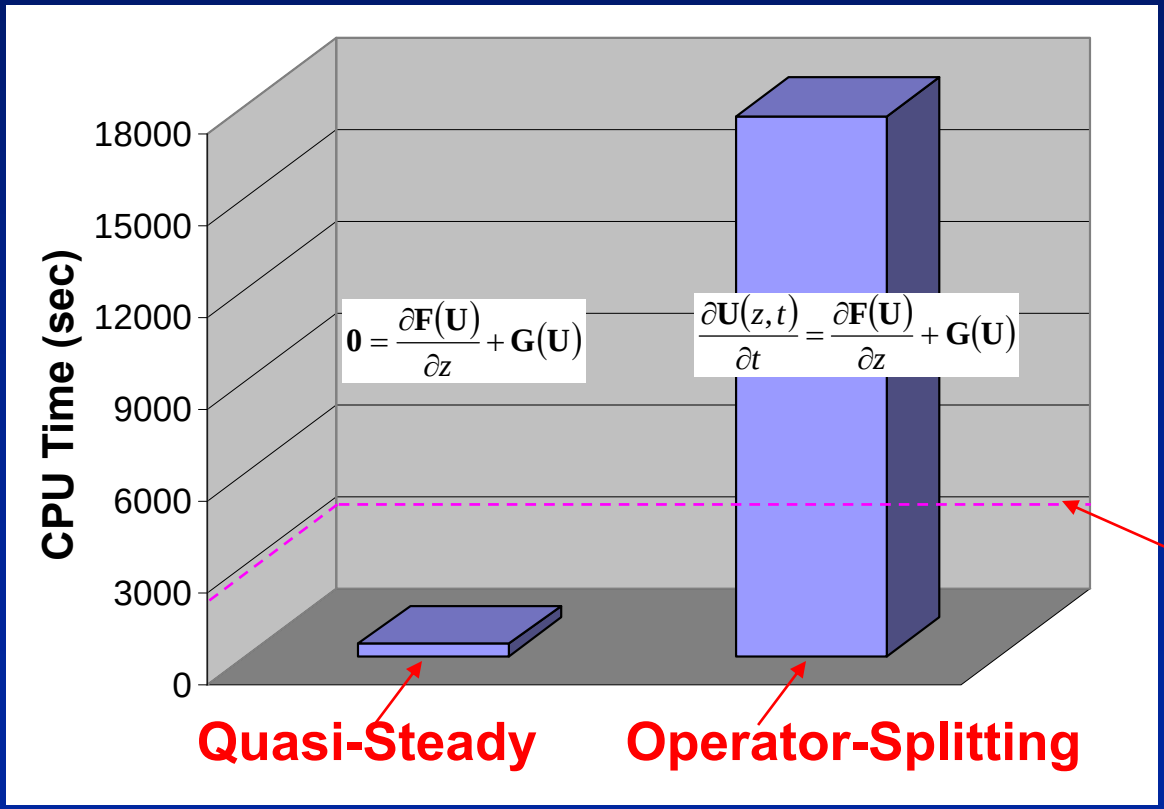
cycle emissions prediction



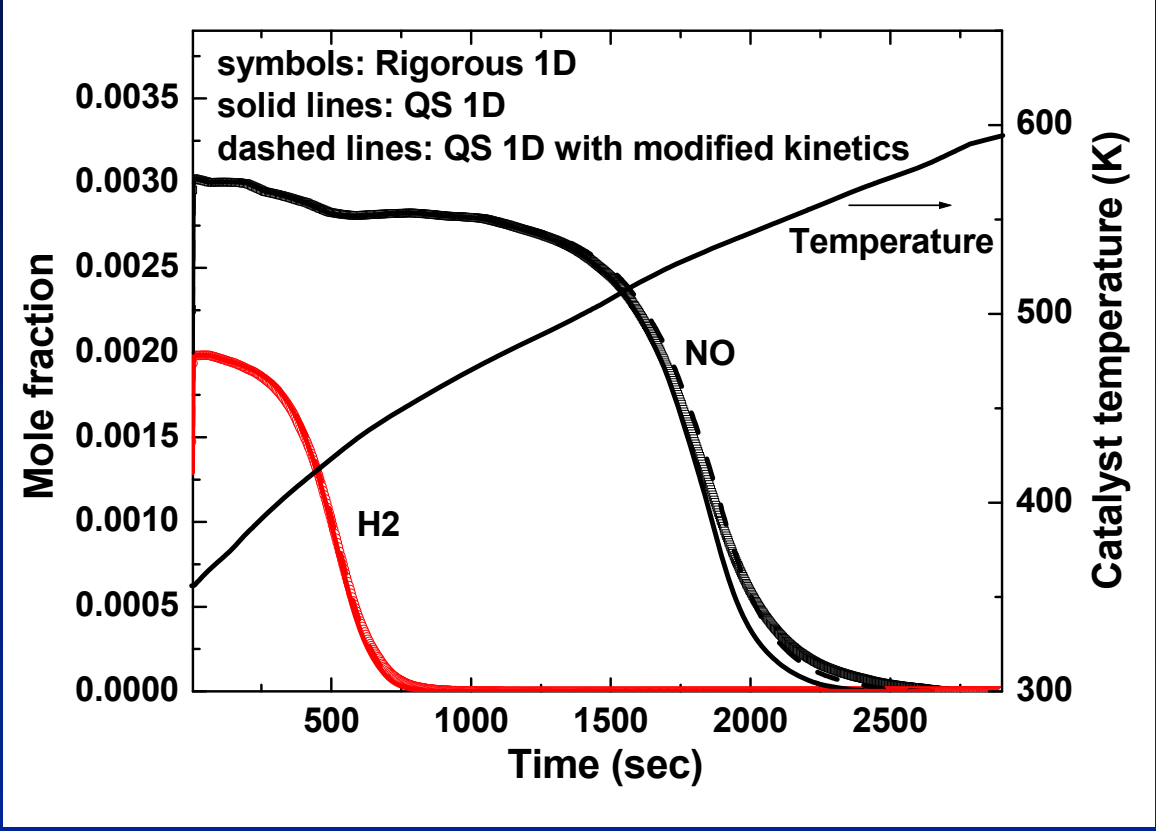
All in a one integrated environment

Computational Efficiency of Q-S Solver (SAE 2008-01-0866)

- TWC kinetic model
- Simulation duration: 2942 seconds
- 20 sub-volume, dt = 0.1 seconds
- QS can be 10-100 times faster than real time



Accuracy of QS Approach



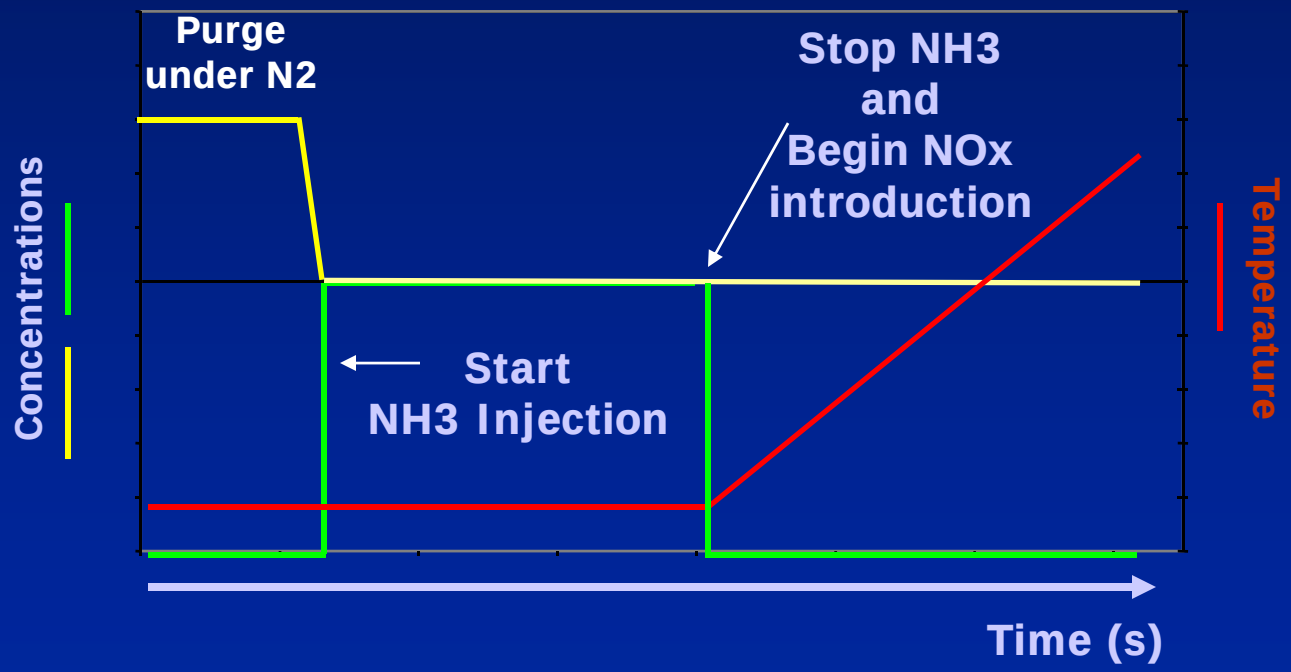
$$\frac{\partial \mathbf{C_g}}{\partial t} + u\frac{\partial \mathbf{C_g}}{\partial z} = \dot{\mathbf{R}}\left(\mathbf{C_s}, \theta, T_s\right)$$

$$u\frac{\partial \mathbf{C_g}}{\partial z} = \dot{\mathbf{R}}\left(\mathbf{C_s}, \theta, T_s\right) - \frac{\mathbf{C_g} - \mathbf{C_g^o}}{\Delta t} = \dot{\mathbf{R}}'\left(\mathbf{C_s}, \theta, T_s\right)$$

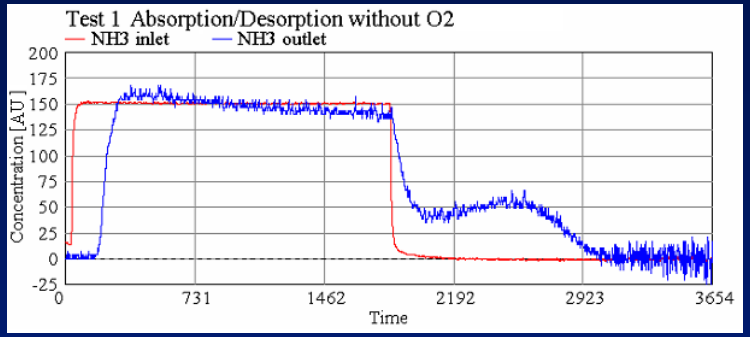
Component Level Modeling
Zeolite Based SCR

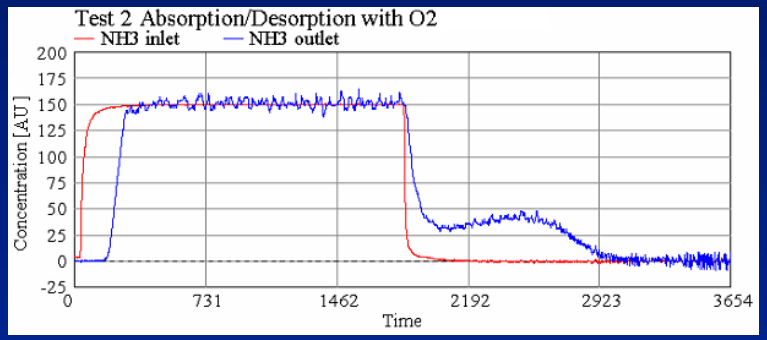
- Experimental data was provided by PSA Peugeot Citroën
- Five set of calibration data aimed at determination of parameters involving
  - Test 1: Storage capacity, absorption/desorption
    $* + NH_3 <=> *NH_3$
  - Test 2: Ammonia oxidation
    $4NH_3 + 3O_2 => 2N_2 + 6H_2O$
  - Test 3: “Standard” SCR reaction
    $4NH_3 + 4NO + O_2 => 4N_2 + 6H_2O$
  - Test 4: “Slow” SCR reaction
    $8NH_3 + 6NO_2 => 7N_2 + 12H_2O$
  - Test 5: “Fast” SCR reaction
    $4NH_3 + 2NO + 2NO_2 => 4N_2 + 6H_2O$

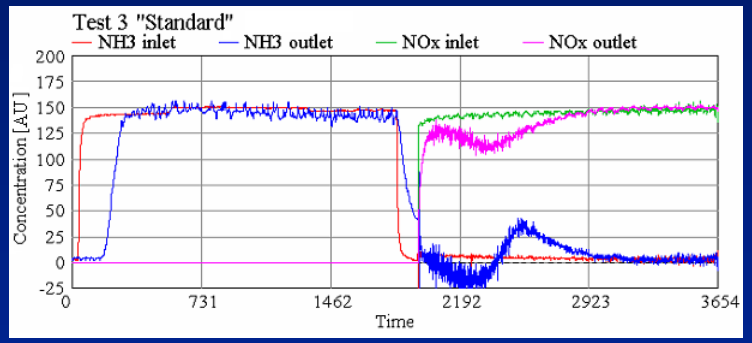
SGB protocol for testing
SCR catalyst

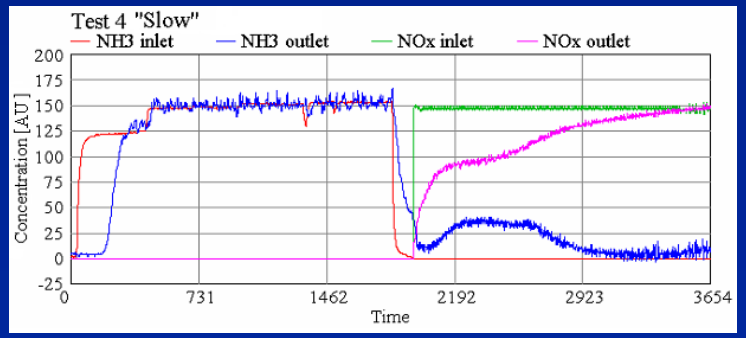


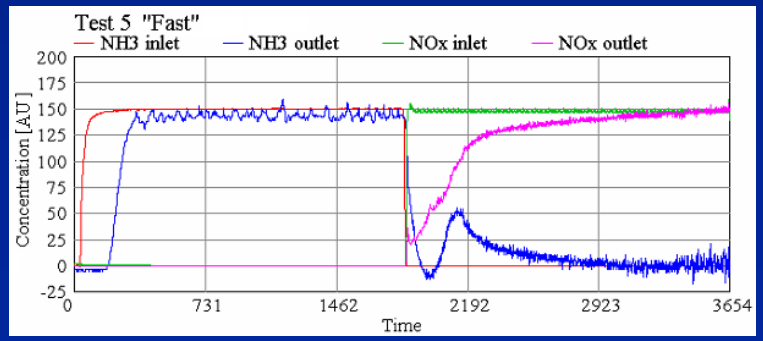
Processed NH3 and Pollutant Sensors Data



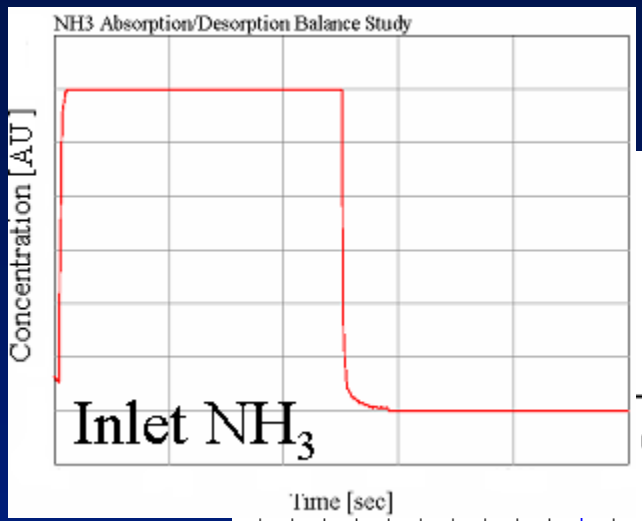


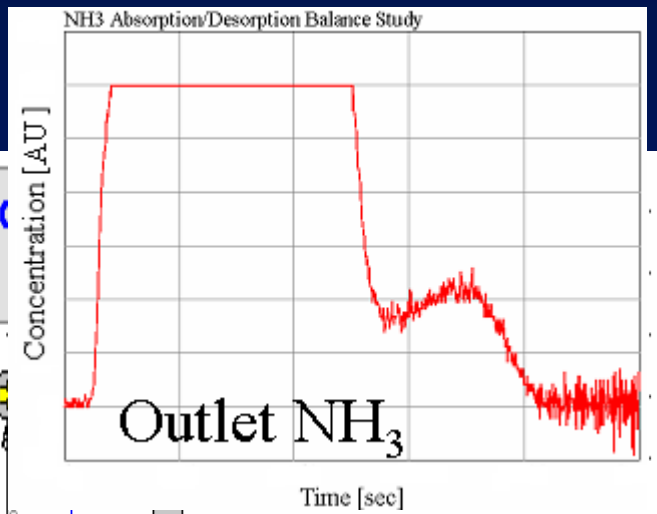


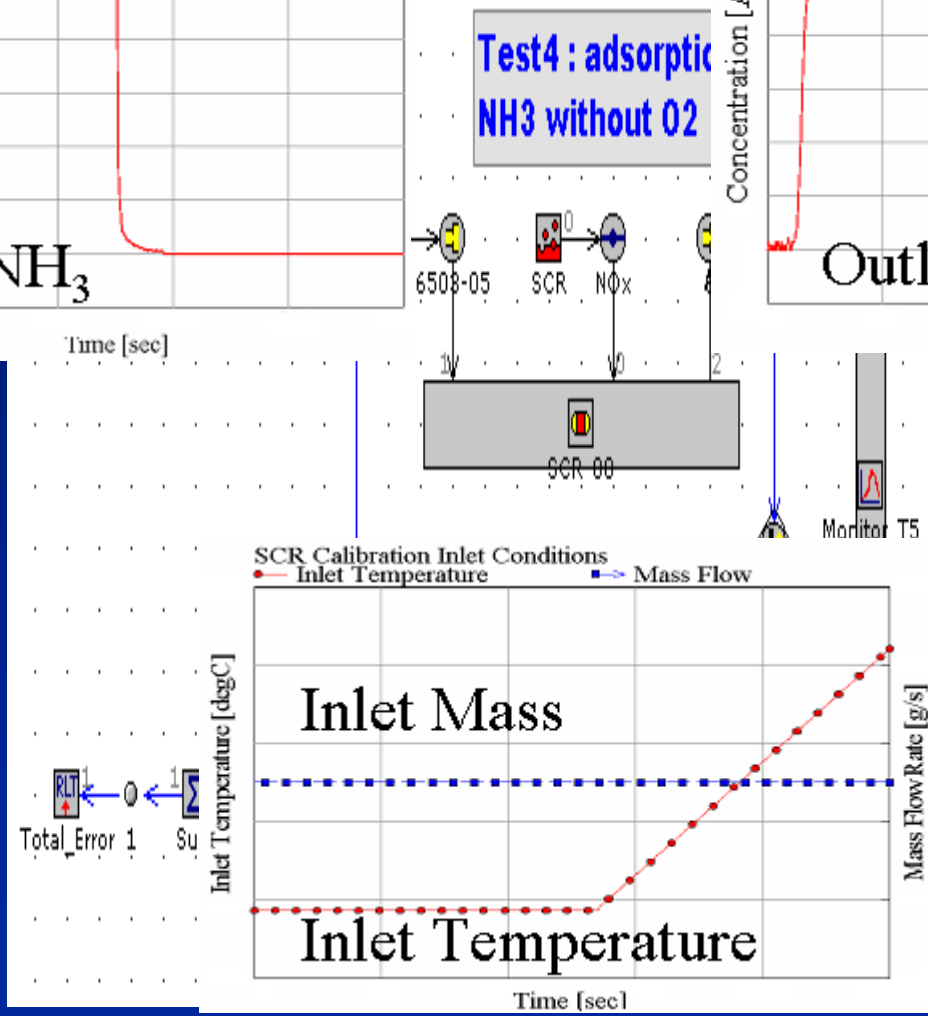




Calculation of Storage Capacity

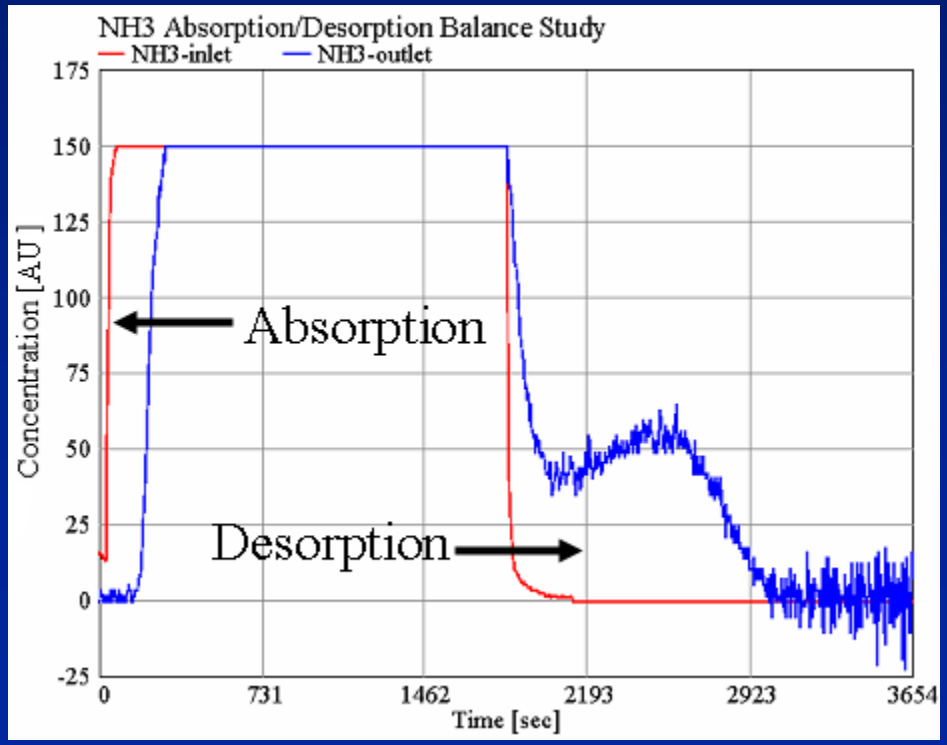






Storage Capacity (cont.)

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

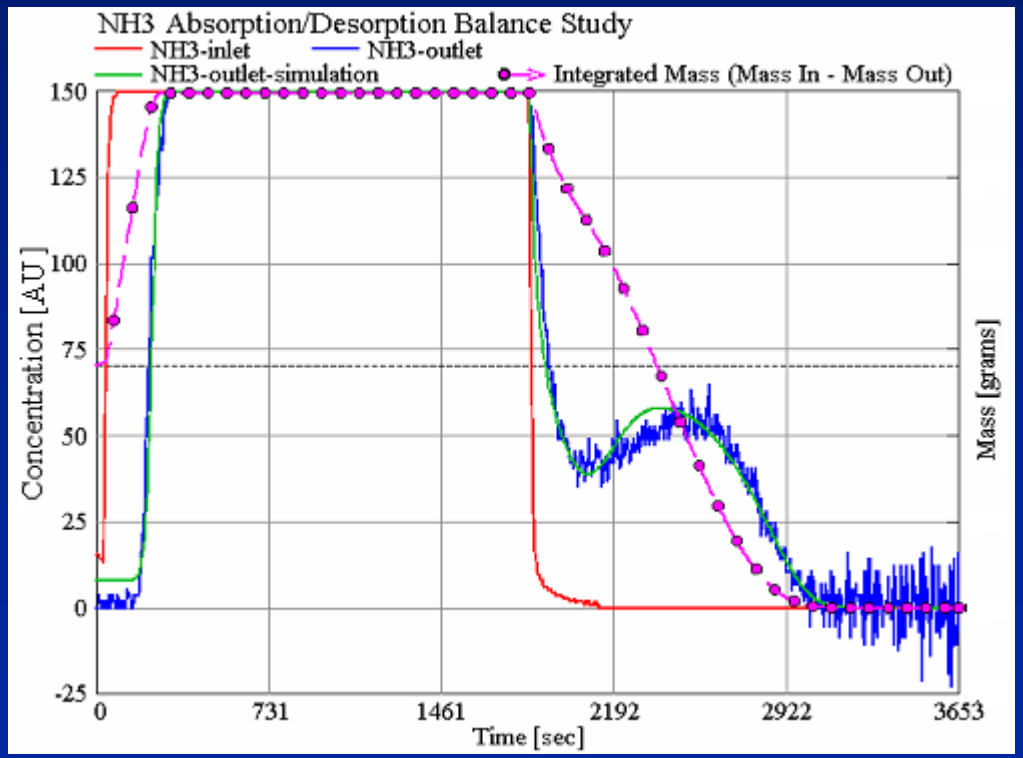


Storage Capacity (cont.)

- 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 direct optimizer (Brent) was used

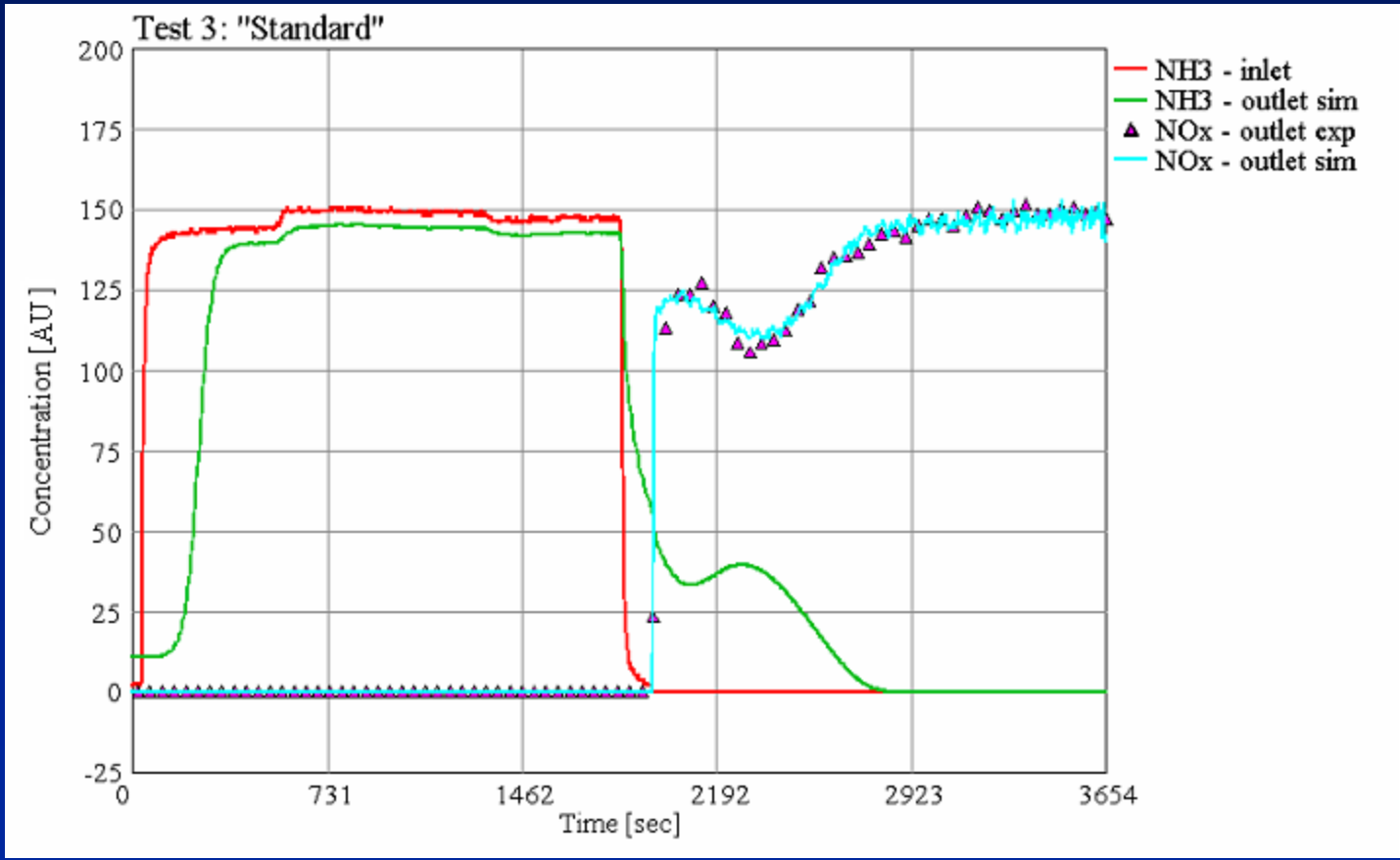
Storage Capacity (cont.)

- 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



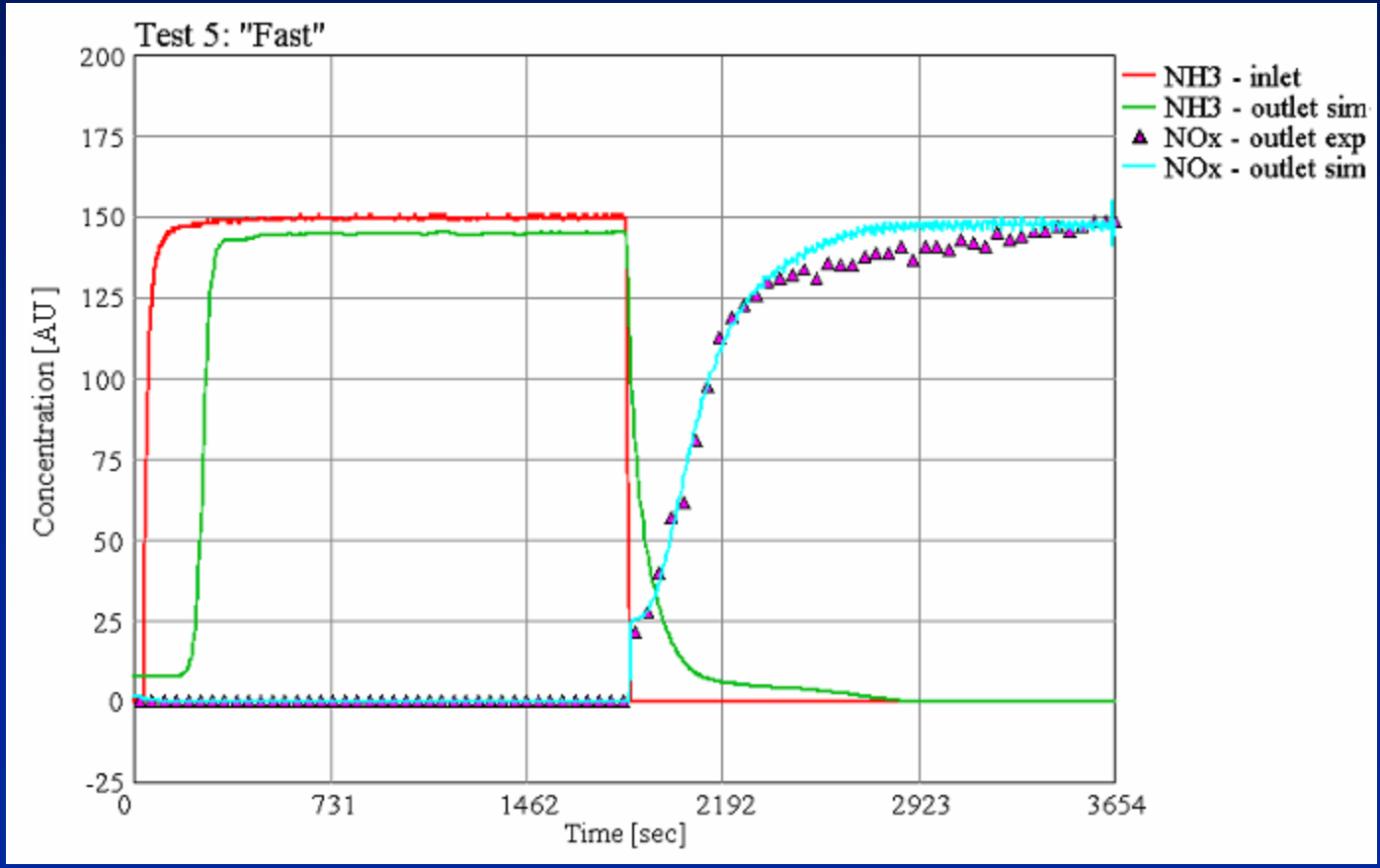
Standard Reaction

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



Fast Reaction

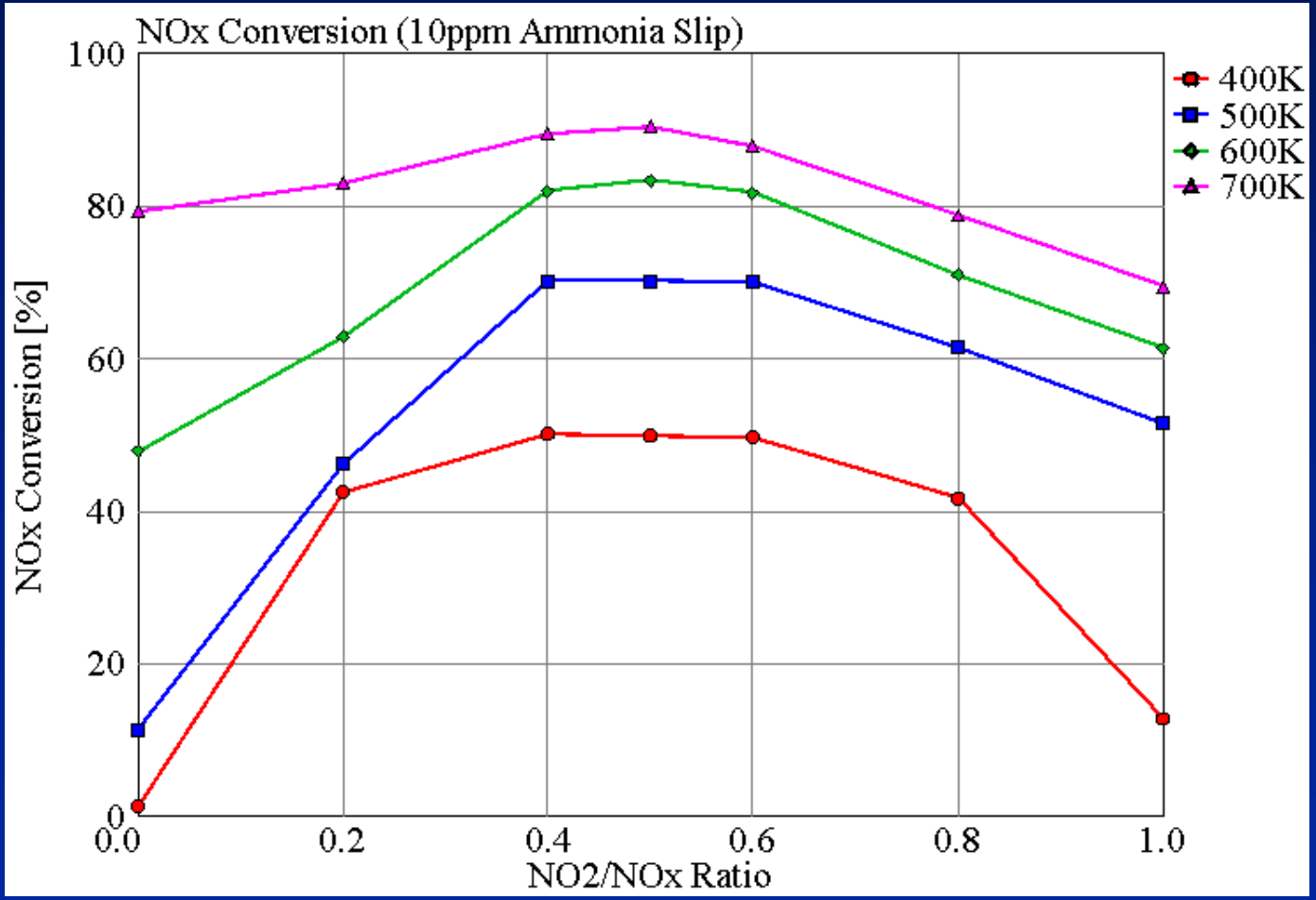
$$4NH_3 + 2NO + 2NO_2 \Rightarrow 4N_2 + 6H_2O$$



SCR NO_X Selectivity Study

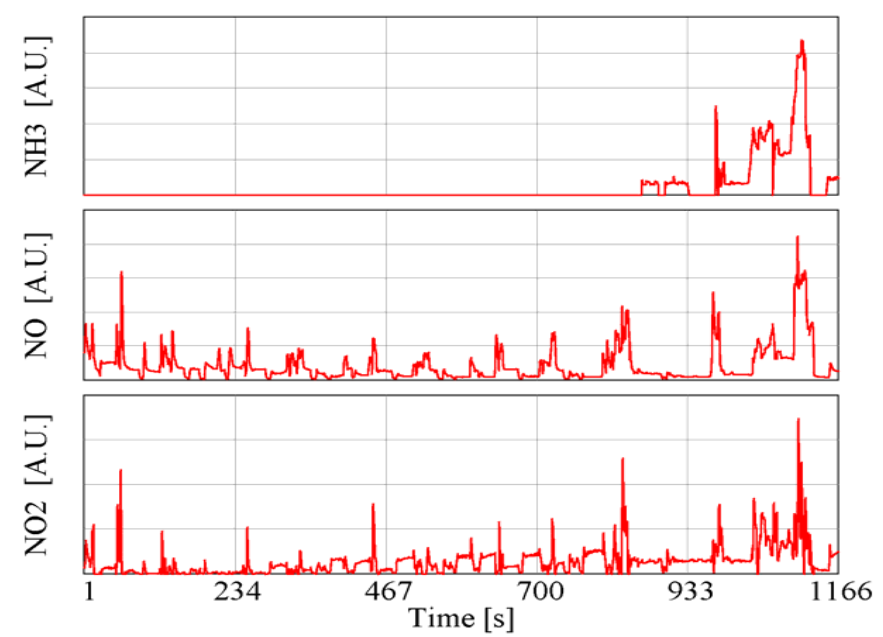
- NO_X conversion should be highest at NO_2/NO_X ratio of 0.5 (or $NO:NO_2$ = 1:1)
- Study was performed using
  - Vary NO_2/NO_X ratio from 0-1
  - Vary temperature from 400-700K
  - 10 ppm NH_3 slip
  - 150 ppm NO_X, NH_3 (variable), 10% H_2O, 10% O_2, balance N_2
  - Constant volume flow rate = 0.55 liter/s

SCR NO_X Selectivity Study



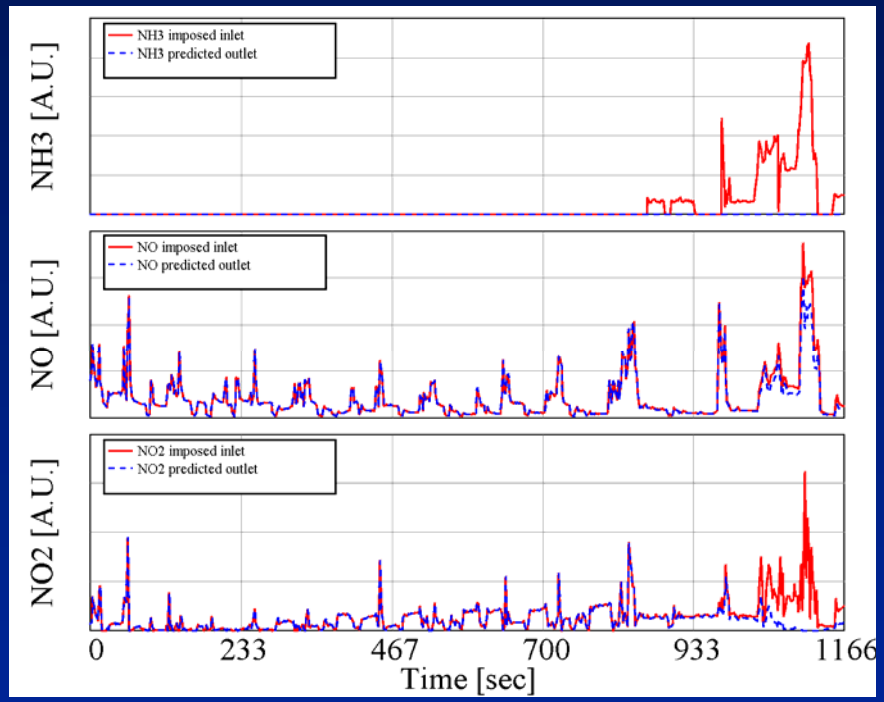
Transient Emission Predictions

- Calibrated SCR model used for Transient NDEC cycle
- Model ran under two conditions:
  - Absorption site 100% “open” (no NH_3 prestorage)
  - Absorption site 0.0% “open”



Emission Predictions (cont.)

- All sites "open" (no NH_3 prestored)



- Cumulative Mass Changes:

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

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

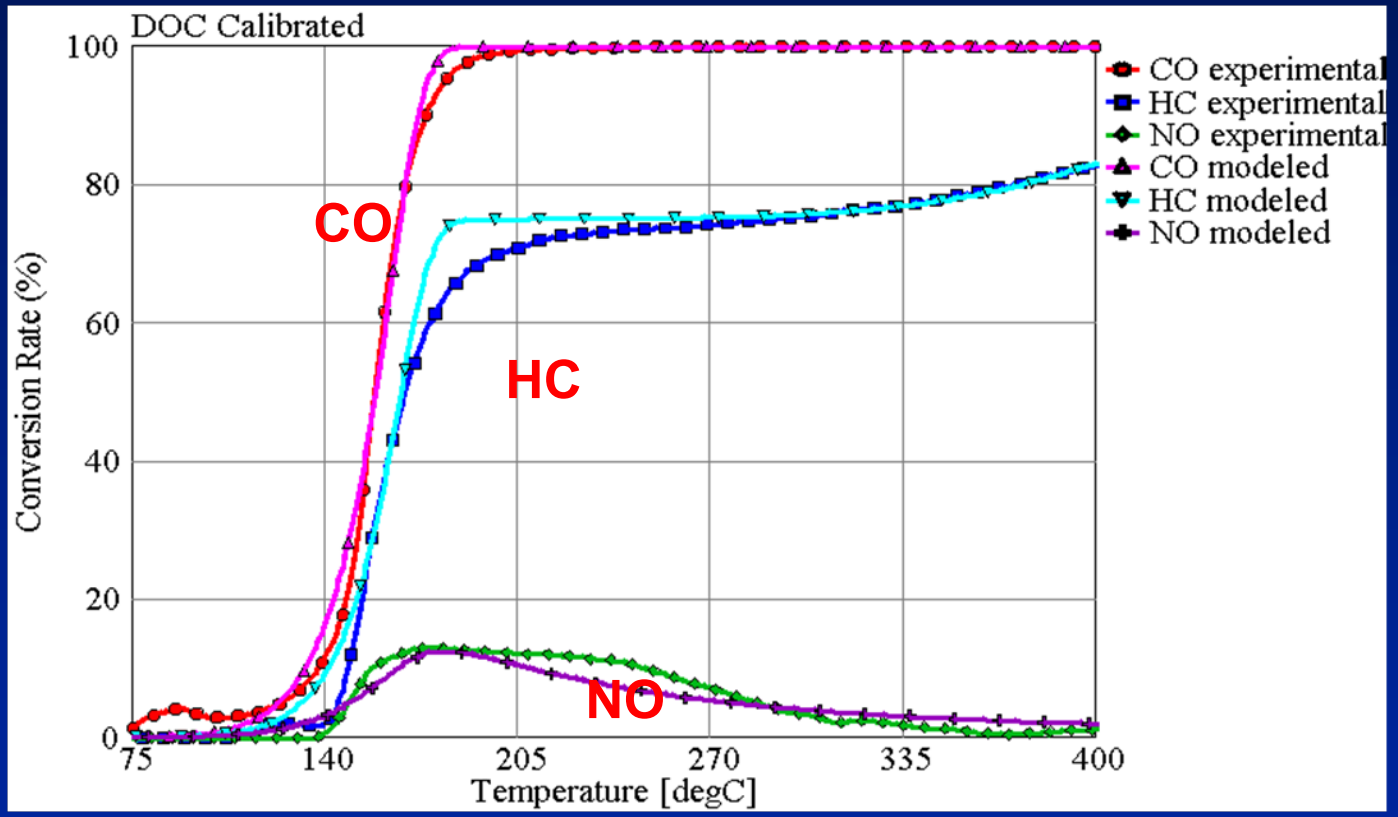
Computational Efficiency: SCR

- Simulations were performed on a Pentium 4 3.4GHz processor with 1 GB of RAM

	Time Step Size (s)	Simulation Time (s)	Computational Time (s)
Abs/Des without O2	0.50	3654	31
Abs/Des with O2	0.50	3654	43
Standard Reaction	0.50	3654	45
Slow Reaction	0.50	3654	49
Fast Reaction	0.50	3654	57
Transient without NH_3 prestored	0.25	1166	85
Transient with NH_3 prestored	0.25	1166	87

Component Level Modeling: DOC

- Step 1: Kinetic model calibration

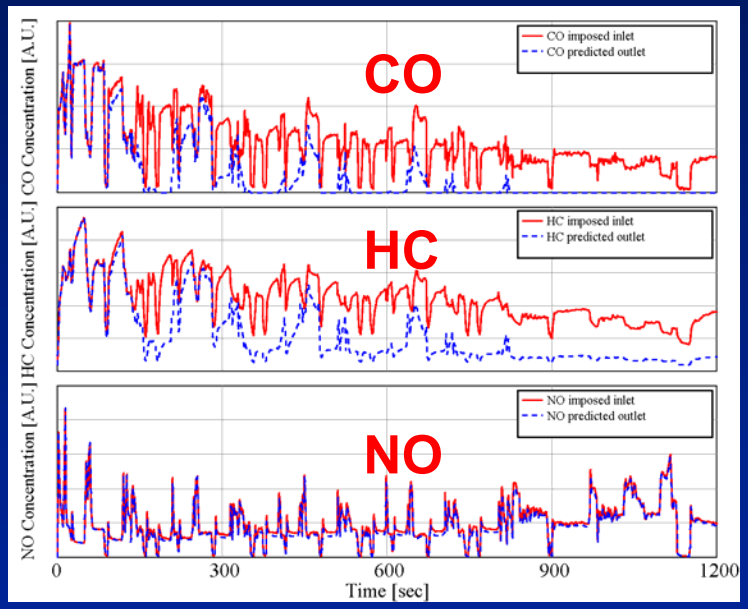


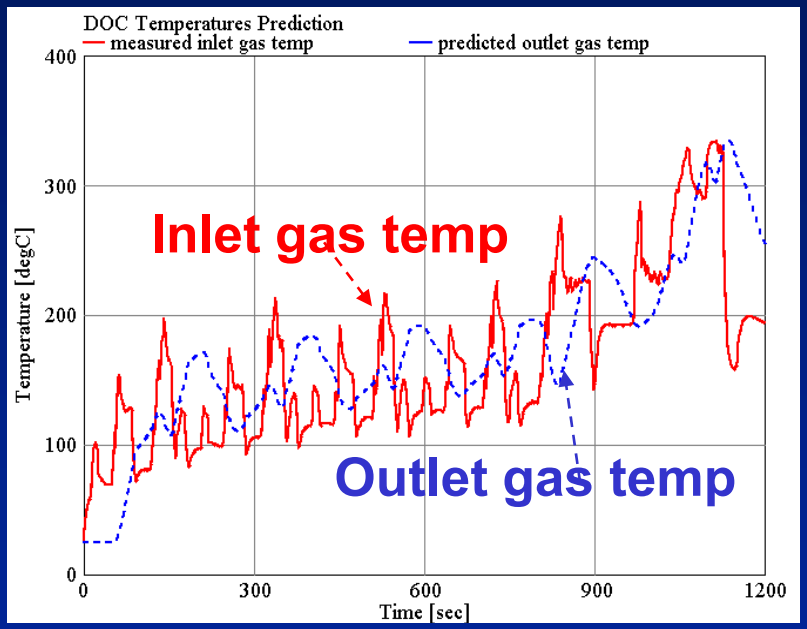
Experiment was done at PSA Peugeot Citroen

NEDC Test Cycle Emissions: DOC

❑ Step 2: Emission predictions

- **Transient NEDC cycle**





- **Cumulative mass conversions predicted to be:**

CO = 61%
HC = 49%
NO = 6%

Computational Efficiency: DOC

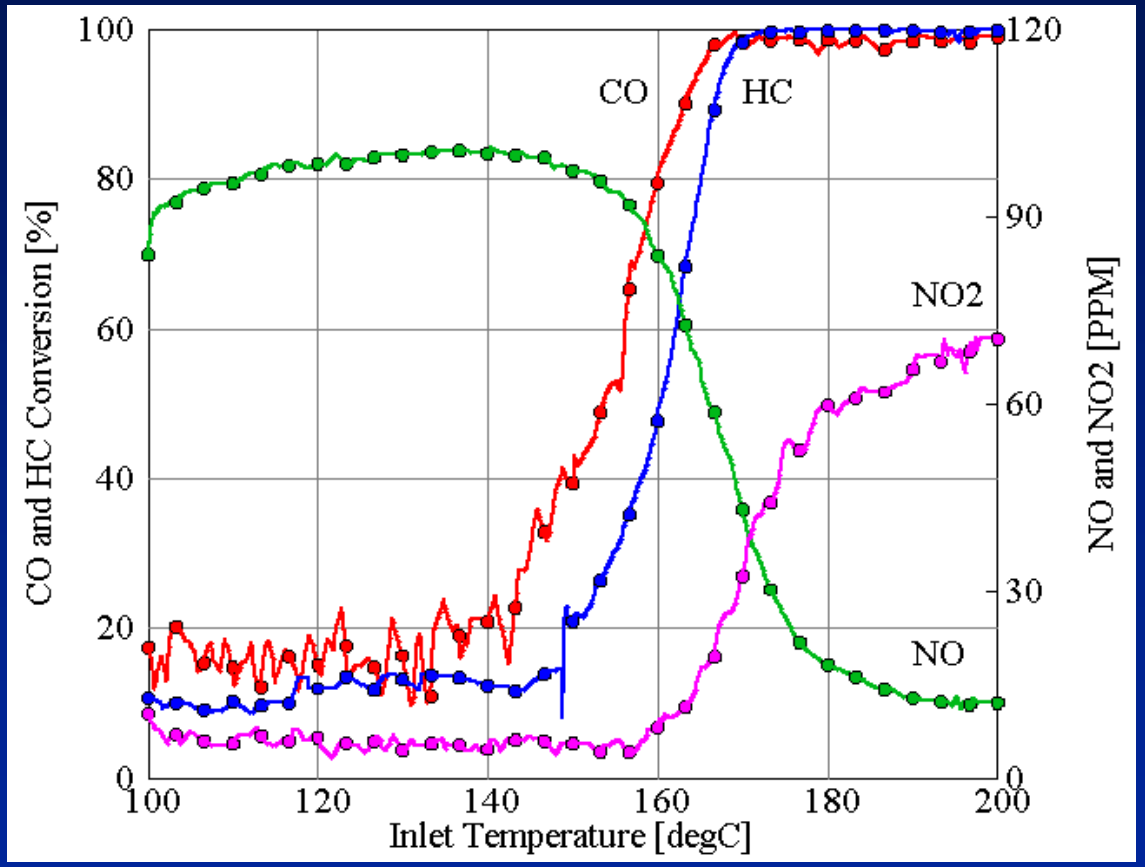
- Simulations were performed on a Pentium 4 3.4GHz processor with 1 GB of RAM

	Time Step Size (s)	Simulation Time (s)	Computational Time (s)
Step 1: Calibration	0.25	327	11
Step 2: Prediction	0.25	1200	71

Aged DOC Modeling

Gas	Exp 1
CO(ppm)	1000
C_2H_4(ppm)	300
H_2(ppm)	333
NO_2(ppm)	100
NO(ppm)	0
H_2O(Vol.-%)	4.5
CO_2(Vol.-%)	5
O_2(Vol.-%)	10

*Balance consists of N2



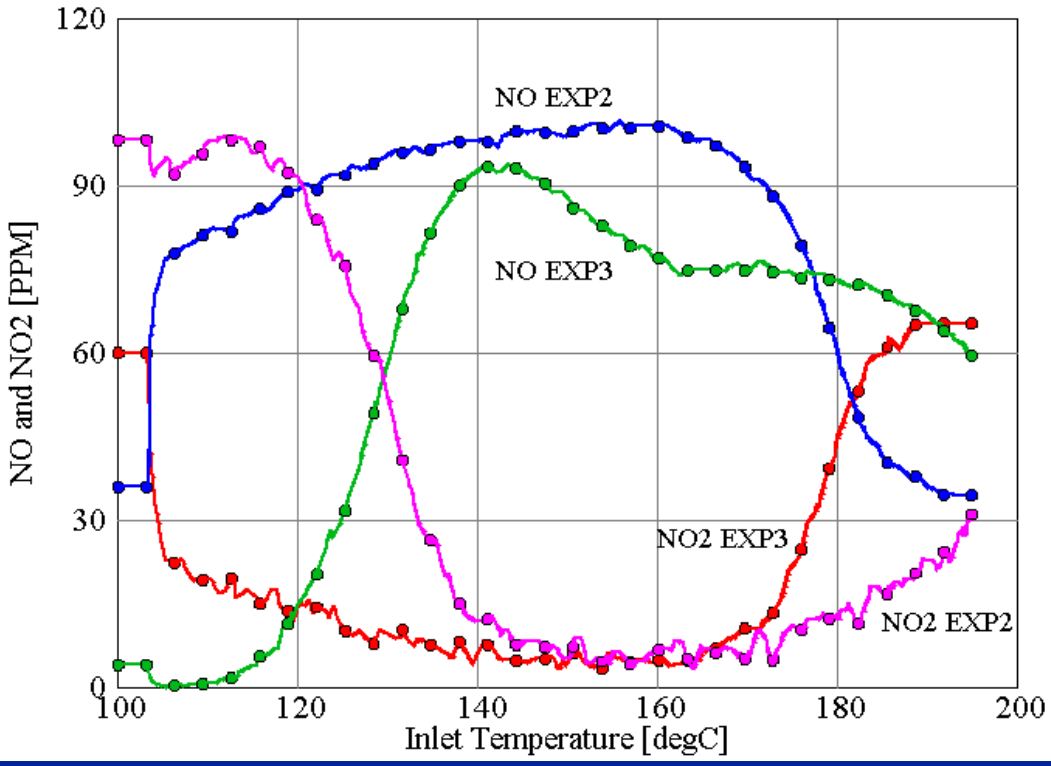
Measurements from Santhoji and coworkers:

"Aged DOC is a Net Consumer of NO2: Analysis of Vehicle, Engine-dynamometer and Reactor Data", SAE NO. 2007-01-3984

Aged DOC Modeling

Gas	Exp2	Exp3
CO(ppm)	1000	0
C_2H_4(ppm)	0	300
H_2 (ppm)	0	0
NO_2 (ppm)	100	100
NO (ppm)	0	0
H_2O (Vol.-%)	4.5	4.5
CO_2 (Vol.-%)	5	5
O_2 (Vol.-%)	10	10

*Balance consists of N2



Measurements from Santhoji and coworkers:

"Aged DOC is a Net Consumer of NO2: Analysis of Vehicle, Engine-dynamometer and Reactor Data", SAE NO. 2007-01-3984

Aged DOC Modeling

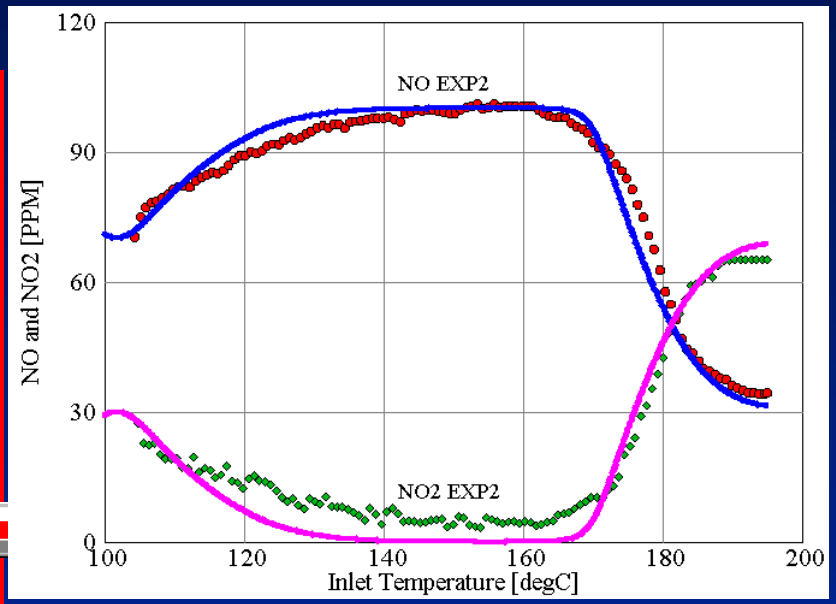
- **Introduce additional reactions:**

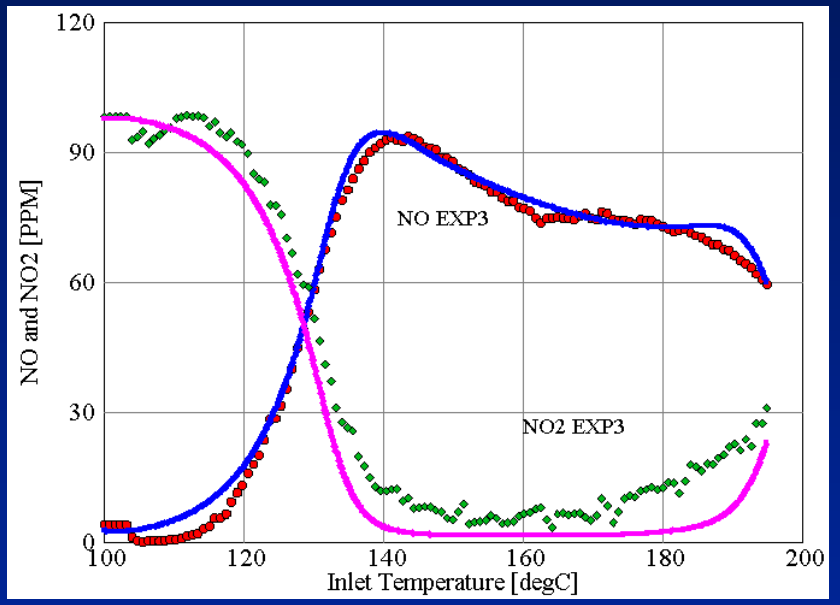
R1: $CO + NO_2 \Rightarrow CO_2 + NO$

R2: $C_2H_4 + 4NO_2 \Rightarrow 2CO_2 + 6NO + 2H_2O$

R3: $C_2H_4 + 6NO_2 \Rightarrow 2CO_2 + 3N_2 + 2H_2O$

Aged DOC Modeling





R1: $CO + NO_2 \Rightarrow CO_2 + NO$

Exp. .....

Sim. ——

R2: $C_2H_4 + 4NO_2 \Rightarrow 2CO_2 + 6NO + 2H_2O$

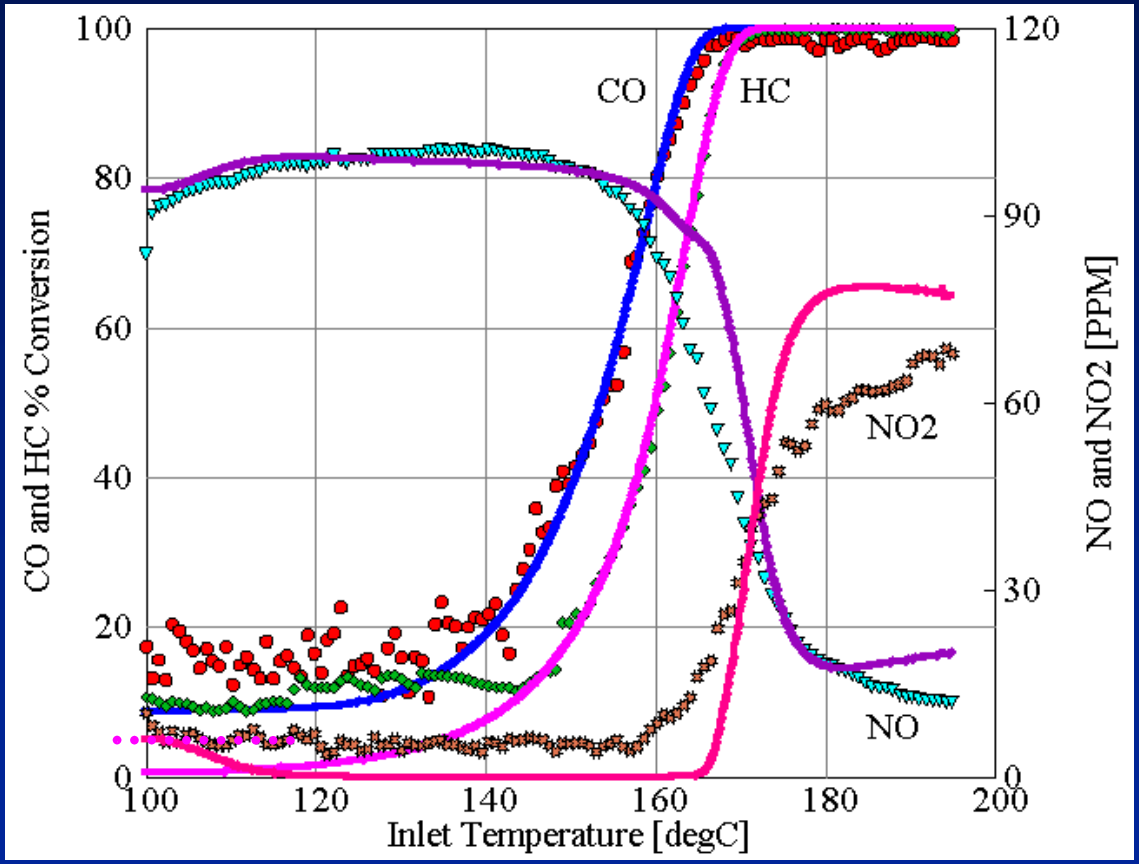
R3: $C_2H_4 + 6NO_2 \Rightarrow 2CO_2 + 3N_2 + 2H_2O$

Measurements from Santhoji and coworkers:

"Aged DOC is a Net Consumer of NO2: Analysis of Vehicle, Engine-dynamometer and Reactor Data", SAE NO. 2007-01-3984

Aged DOC Modeling

Exp. ..... Sim. ——



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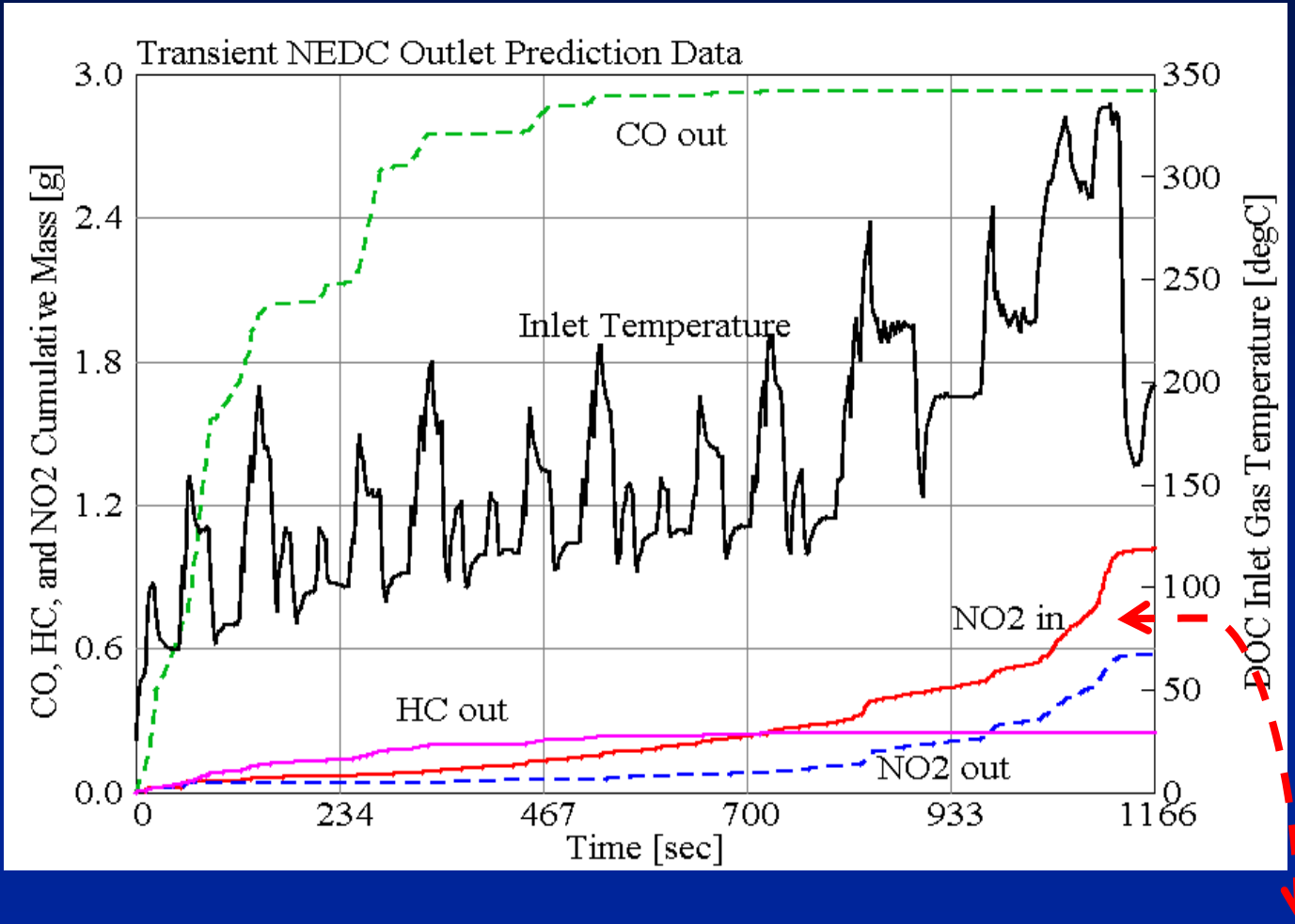
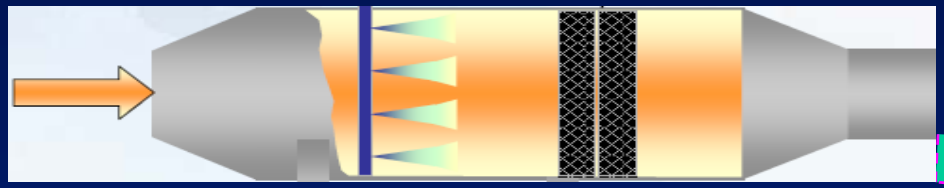
Aged DOC Modeling

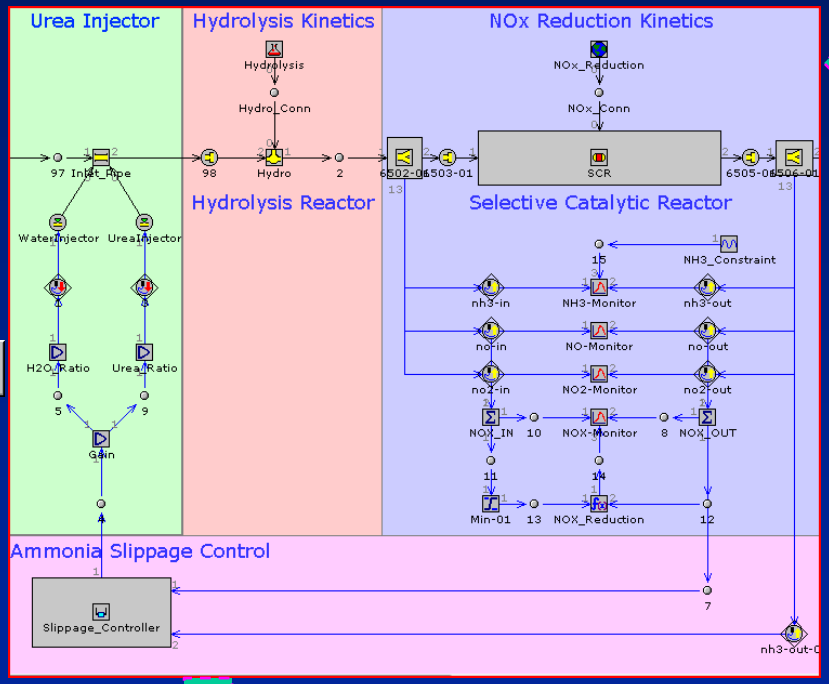


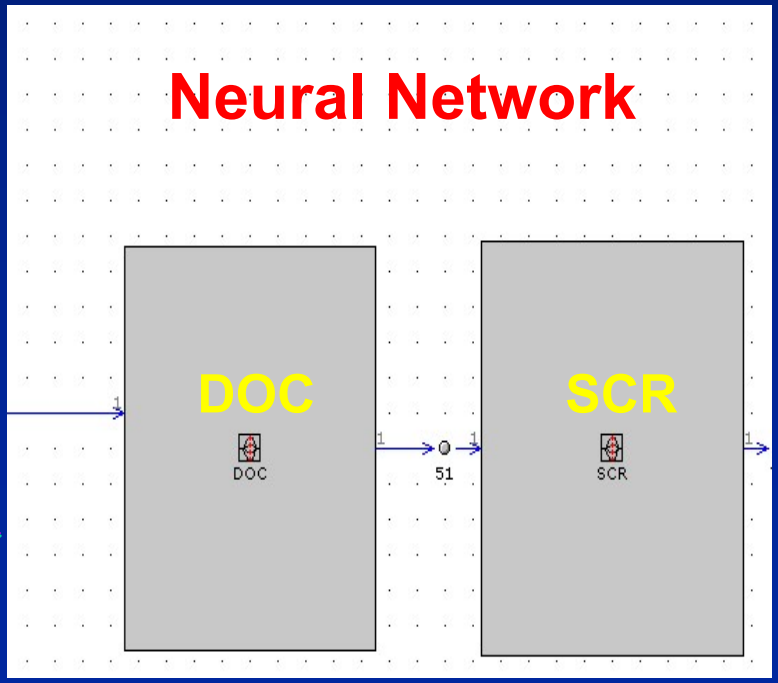
Model predicts cumulative NO_2 reduction = 44%

Experimental inlet conditions provided by PSA Peugeot Citroen

SIL/HIL Model Generation

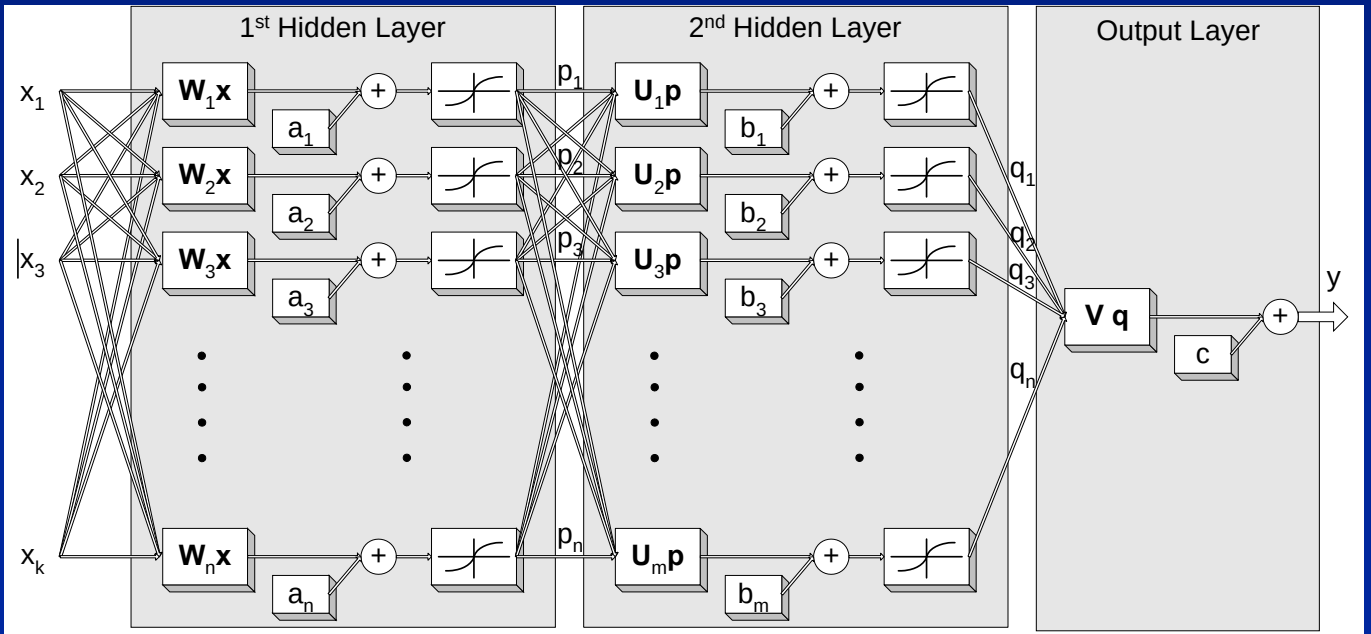






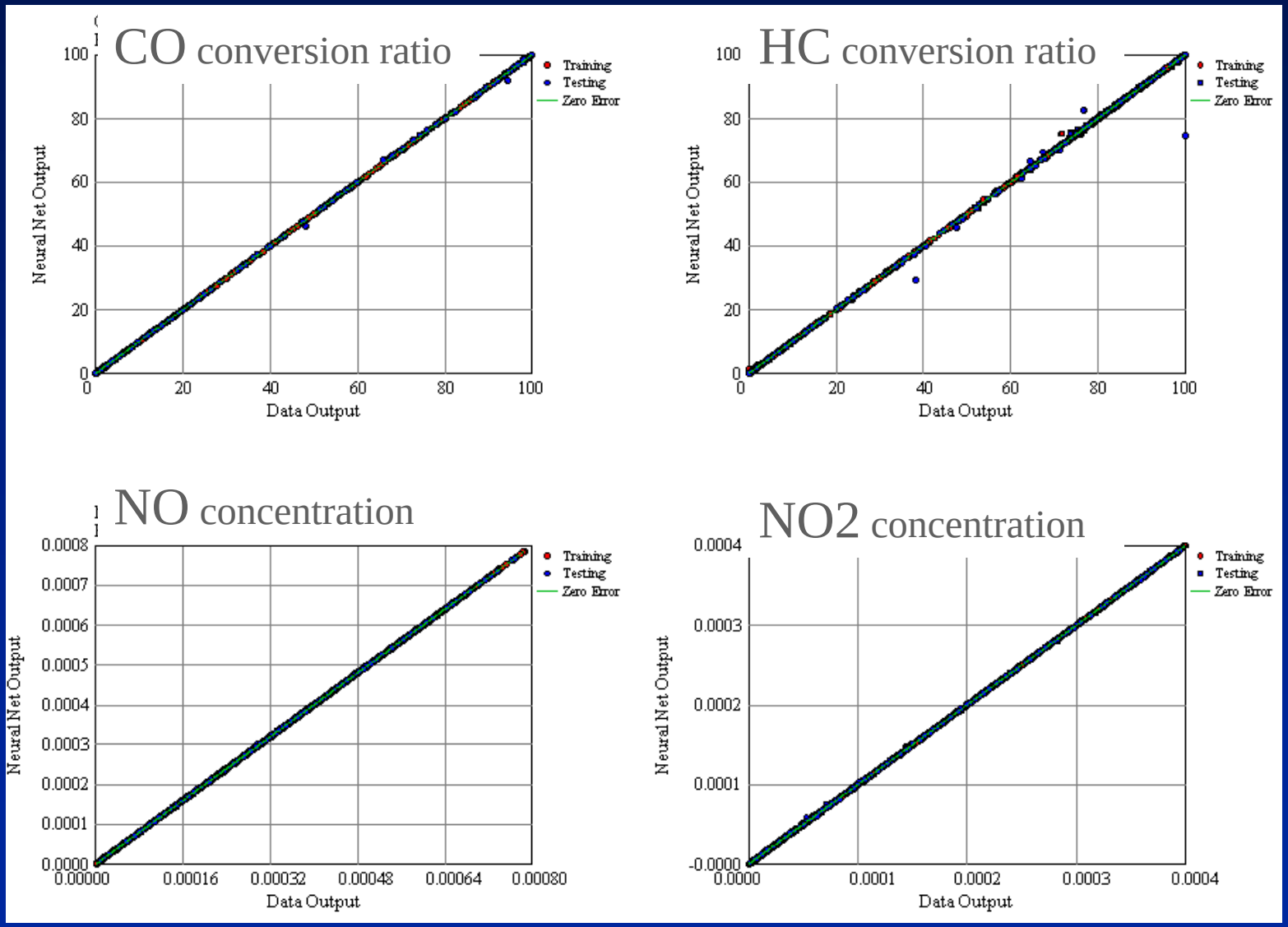
Neural Network Training

- 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")



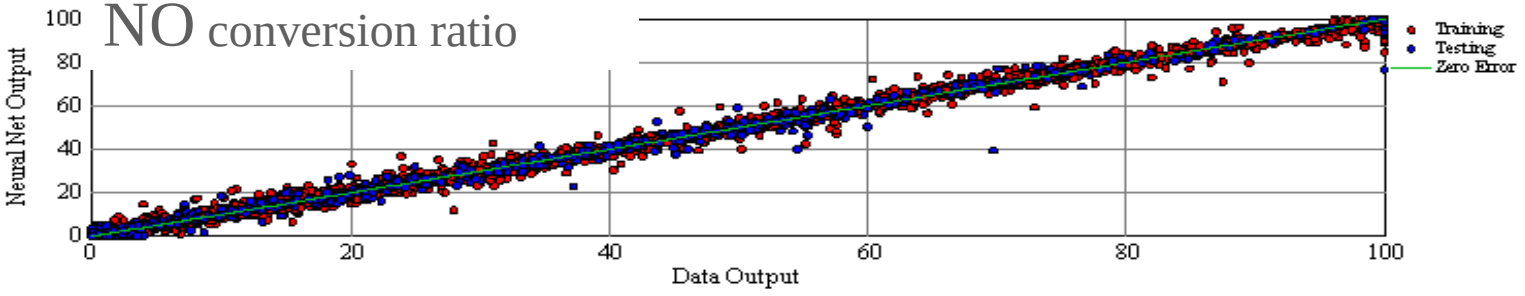
Conversion Efficiency

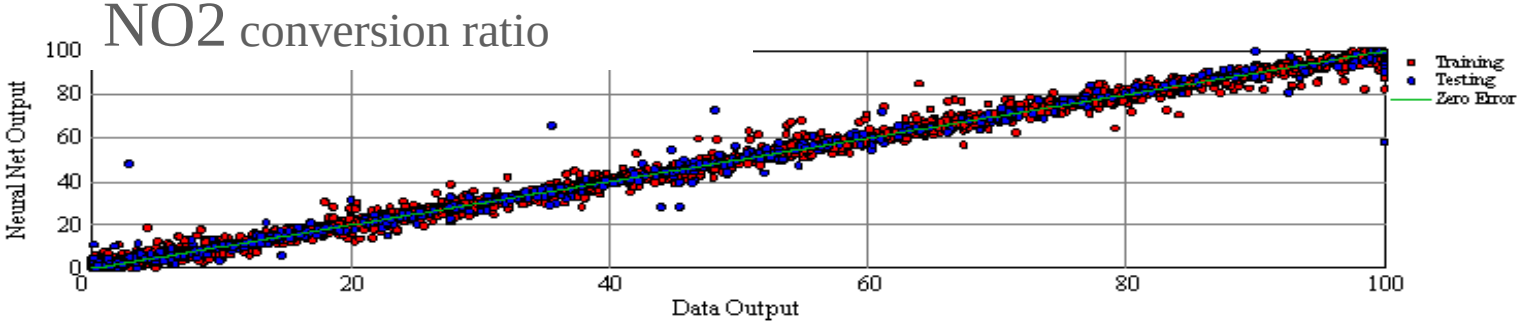
- DOC

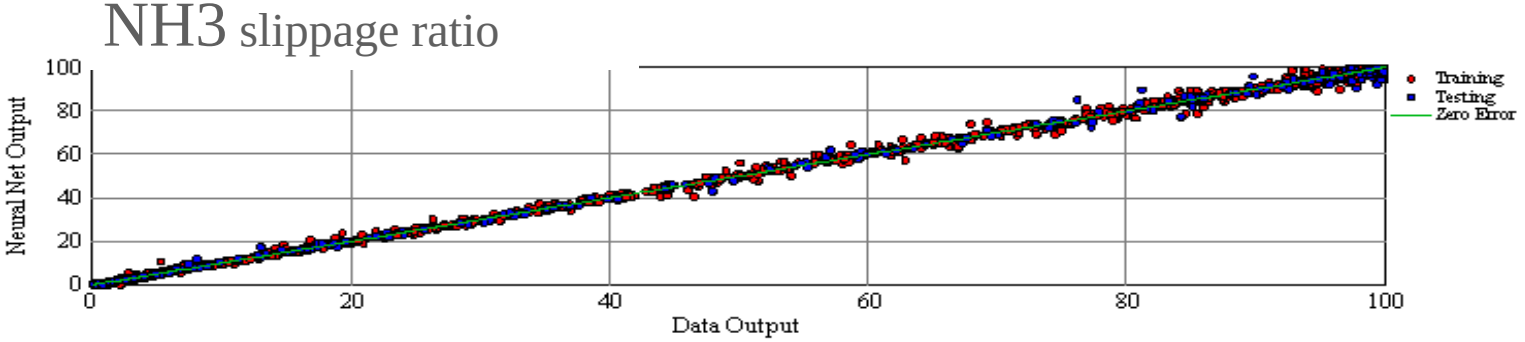


Conversion Efficiency

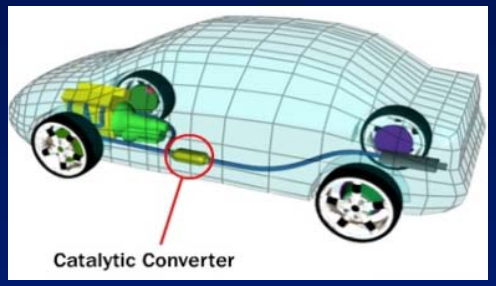
- SCR

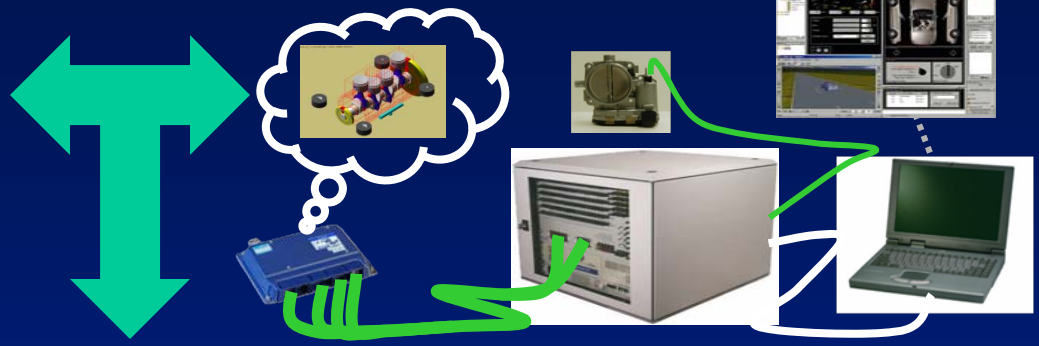


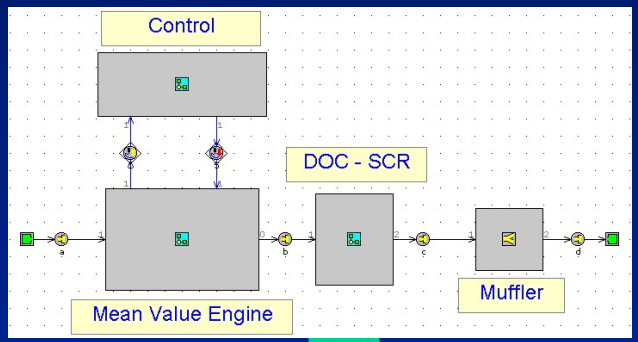


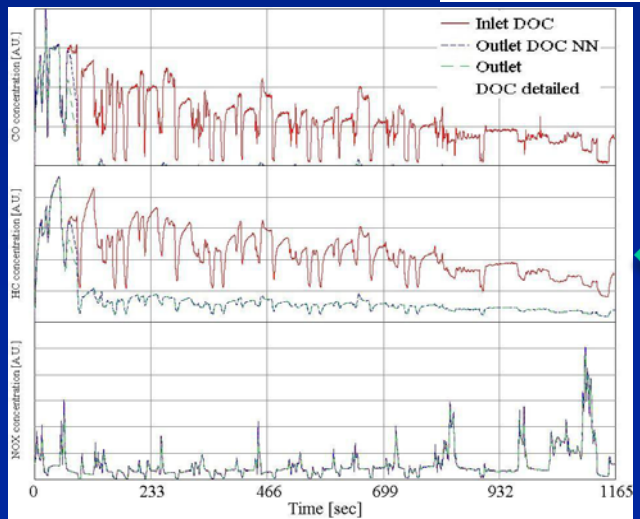


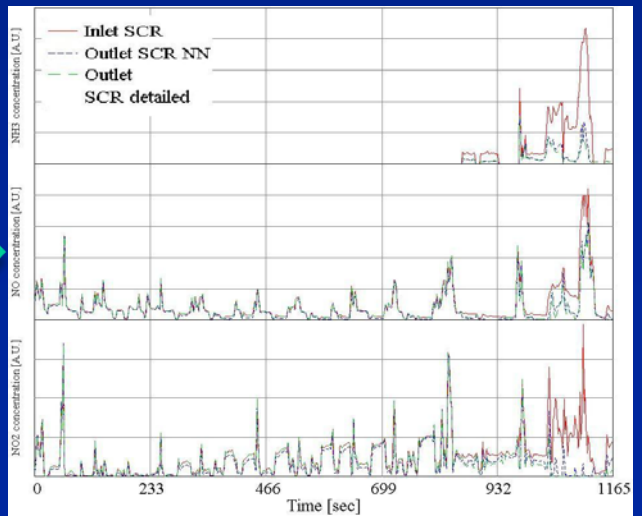
SIL/HIL Enabled Engine/NN-AT Model











Computational Speed Comparison (1180s NDEC)

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

Pseudo-Multi-D Methodologies

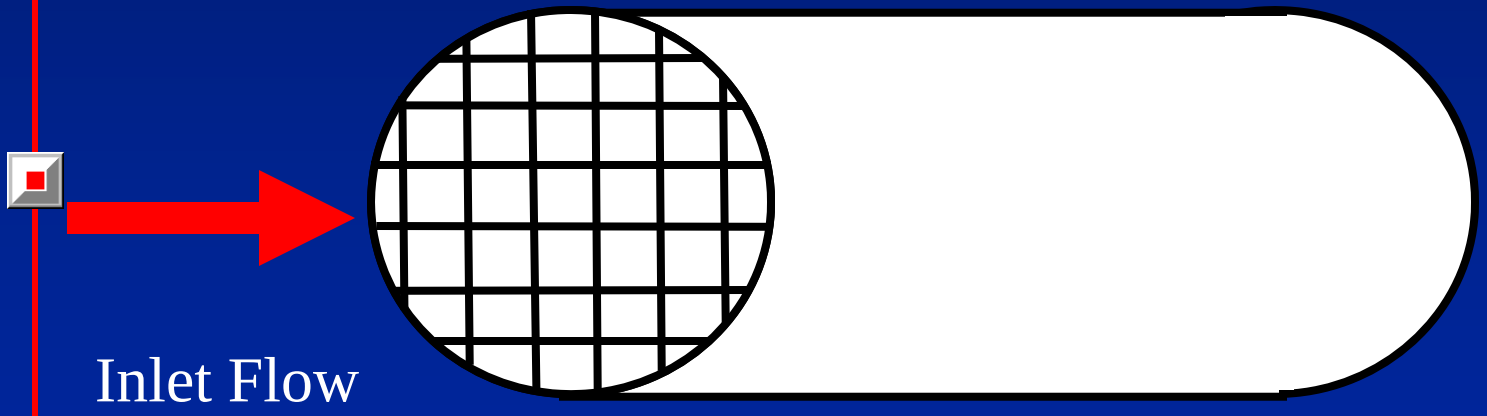
Are real time 3-D simulations possible?

3D - vs- 1D

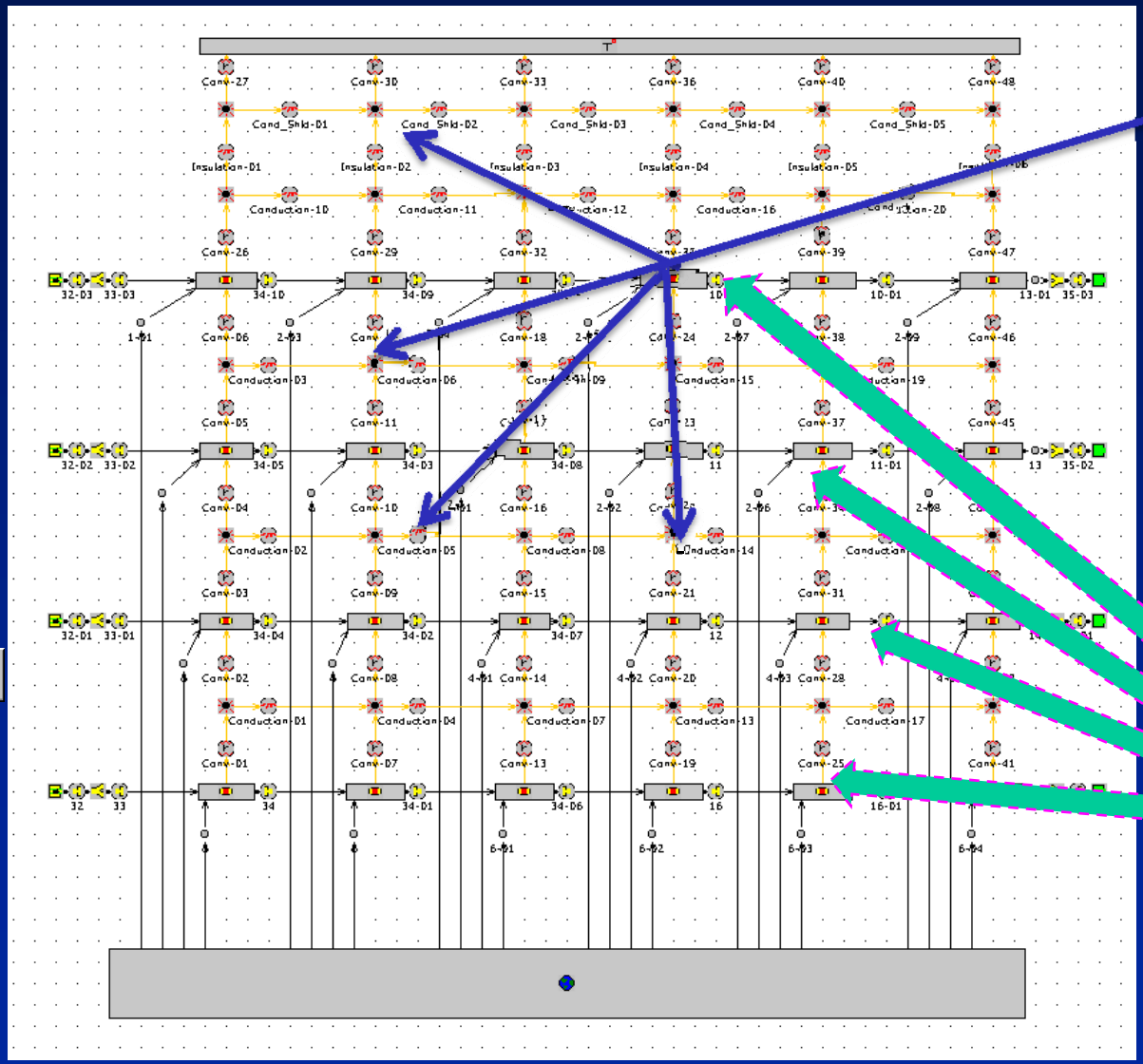
- Based on thermal object
  - Explicit discretization
  - Discretized CatalystBrick and thermal objects
- Based on Mathematical formulation (3-D conduction solution)
  - Implicit discretization
  - Diesel particulate ilters

Aftertreatment Simulation

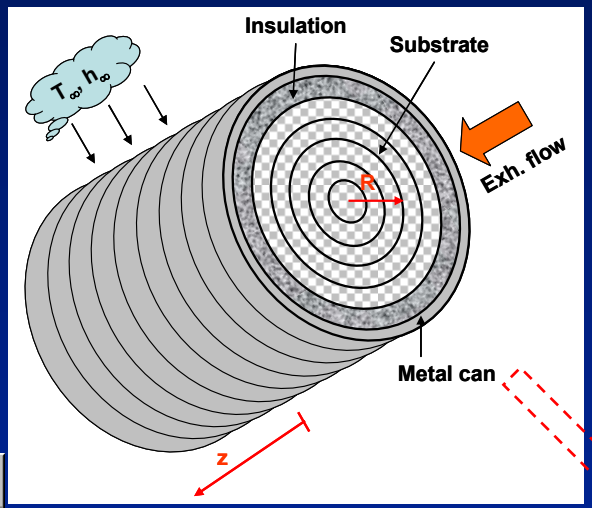
- **Modeling Techniques**
  - 3D: model discretized in X ,Y, and Z direction
    - captures heat loss to environment
    - allows for non-uniform inlet flow
    - most computationally demanding

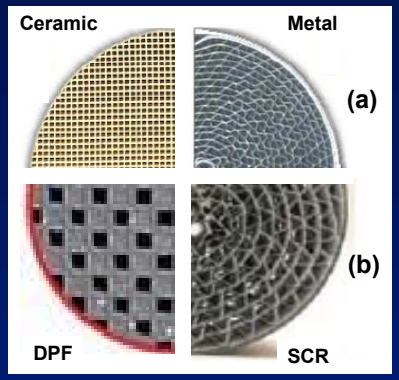


Aftertreatment Simulation



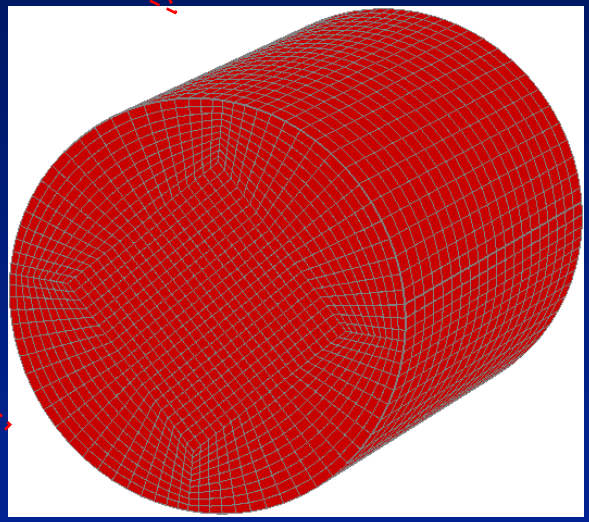
Representative Channel Approach

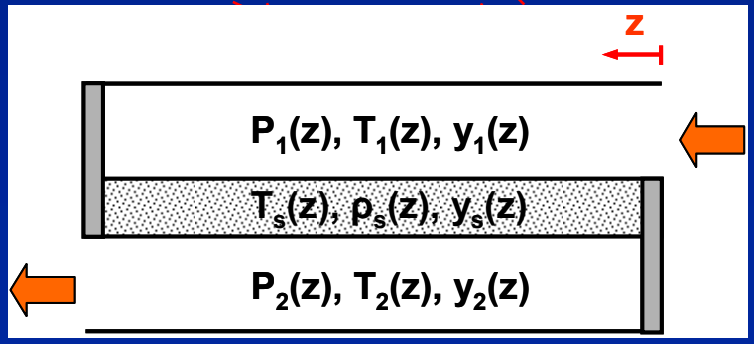




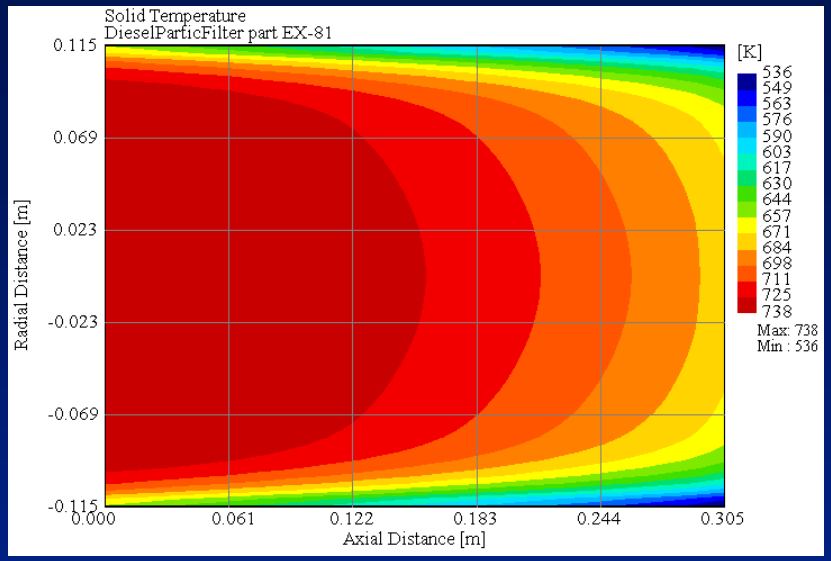
2D

3D

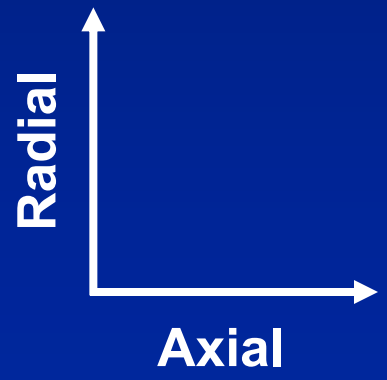




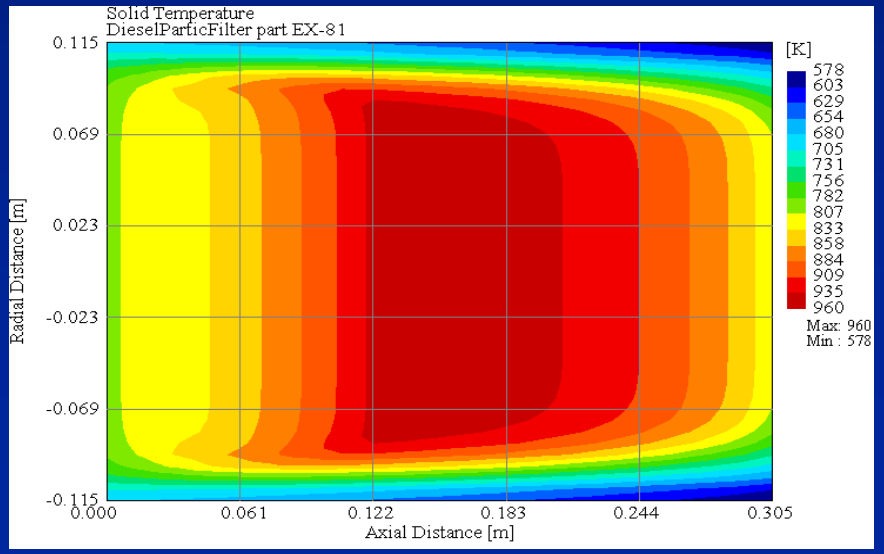
Typical Transient 2D Results



Warm-up



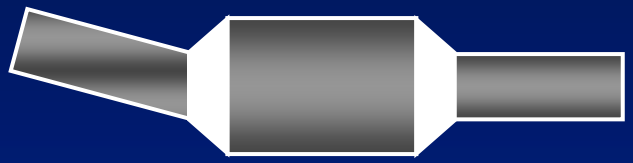
Regeneration



Non-uniform Flow Distributions

Physical layout out

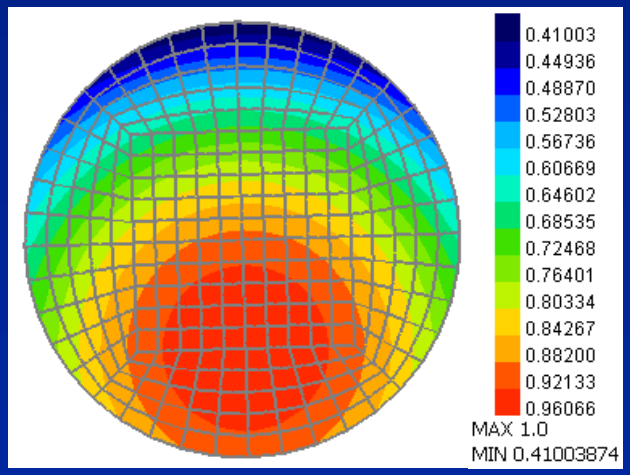
(A)



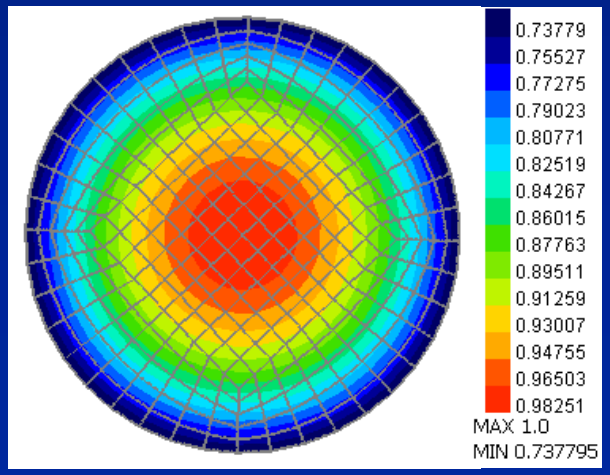
(B)

Pseudo front inlet mass flow rate intensity

(A)

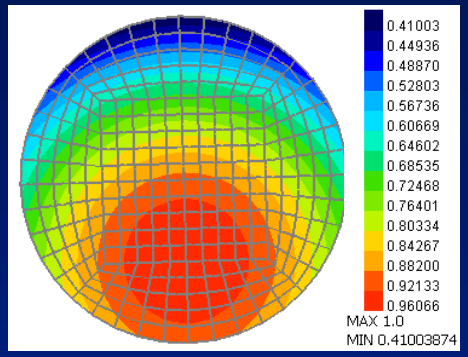


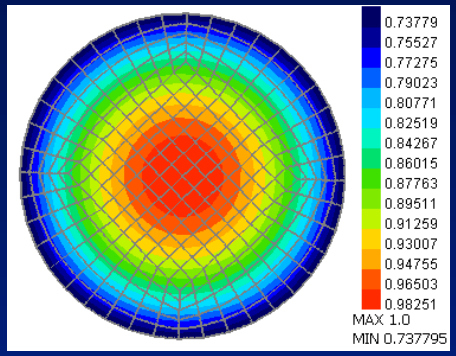
(B)

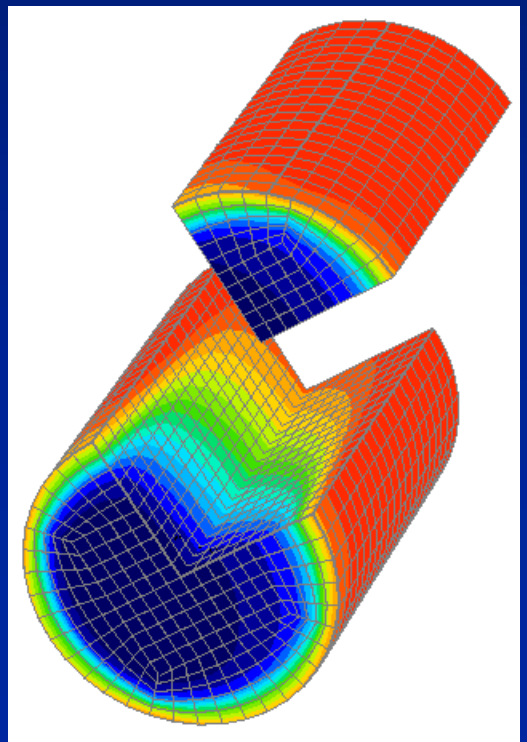


Typical Transient 3D Results

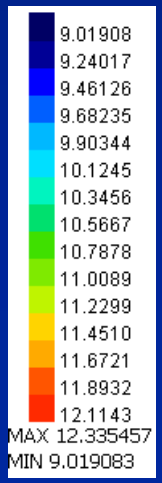
Non-uniform front inlet mass flow rate intensity

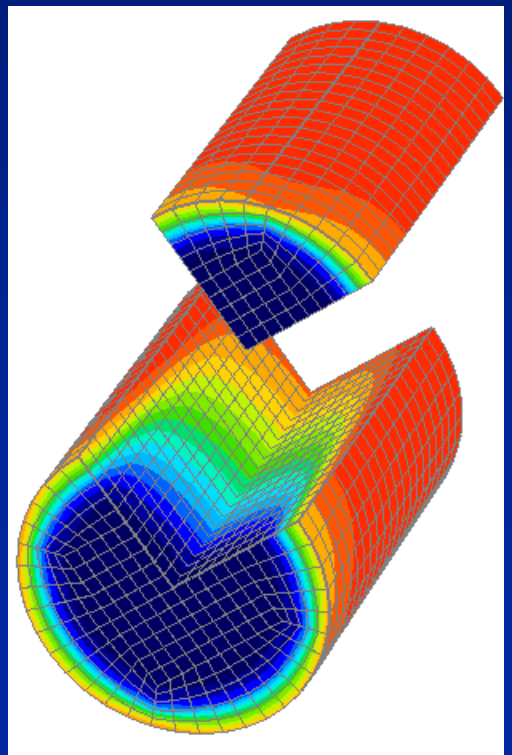






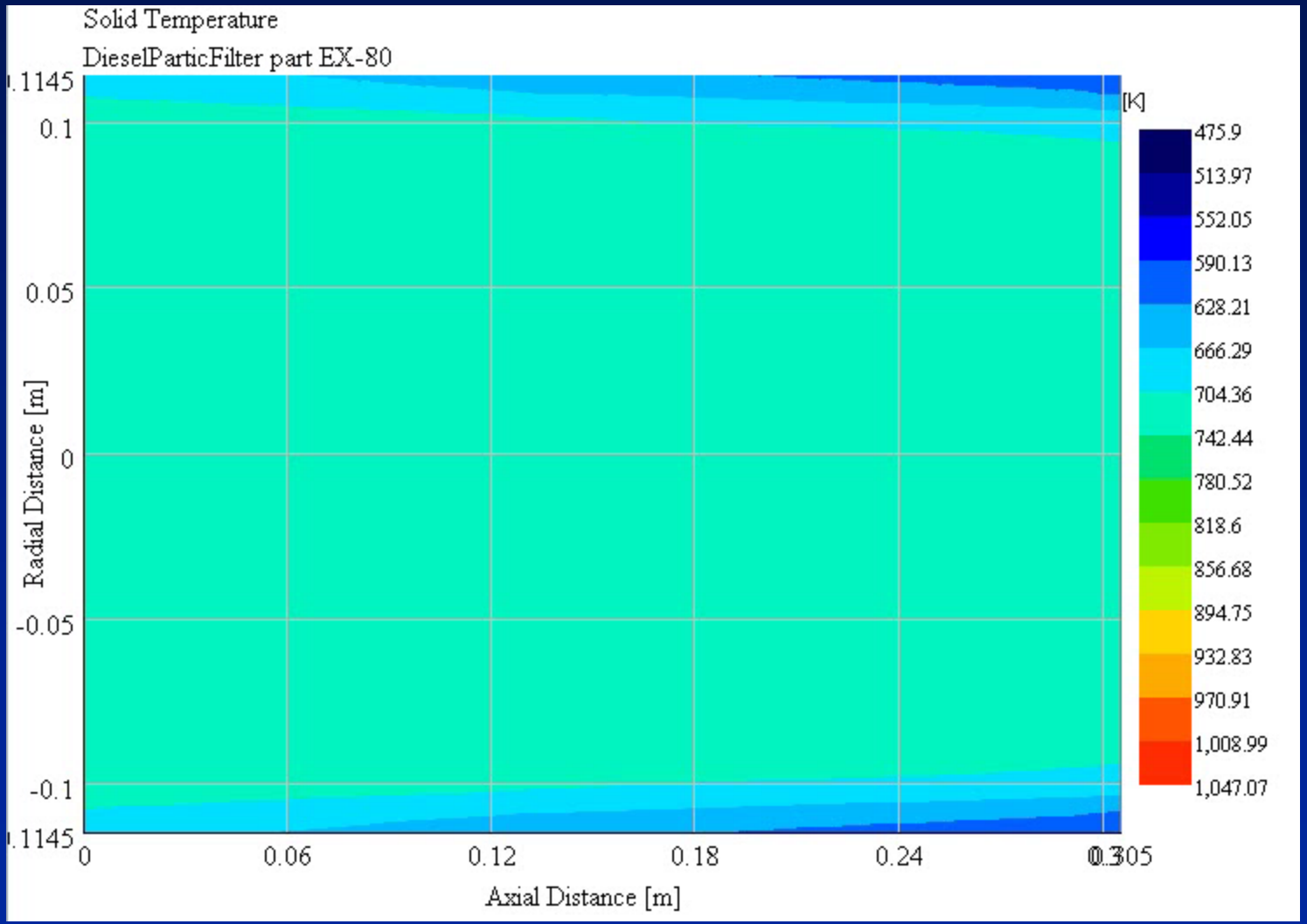
Loading Density at 110 sec. (g/L)





Typical Transient 2D Results

DPF Regeneration Animation

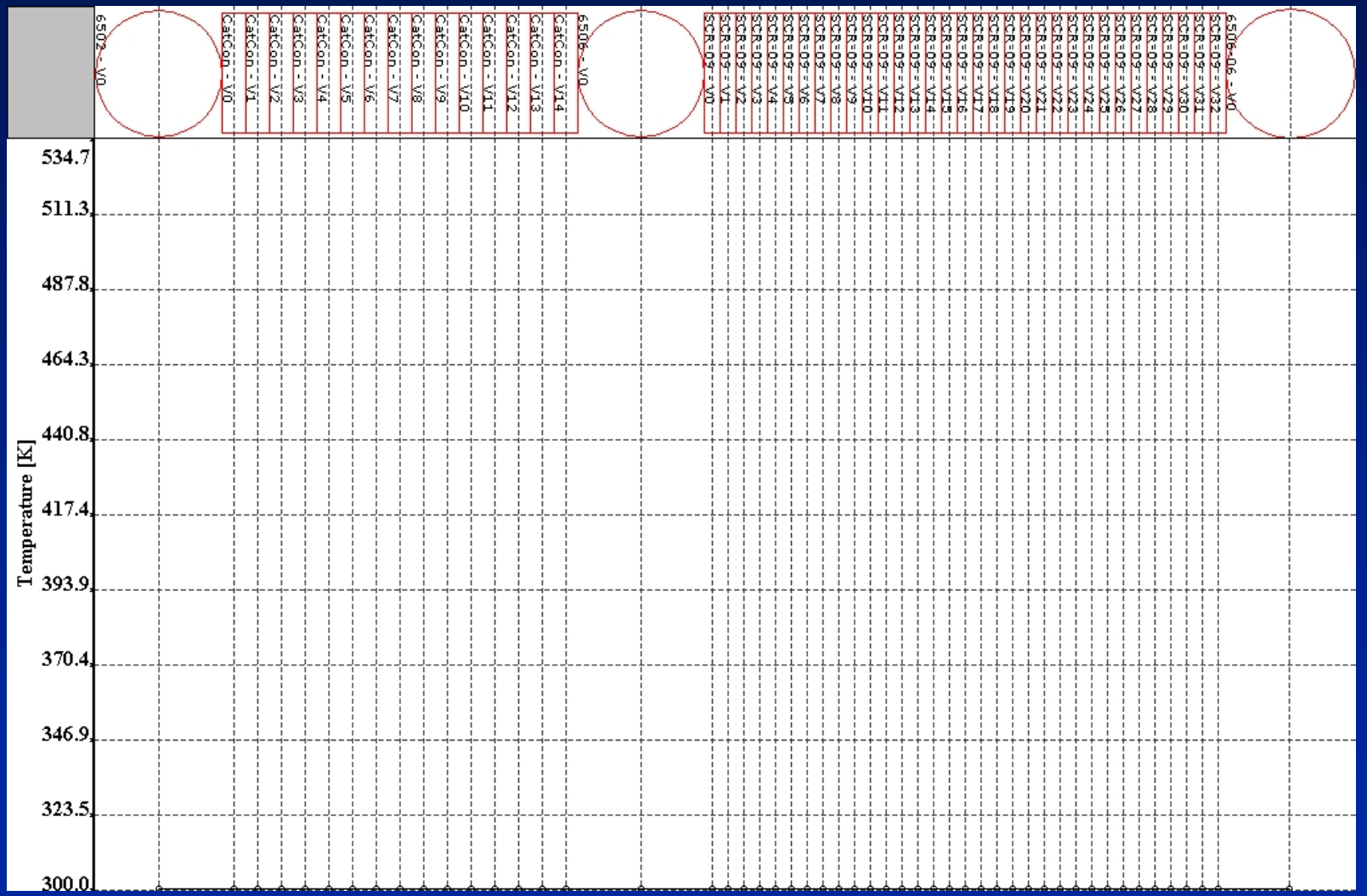


Conclusion

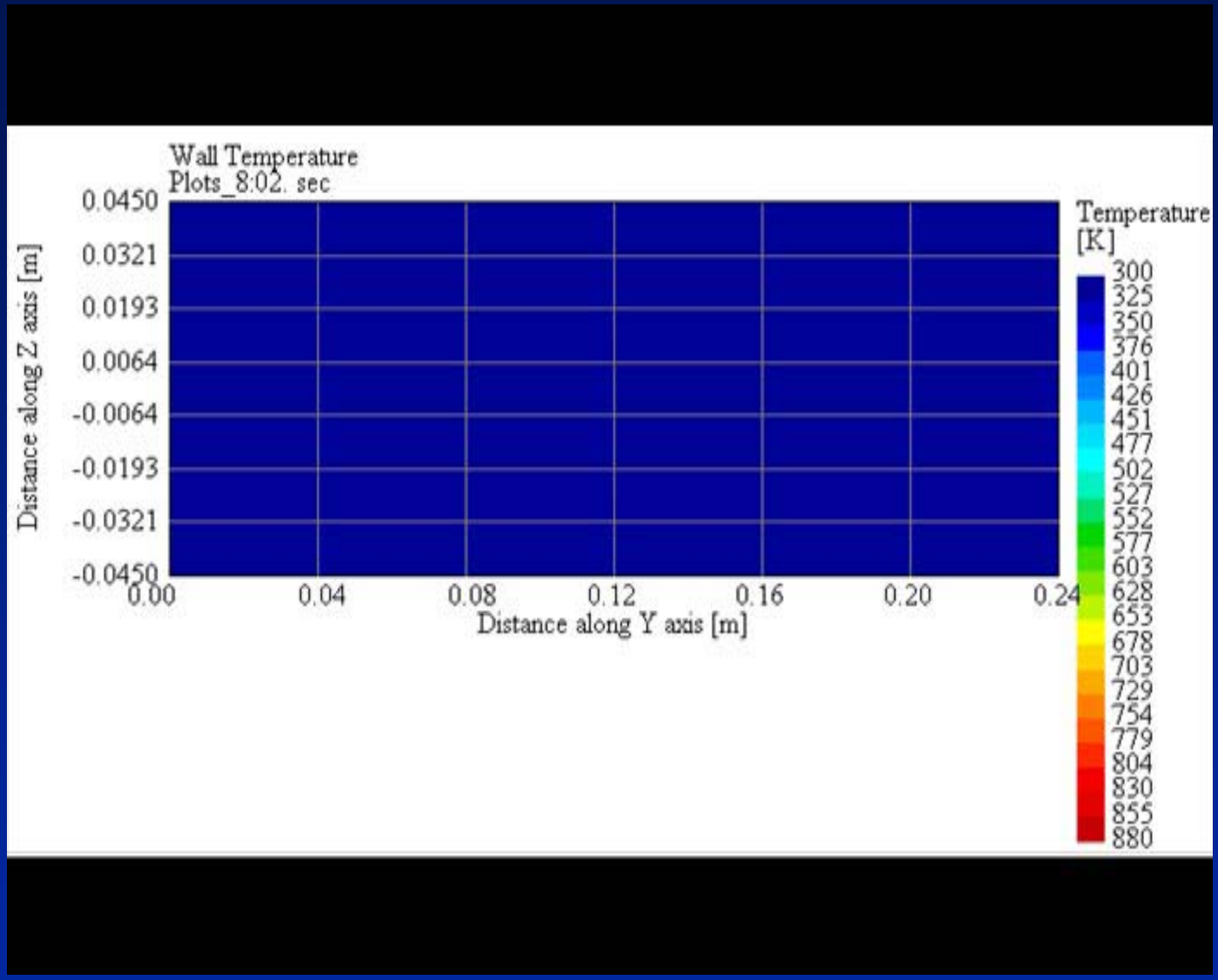
- A *Quasi-steady* (*QS*) based solver have been implemented that conserves accuracy of the computationally demanding fully explicit solver
- Calibration of global kinetics was shown to be computationally efficient using DOE direct optimizers
- Feasibility of SIL/HIL compatible model generation was demonstrated using detailed kinetic model
- Various levels of modeling were demonstrated:
  *D*etailed engine/vehicle + detailed kinetics to mean-value engine/vehicle + NN/AT model
- 1-D methodology was extended to simulate multi-dimensional effect s using QS based quasi 2D/3D development

1-D Catalyst Simulation

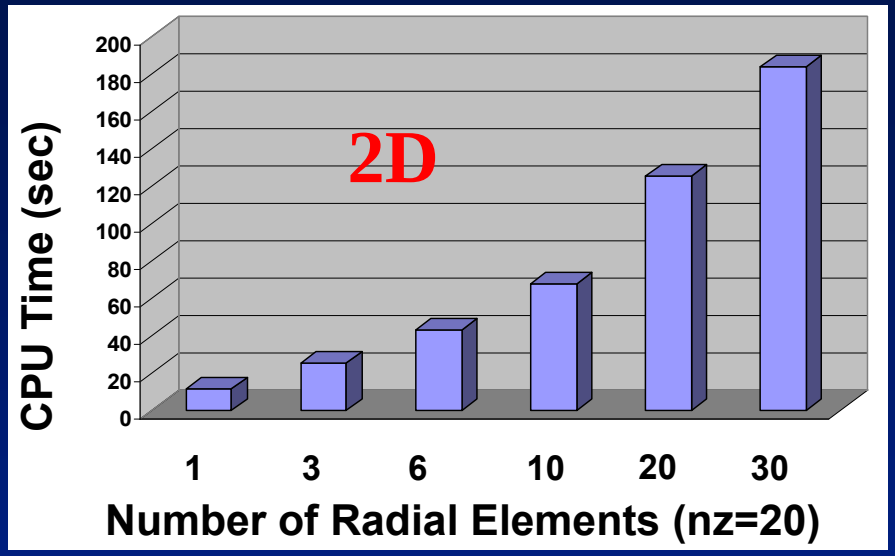
- Solution Overview
- Calibration
- Q-S Solver
- SCR
- DOC
- Aged DOC
- SIL/HIL /NN
- 2D/3D Model
- Conclusions



2-D Catalyst Simulation



Computational Speed Consideration



With regeneration rxn
Axial nodes = 21
300 second duration
dt = 0.1 sec.
AMD 1.8 GHz, 1.28 GB RAM

Real time is POSSIBLE for 2D/3D AT simulation