SCR Model Calibration

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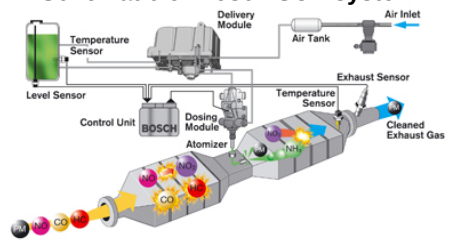
SCR Model

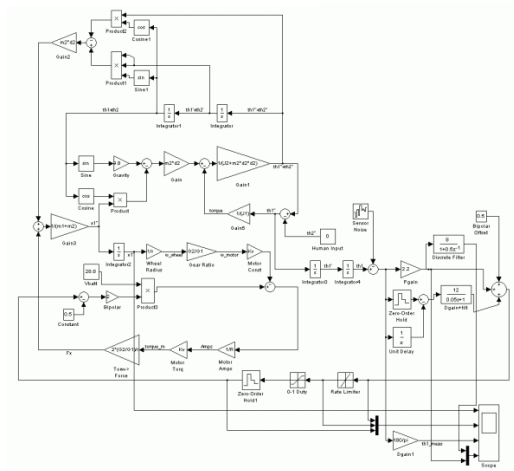
Relevance to Real World Applications, E.g. Tier 4 Machines

- Research and development
  - Technology capabilities
  - Different catalyst formulations and suppliers
  - Interaction of SCR with DOC/DPF

Schematic of Bosch SCR system



- Development of model based controls
  - Achieve high NOx conversion with low NH_3 slip
  - Account for catalyst aging
  - Improved BSFC and packaging



SCR Model

Chemical Kinetics

- Simplified single site SCR mechanism

- Six global reactions to approximate SCR chemistry
  - NH_3 adsorption and desorption
  - Standard, NO SCR
  - Fast, NO+NO_2 SCR
  - NO_2 SCR
  - NH_3 oxidation

$$NH_3 + S \rightarrow NH_3^* \quad (1)$$

$$NH_3^* \rightarrow NH_3 + S \quad (2)$$

$$4NH_3^* + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \quad (3)$$

$$2NH_3^* + NO + NO_2 \rightarrow 2N_2 + 3H_2O \quad (4)$$

$$4NH_3^* + 3NO_2 \rightarrow 3.5N_2 + 6H_2O \quad (5)$$

$$4NH_3^* + 3O_2 \rightarrow 2N_2 + 6H_2O \quad (6)$$

SCR Model

Chemical Kinetics

Reaction rates modeled based on Arrhenius equation

$$r = k e^{\left(\frac{-E_a}{RT}\right)} [C_1][C_2]$$

- Two unknowns per reaction
  - –Corresponding to pre-exponential term (k) and the activation energy (E_a)
- Additional calibration parameters such as ammonia storage capacity and ammonia saturation effect etc

SCR Model

Calibration Process

Difficult optimization problem

- Strongly coupled variables
  - *Pre-exponential terms and activation energies*
- Strongly coupled chemistry
  - *NO, NO_2 and NH_3 reactions depend on reactions interacting with each other*

Conventional approach

- Manual iteration + stochastic runs
  - *Requires knowledge of fundamental SCR chemistry*
  - *Time and effort intensive (~ 1 month)*
- Manual iteration + non linear optimization software
  - *Highly dependent on initial starting point*
  - *Time intensive and not very effective*

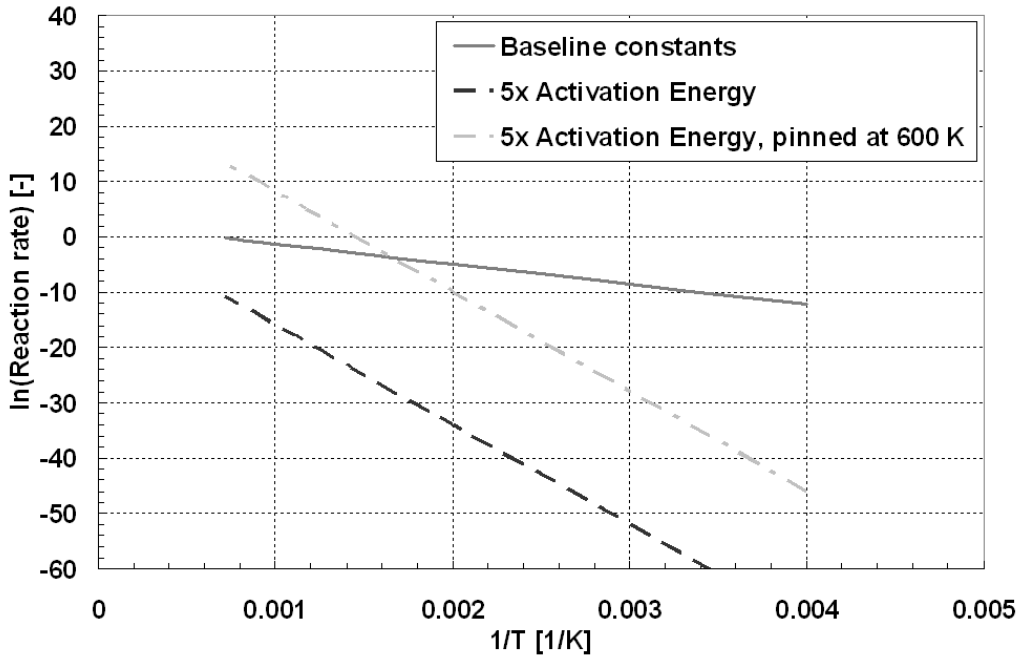
SCR Model

"Pinned" activation energies

Introduce additional term in Arrhenius equation to reduce interaction between pre-exponential term and activation energy

$$r = A' \exp\left(-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{600}\right)\right)$$

$$A' = \frac{A}{\exp\left(\frac{E}{R.600}\right)}$$

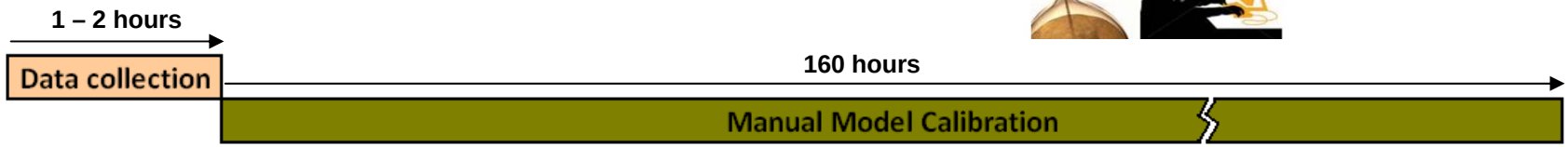


SCR Model

Calibration Process

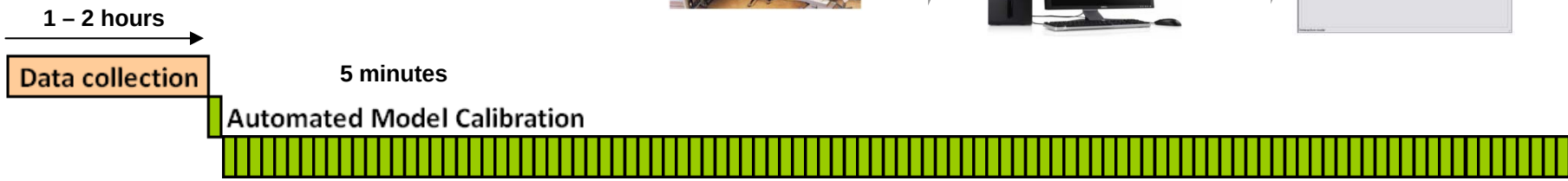
Old process

- Manual process (combination of manual tweaking and stochastic runs)
- Time consuming (~160 hrs)
- Expert user required



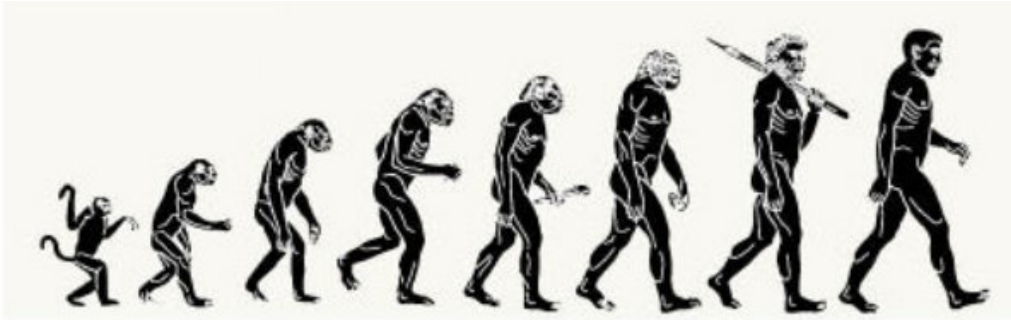
New process

- Automated process based on genetic algorithm
- Significantly faster (setup time ~5 min)
- Expert user ***NOT*** needed



SCR Model

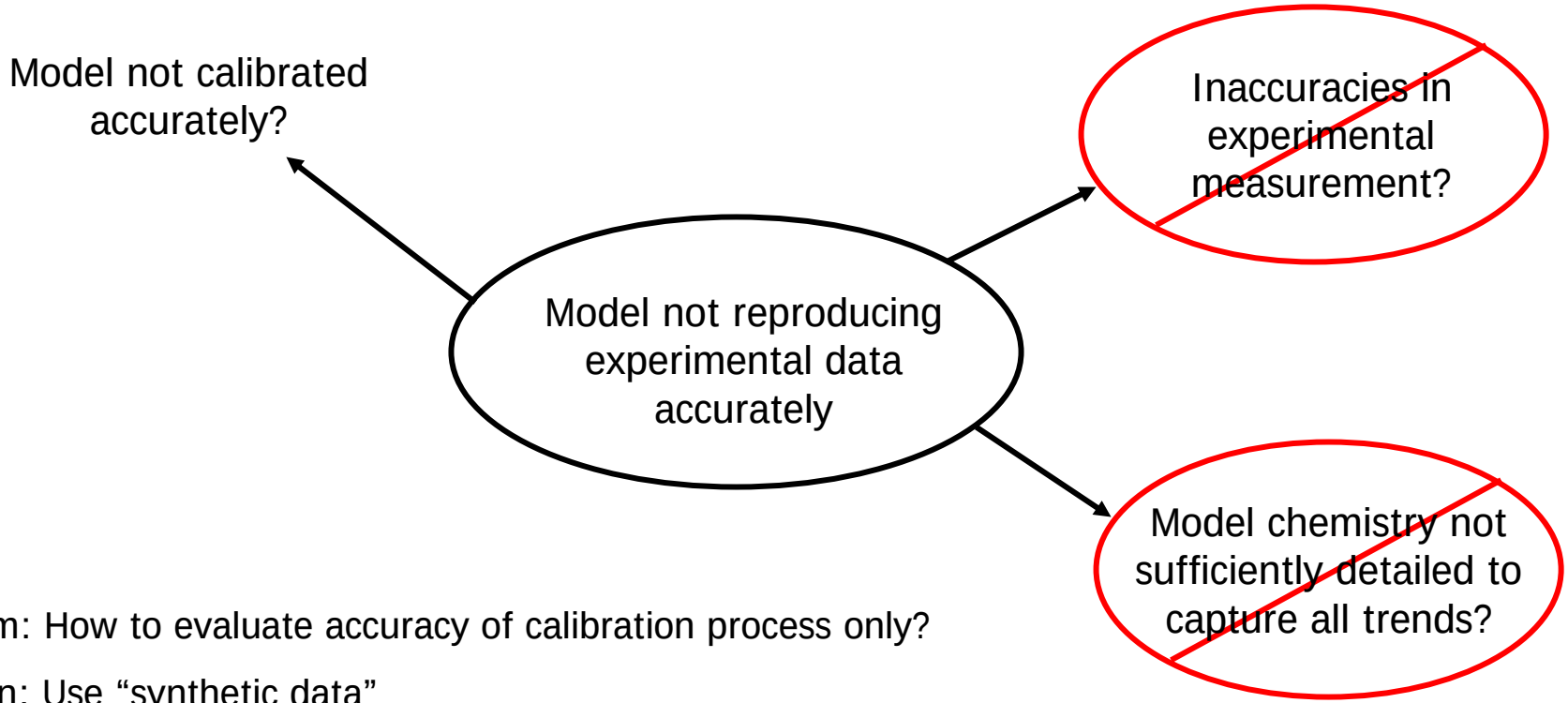
Calibration based on Genetic Algorithm



- Calibration based on optimization of constants using a multiple crossover, multi-elitist genetic algorithm
- Genetic information encoded in base 10 format

SCR Model Calibration

Validation Process



Problem: How to evaluate accuracy of calibration process only?

Solution: Use “synthetic data”

“Synthetic data” is data that has been created using a model

SCR Model

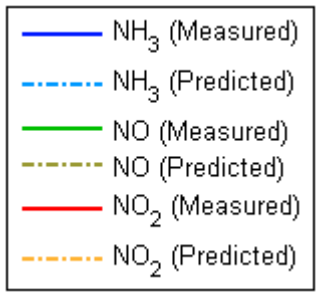
Validation using "synthetic data"

Benefits of using "synthetic data"

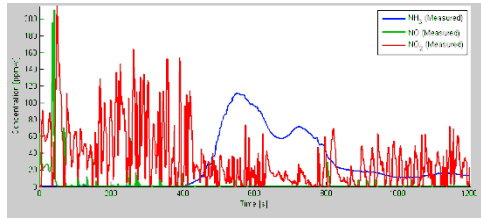
- Eliminates experimental inaccuracies
- Eliminates concern about model chemistry detail
- Quick and inexpensive to generate
- Allows many different cycles to be generated and evaluated for use in calibration process to mimic what can be generated on the bench and in engine test cells

SCR Model

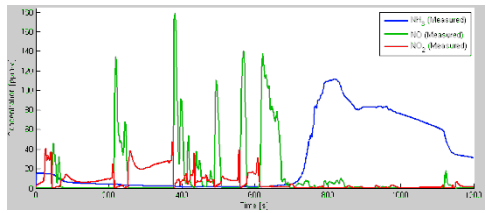
Transient Engine Cycles



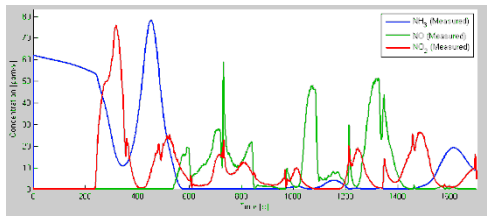
NRTC	Non Road Transient Cycle
FTP	Federal Test Protocol
ESC	European Steady-state Cycle
RMC	Ramped Modal Cycle



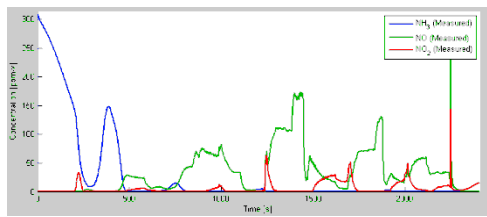
NRTC



FTP



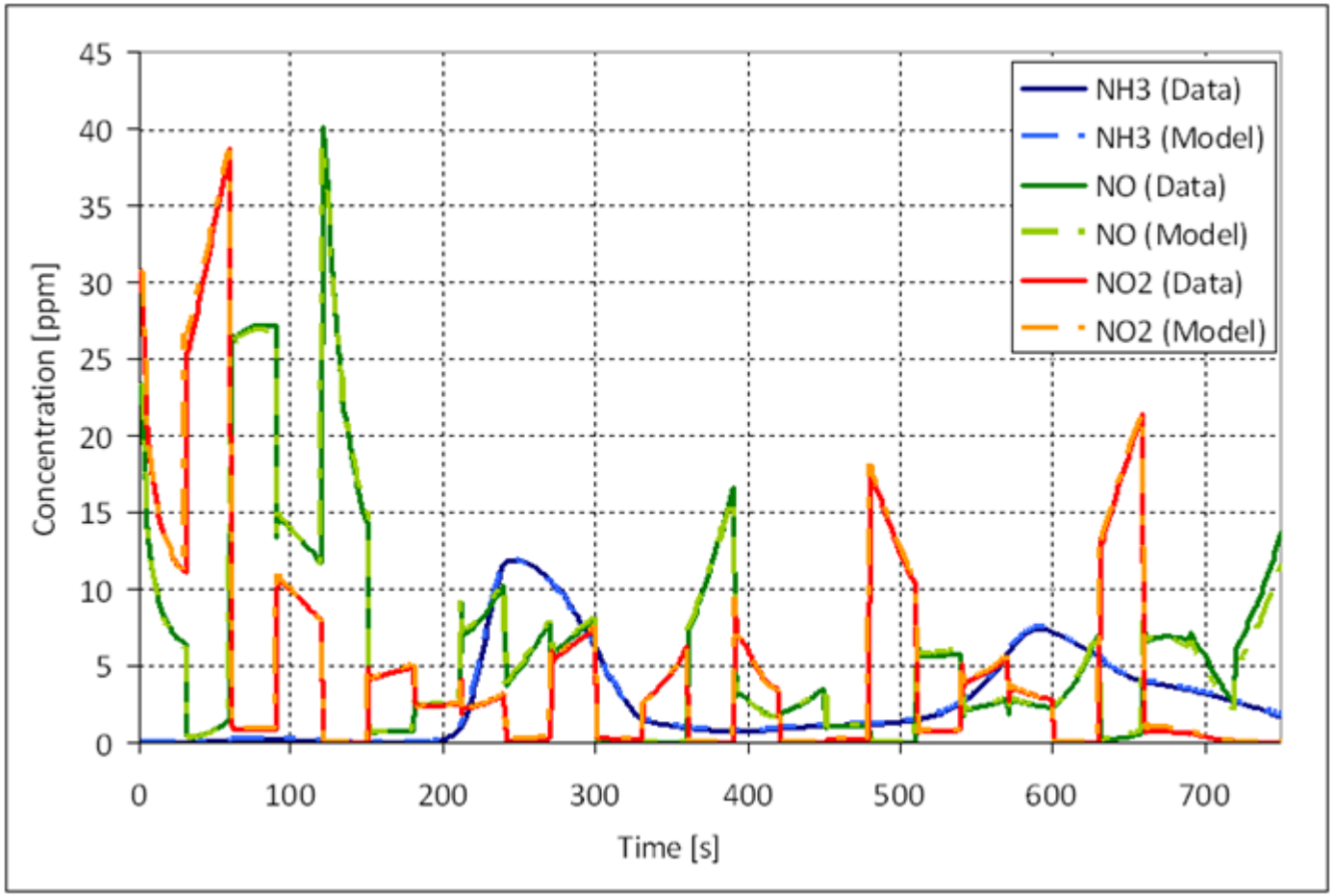
ESC



RMC

SCR Model

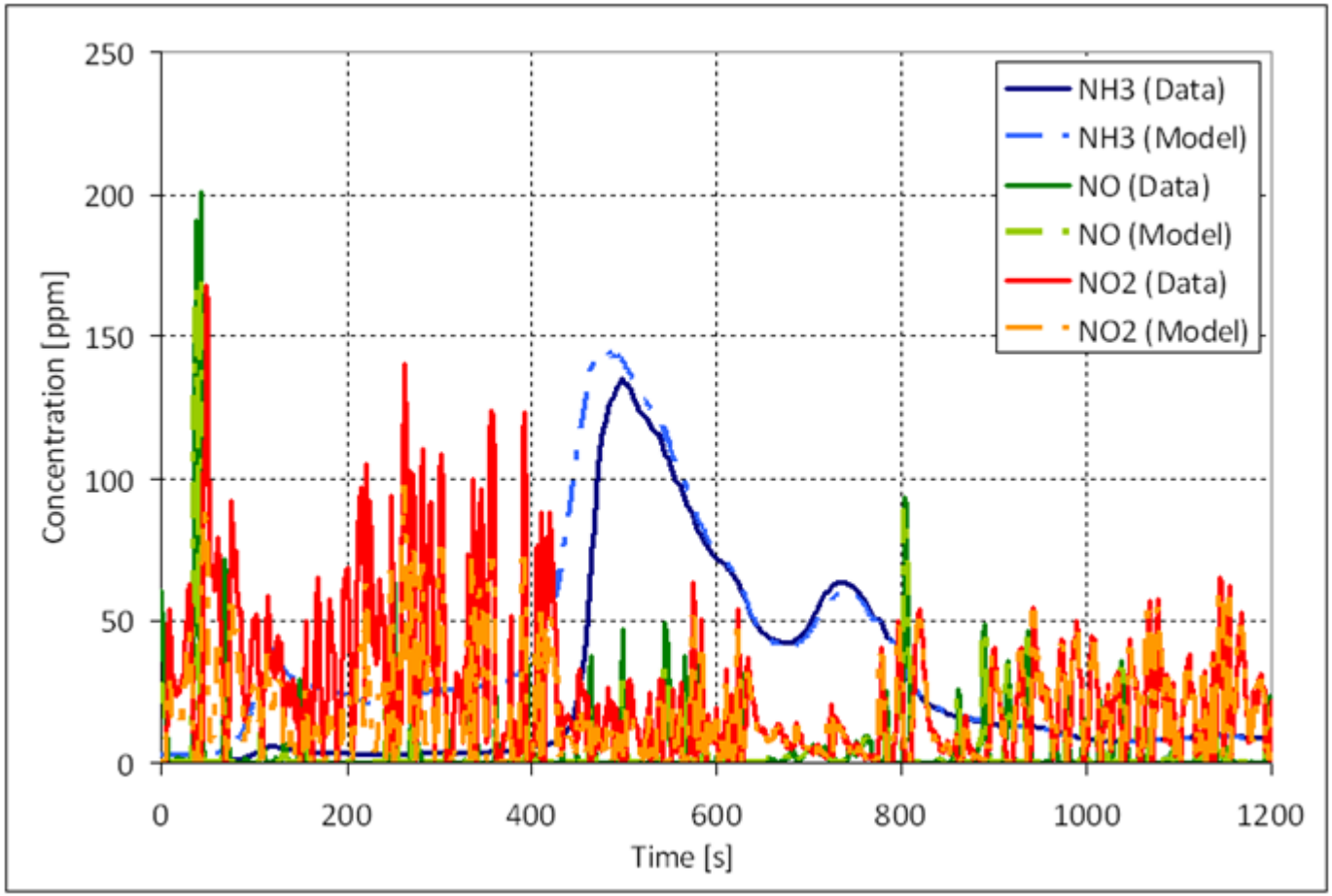
Calibration using 25 randomly selected points



Note: Data generated using a model and not necessarily representative of a physical catalyst.

SCR Model

Validation using NRTC



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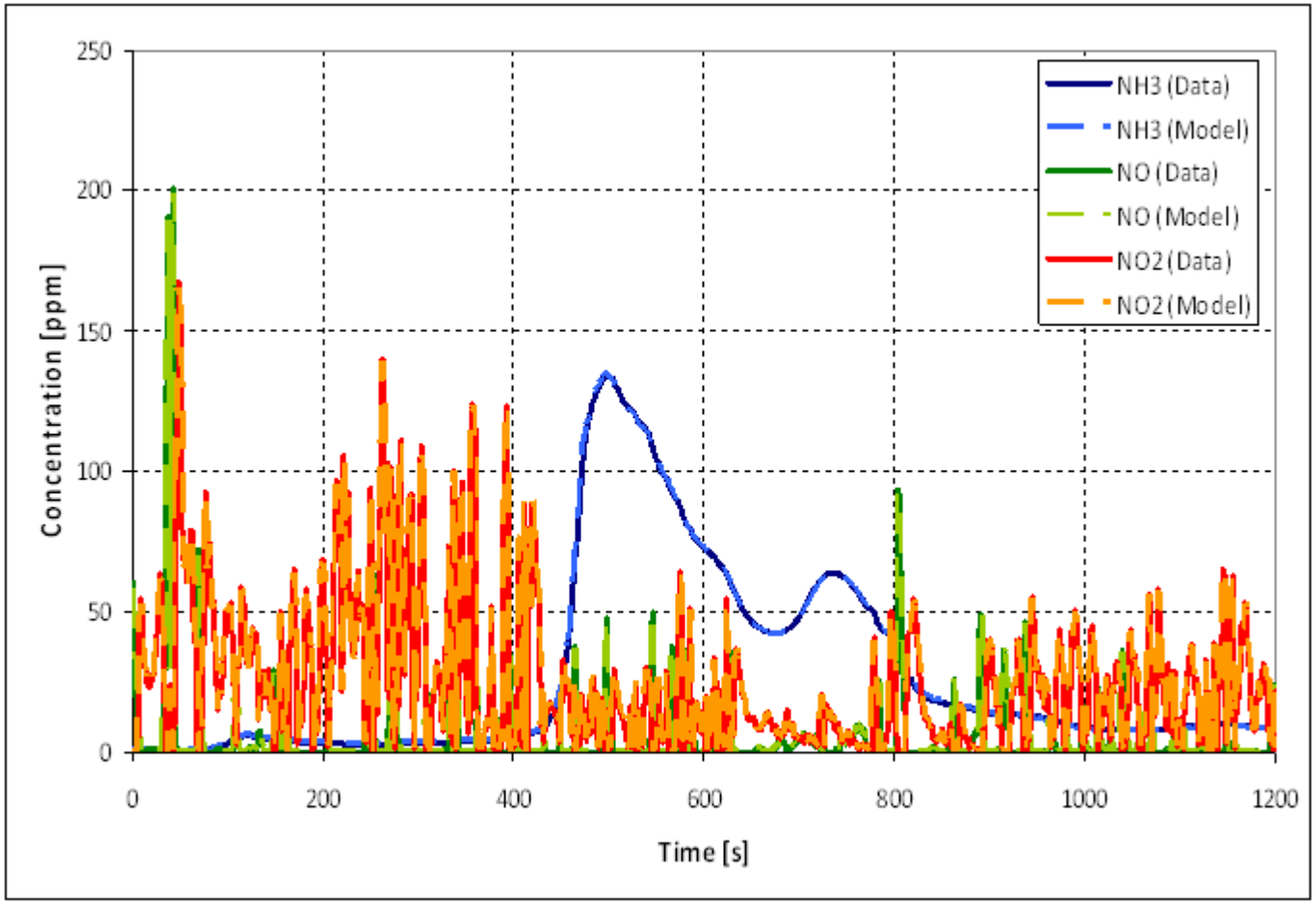
SCR Model

Calibration using NRTC



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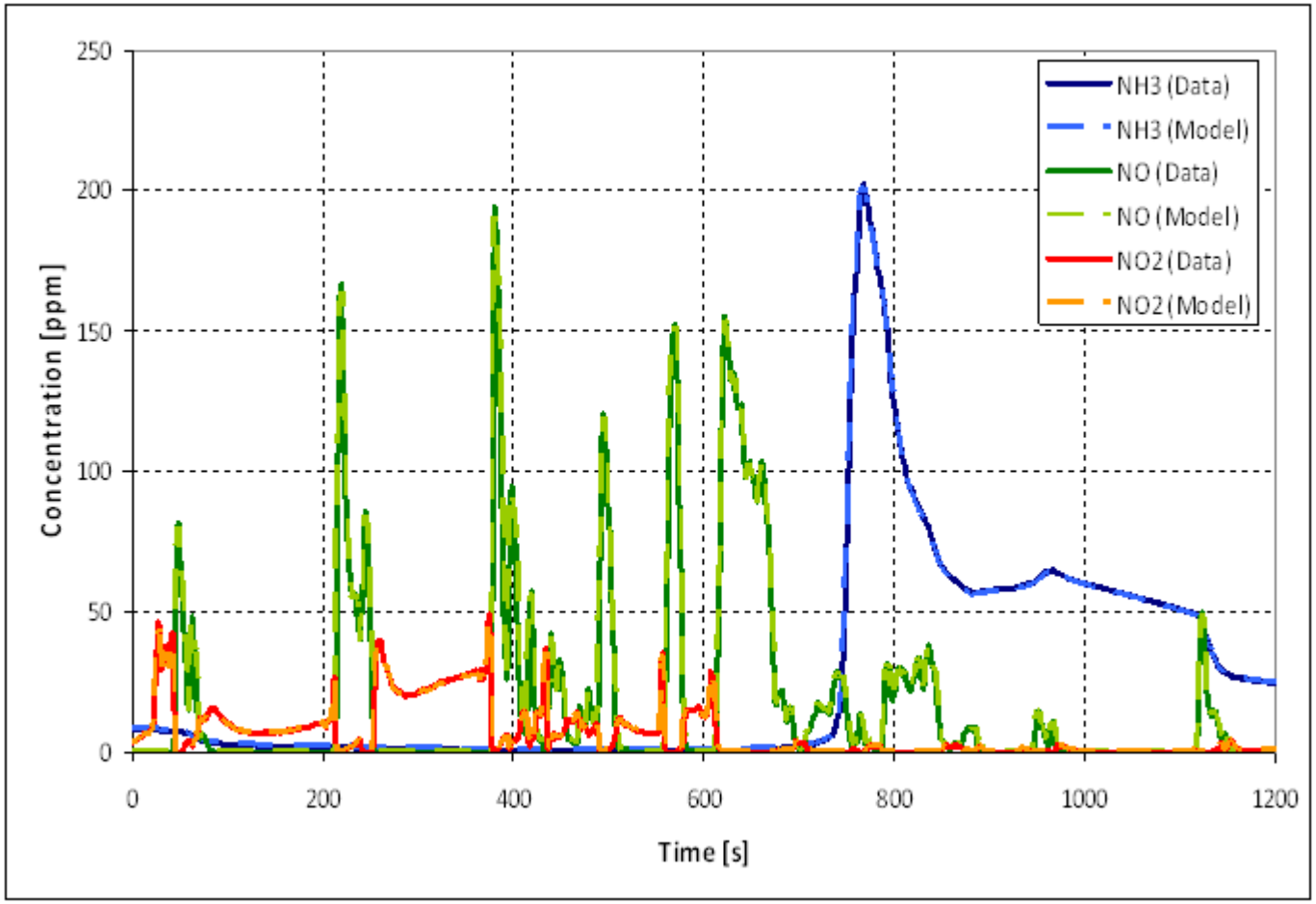
SCR Model

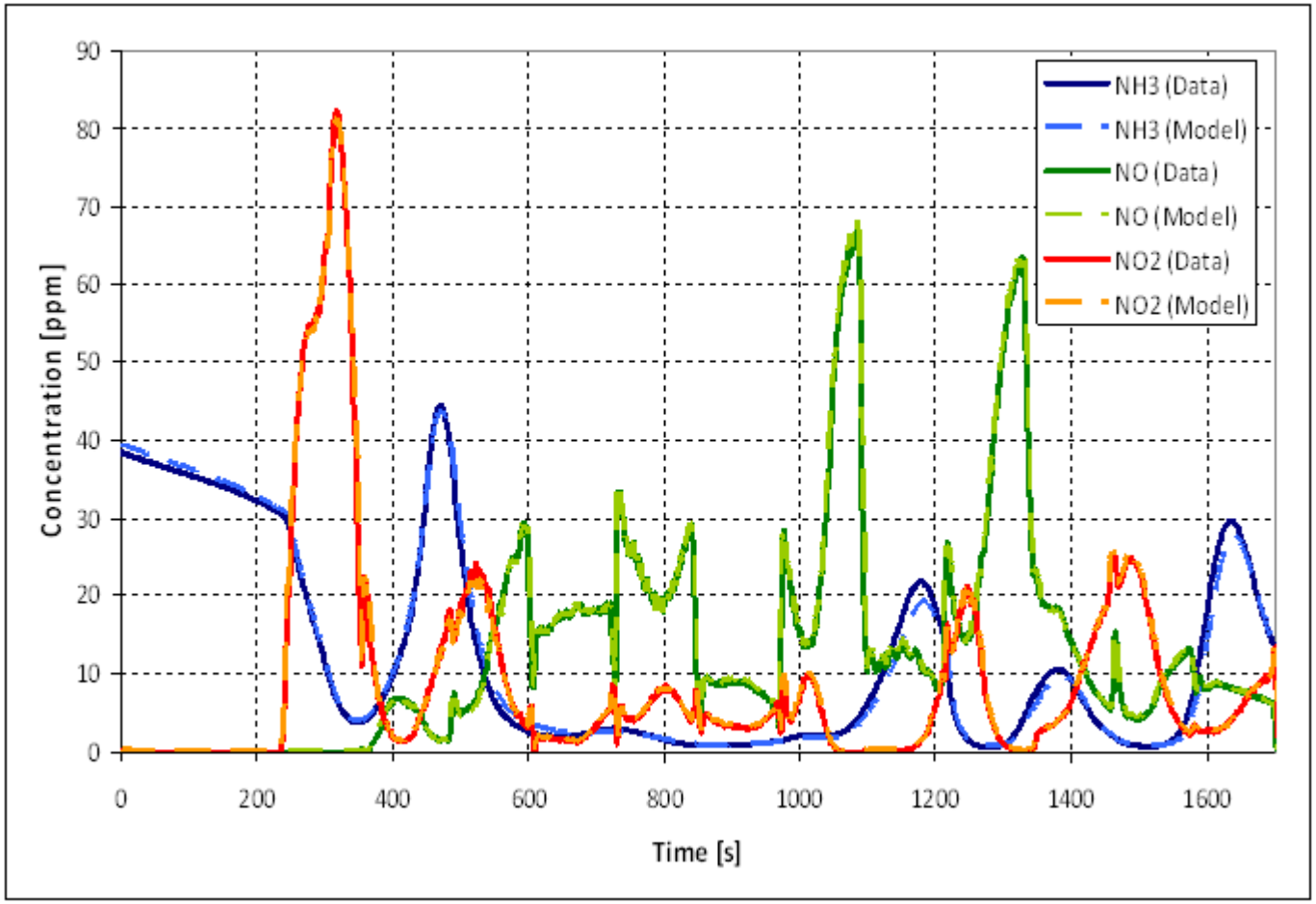
Validation using FTP



Note: Data generated using a model and not necessarily representative of a physical catalyst.

SCR Model

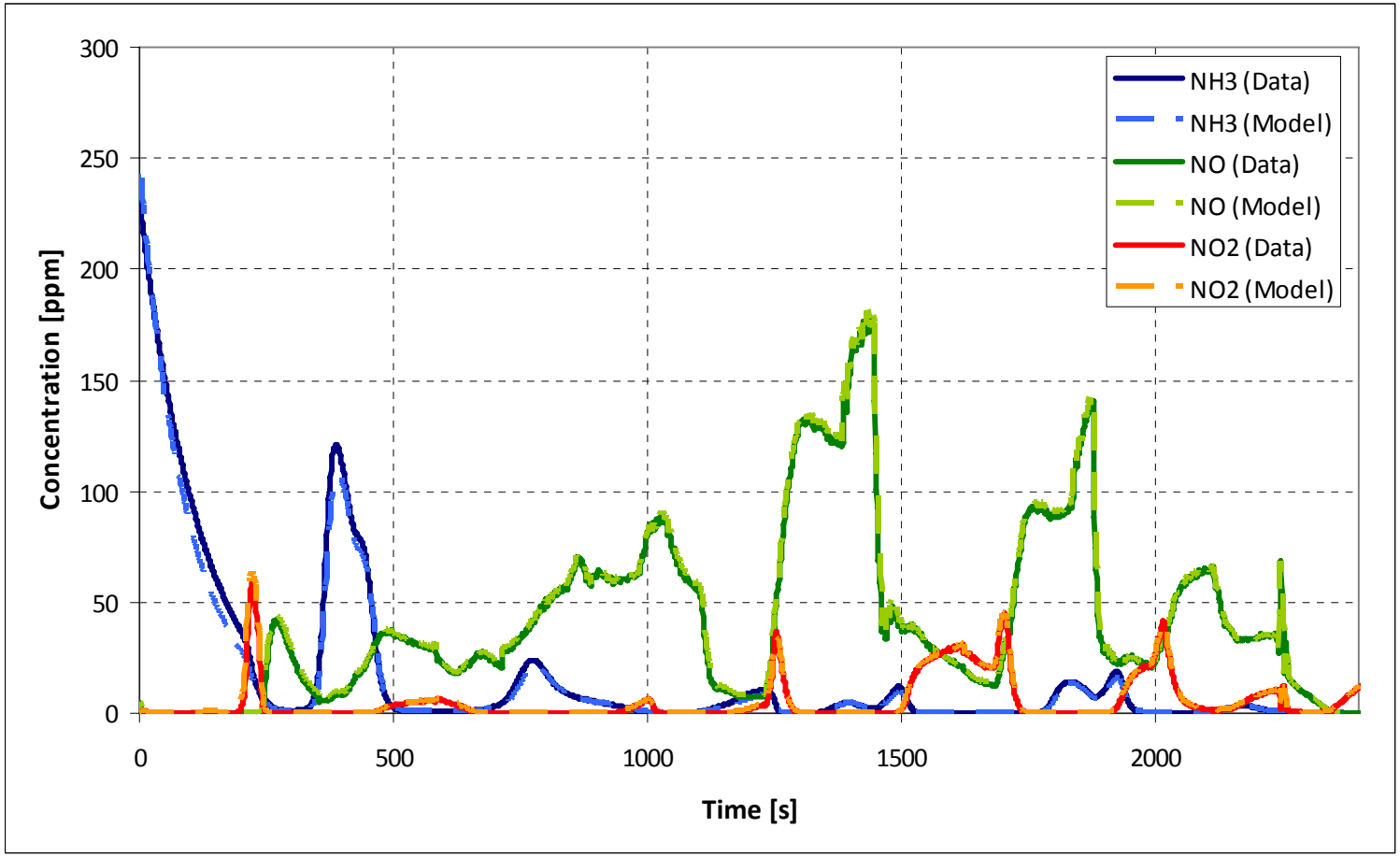
Validation using ESC



Note: Data generated using a model and not necessarily representative of a physical catalyst.

SCR Model

Validation using RMC



Note: Data generated using a model and not necessarily representative of a physical catalyst.

SCR Model Calibration

Summary

- Genetic algorithm based SCR model calibration tool is capable of determining appropriate constants for the SCR model
- Improvement in model prediction accuracy
  - 2x to 5x depending on cycle
- Significant reduction in time required for calibration
  - 2000x (160 hrs → 5 min)

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