Simulation Based Control System Analysis of a Urea-SCR Aftertreatment System Based on NOx and NH3 Sensor Feedback

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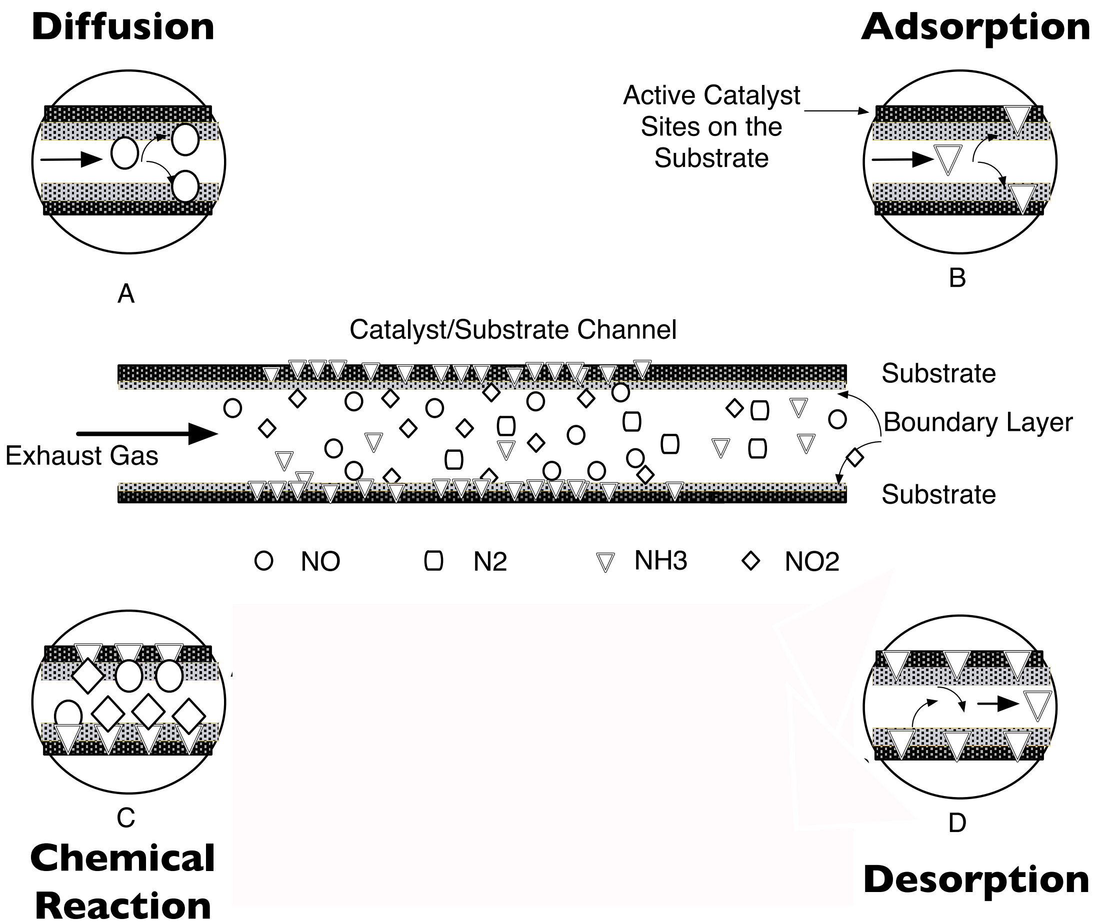
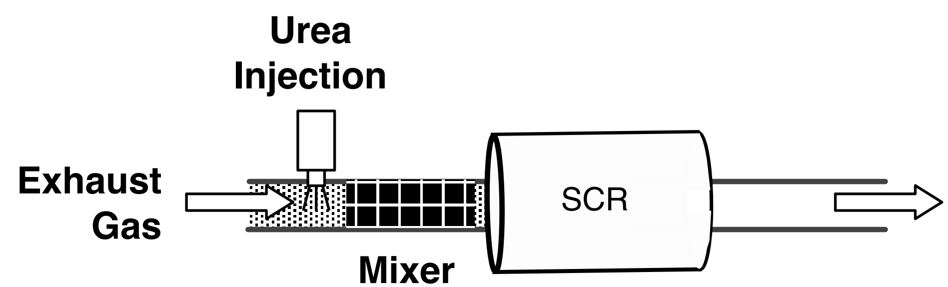
Brief Introduction to Urea-SCR Modeling

- Model Based Estimator and Control System Design
- Development of Sensor Models
- Simulation Based Analysis of NH3 Sensor Feedback
- Results

Phenomena in a SCR Catalyst - An Overview



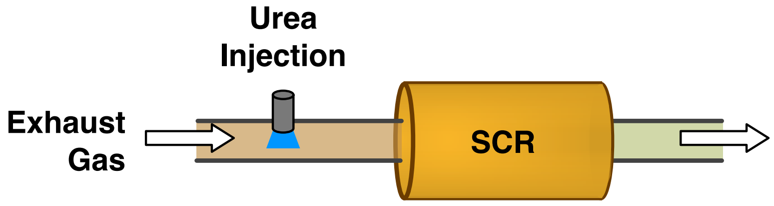


NH3 is the only species assumed to adsorb/desorb from the active sites of the catalyst.

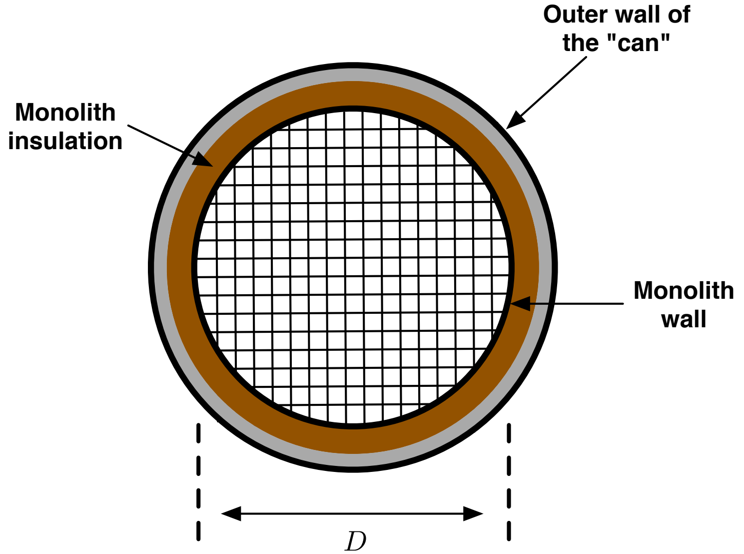
According to Eley Rideal mechanism, strongly adsorbed NH3 reacts with a weakly adsorbed NO and NO2 (gas/surface phase NO and NO2) on the monolith wall.

Lietti, 1998., Nova, 2001

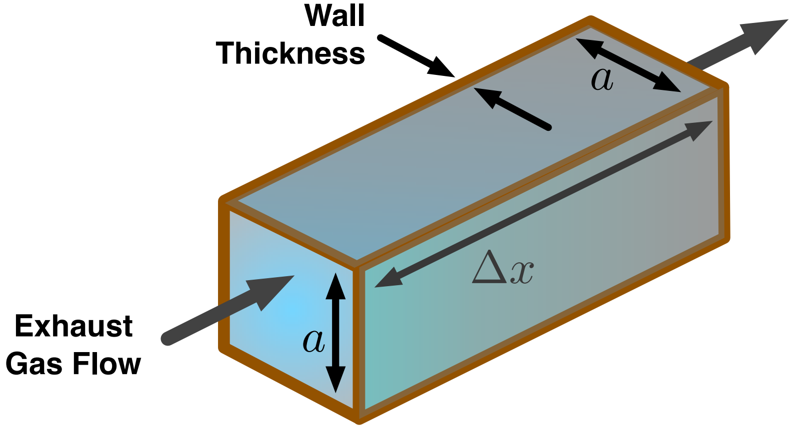
The objective of the higher order model (HOM) is to accurately predict the concentrations of NO, NO2 and NH3 species based on mass transfer and chemical kinetics of various reactions.



High-Level Illustration of the Urea-SCR Aftertreatment System



Idealized Illustration of a Flow Through Catalyst Cross-section



A Single Square Channel of a Urea-SCR Catalyst

Reaction Name	**Chemical Reaction**	**Reaction Rate**
Fast SCR	$4NH_3 + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O$	$R_1 = k_1 C_{s,NO} C_{s,NO_2} \theta \Omega$
Standard SCR	$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$	$R_2 = k_2 C_{s,NO} C_{O_2} \theta \Omega$
Slow SCR	$4NH_3 + 3NO_2 \rightarrow 7/2N_2 + 6H_2O$	$R_3 = k_3 C_{s,NO_2} \theta \Omega$
Fast NH3 Oxidation	$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$	$R_{fox} = k_{fox} \theta \Omega$ (neglected)
Slow NH3 Oxidation	$4NH_3 + 3O_2 \rightarrow 2N_2 + 3H_2O$	$R_4 = k_4 \theta \Omega$
NO Oxidation	$NO + 1/2O_2 \rightarrow NO_2$	$R_{no,oxi} = k_{no,oxi} C_{NO} C_{O_2}^{\frac{1}{2}}$ (neglected)
NH3 Adsorption	$NH_3 + S \rightarrow NH_3^*$	$R_5 = k_5 (1-\theta) C_{s,NH_3} \Omega$
NH3 Desorption	$NH_3^* \rightarrow NH_3 + S$	$R_6 = k_6 \theta \Omega$

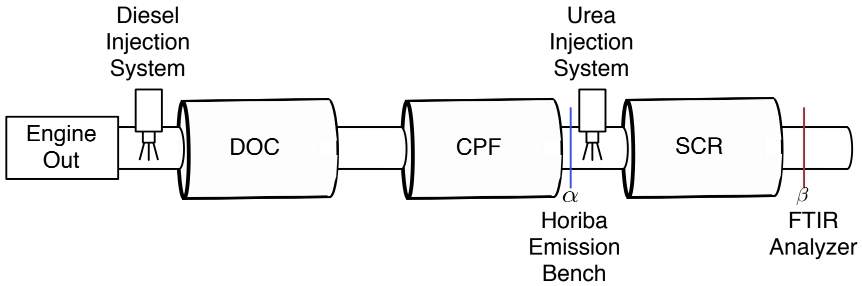
The reaction rate constants (K) are defined by the Arrhenius law defined as

$$k_i = A_i e^{-\frac{E_i}{RT}}$$

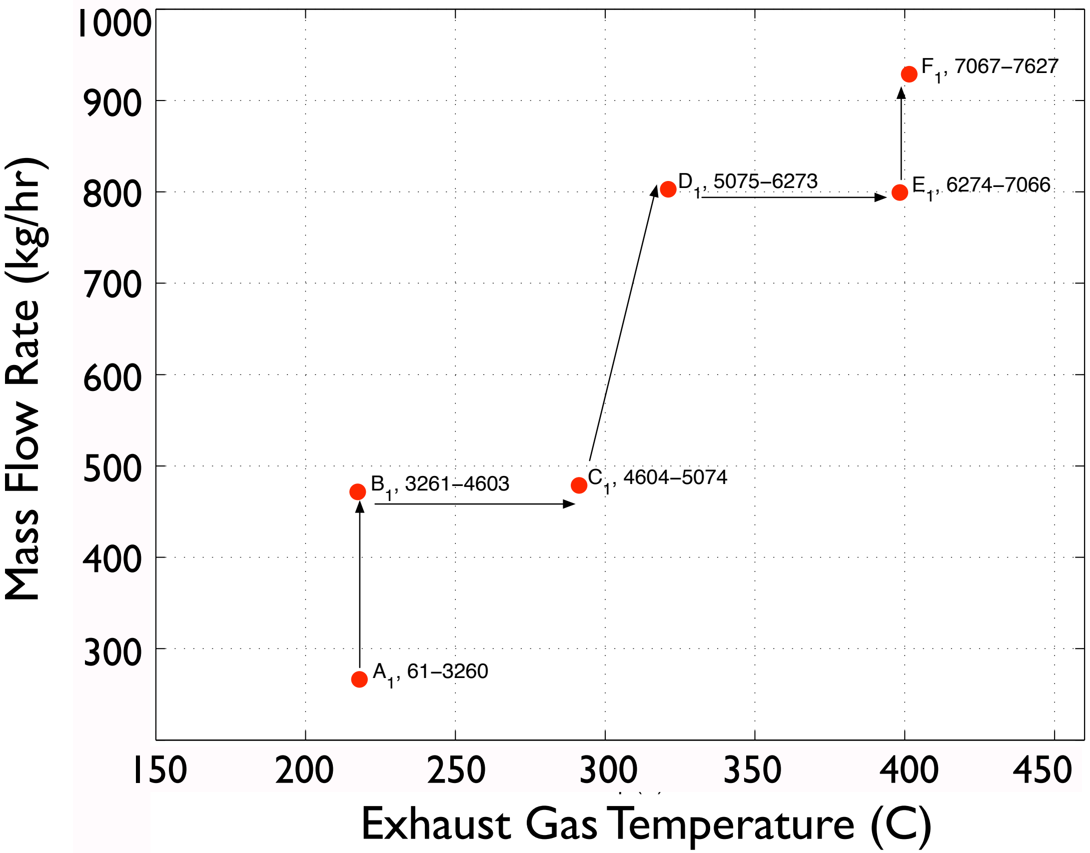
$$(i = 1...6)$$

A - Pre-exponential factor of the reaction
E - Activation energy of the reaction

- Experiments were conducted on a Navistar I6 7.6L engine at Bodycote testing facilities in Toronto, Canada.
- Four independent measurements were taken using 2 FTIR analyzers and 2 Horiba emission benches as shown.

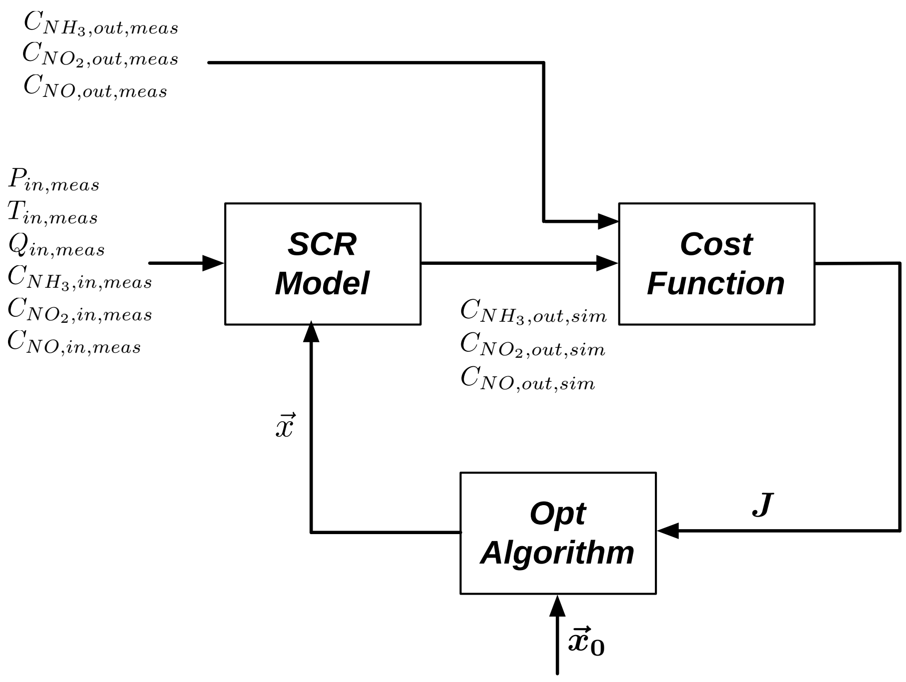


Experimental Set-up



- A total of **13 parameters have to be identified** for the 4 state model. These include the pre-exponential factors (As) and activation temperatures (Es) of the 6 reactions and the total ammonia adsorption capacity (Omega) in the catalyst.

The parameter identification problem is formulated as an optimization problem. Matlab's simplex method based optimization function 'fminsearch' is used.



Find the model parameters (x_i) where x_i are the pre-exponential factors and activation temperatures of the reactions, which

Minimize

$$J = \frac{1}{N}\sum_{i=1}^{N}(y_{i,s} - y_{i,t})^2 \quad y = NO, NO_2, NH_3$$

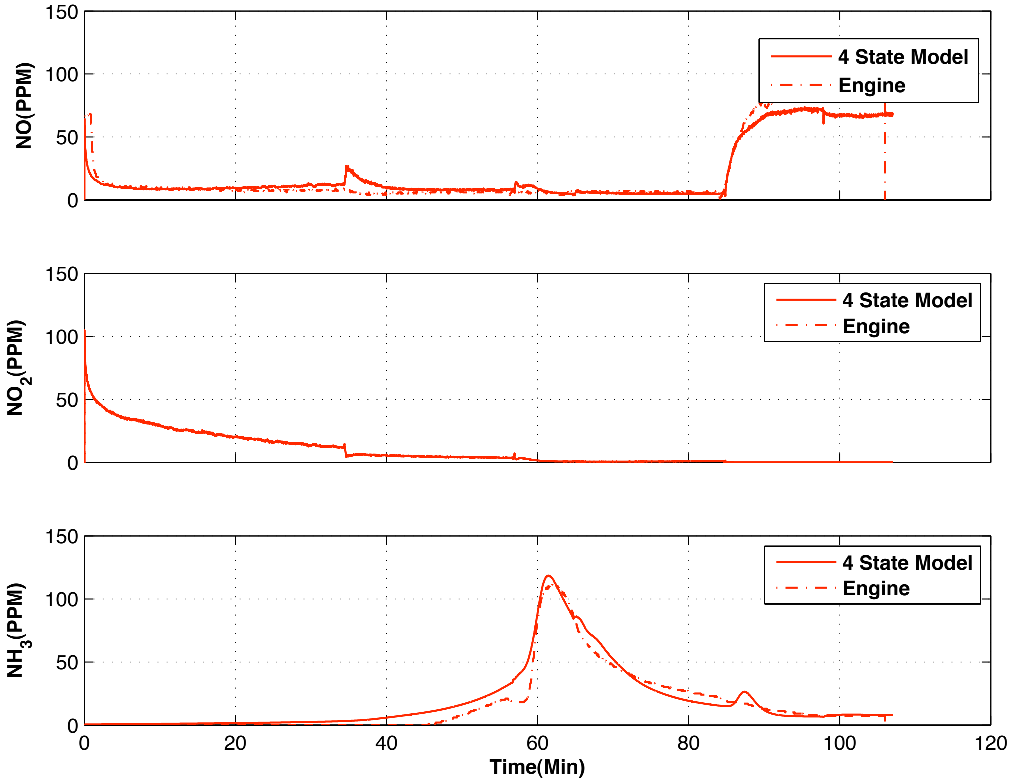
where N is the number of test data points. The cost function can be further expanded and expressed as

$$J = \frac{1}{N}\sum_{i=1}^{N}(y_{NO,s} - y_{NO,t})^2 + (y_{NO_2,s} - y_{NO_2,t})^2 + (y_{NH_3,s} - y_{NH_3,t})^2$$

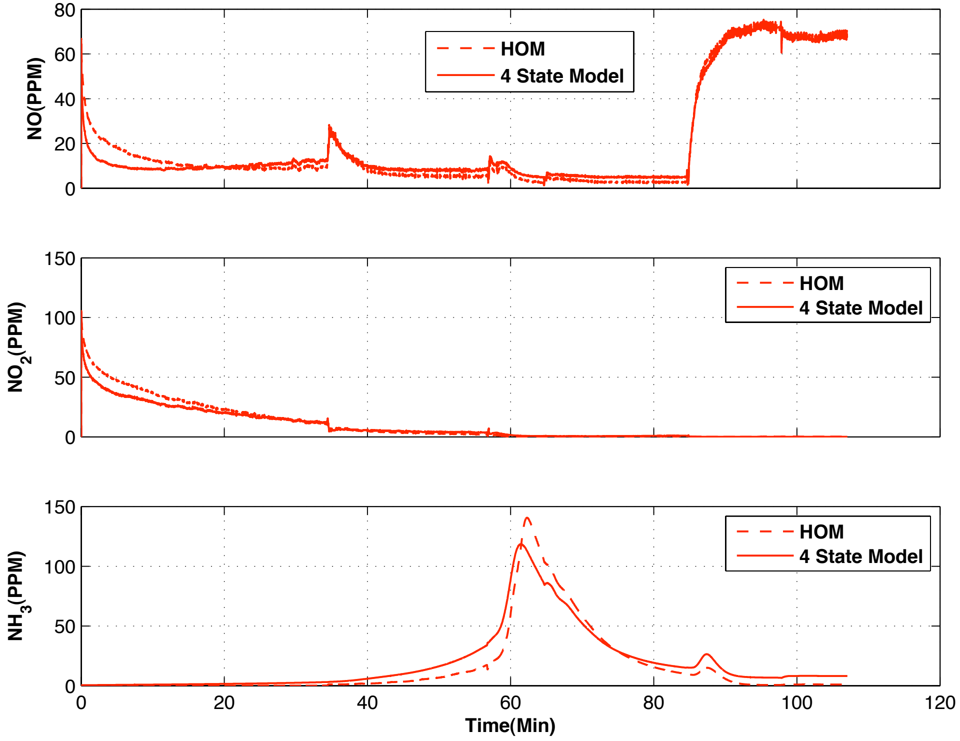
$y_{i,s}$ is the simulated concentration of the species in PPM

$y_{i,t}$ is the concentration of the species from the tests in PPM

4 State Model Validation Based on Test Data



Comparison of the 4 state model and the Higher Order Model (HOM)



Brief Introduction to Urea-SCR Modeling

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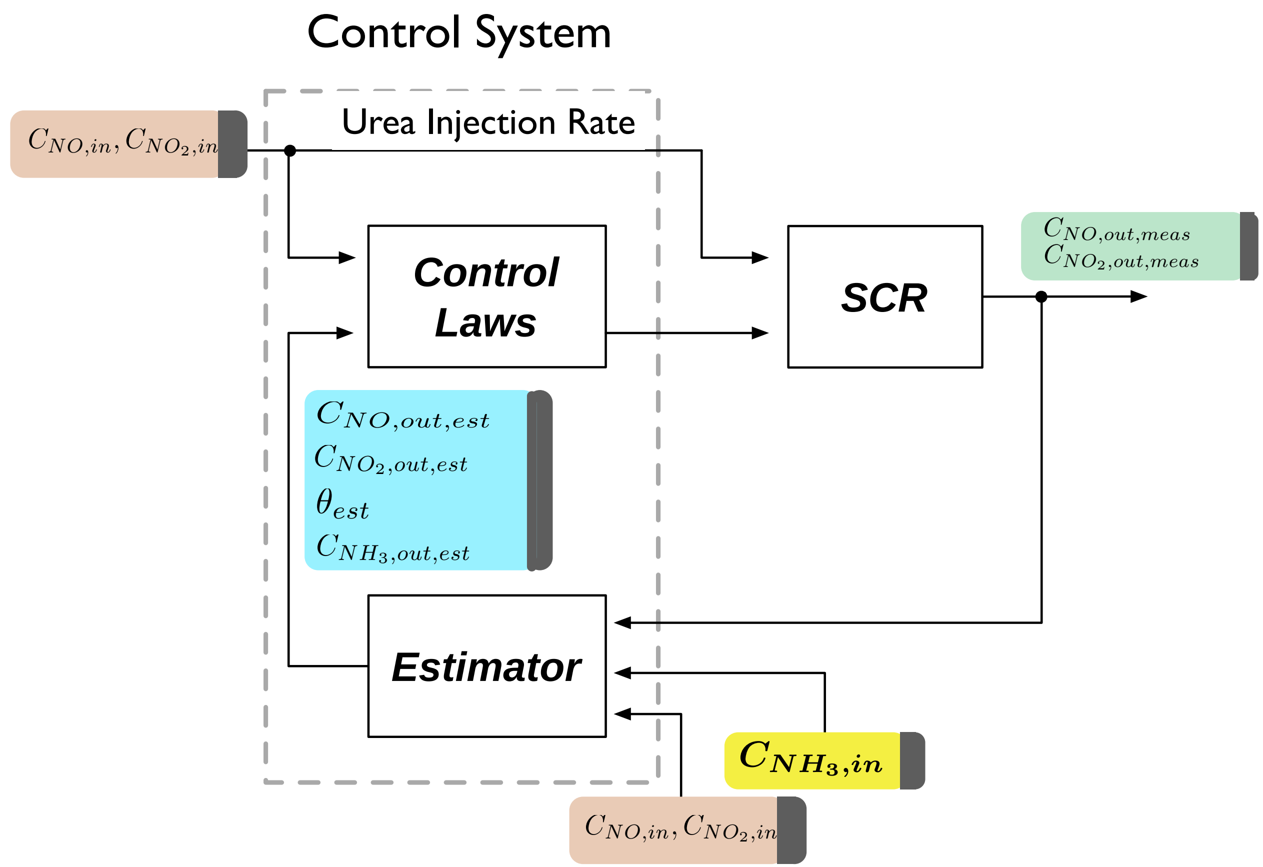
- Model-based state estimator
- Full state feedback, nonlinear control law

Both the estimator and the control strategy are based on a 4-state, reduced order model.



A linear state estimator from the reduced order model can be written as

$$\left\{ \begin{matrix} \dot{C}_{NO,est} \\ \dot{C}_{NO_2,est} \\ \dot{\theta}_{est} \\ \dot{C}_{NH_3,est} \end{matrix} \right\} = \vec{f}(C_{NO,est}, C_{NO_2,est}, \theta_{est}, C_{NH_3,est}, C_{NO,in}, C_{NO_2,in}) + \vec{L}(C_{NO,meas} + C_{NO_2,meas} - C_{NO,est} - C_{NO_2,est})$$

- $\vec{L}$ must be chosen such the estimator is stable. Since the linear portion of $\vec{f}$ is stable, this should be possible.

- If the NO and NO2 states converge quickly, the correction term vanishes and convergence will follow the natural NH3 dynamics.

$$\bar{L} = [-5; -5; 10000; 0]^T$$

Goals

- Minimize NO and NO2 out
- Minimize NH3 out

Performance Metrics

- NOx Conversion Efficiency

$$\eta_{NOx} = \frac{C_{NO,in} + C_{NO_2,in} - C_{NO,out} - C_{NO_2,out}}{C_{NO,in} + C_{NO_2,in}} = 1 - \frac{C_{NO,out} + C_{NO_2,out}}{C_{NO,in} + C_{NO_2,in}}$$

- Modified Conversion Efficiency

$$\eta_T = \frac{C_{NO_x,in} - C_{NO_x,out} - \alpha C_{NH_3,out}}{C_{NO_x,in}} = \eta_{NO_x} - \alpha \frac{C_{NH_3,out}}{C_{NO_x,in}}$$

Ref: Van Nieuwstadt, Upadhyay, IMECE 2002

- For the present work, the efficiency has been modified as a function of NO and NO2, instead of NOx, as cited in the prior art.

$$\eta_T = \frac{C_{NO,in} + C_{NO_2,in} - C_{NO,out} - C_{NO_2,out} - \alpha C_{NH_3,out}}{C_{NO,in} + C_{NO_2,in}} = \eta_{NOx} - \alpha \frac{C_{NH_3,out}}{C_{NO},in + C_{NO_2,in}}$$

SMC Approach

- Use the 4 state model to compute $C_{NH_3,in}$ such that the desired output is achieved, taking into consideration dynamic effects.

- Build in a correction term that guarantees stability and robustness to model, measurement, and disturbance errors.

Desired Response

Recall:

$$\eta_{T,des} = 1 - \frac{C_{NO,des} + C_{NO_2,des} + \alpha C_{NH_3,des}}{C_{NO,in} + C_{NO_2,in}} = 1 - p_{des}$$

Define a new quantity:

$$\bar{p}_{des} = p_{des}(C_{NO,in} + C_{NO_2,in}) = C_{NO,des} + C_{NO_2,des} + \alpha C_{NH_3,des}$$

where $\bar{p} = C_{NO} + C_{NO_2} + C_{NH_3}$ is simply a linear combination of the 4 state model states.

Define: $e_{\bar{p}} = \bar{p}_{des} - \bar{p}$

The response goal can be expressed as: $e_{\bar{p}} = \dot{e}_{\bar{p}} = 0$

or $\dot{\bar{p}}_{des} - \dot{C}_{NO} - \dot{C}_{NO_2} - \alpha \dot{C}_{NH_3} = 0$

Substituting in the 4 state model equations gives the dynamic portion of the control law:

$$\begin{aligned} C_{\mathrm{NH_3},in,dyn} =& C_{\mathrm{NH_3},est} + \frac{1}{\lambda}(C_{\mathrm{NO},est} + C_{\mathrm{NO_2},est} \\ & - C_{\mathrm{NO},in} - C_{\mathrm{NO_2},in}) + \frac{1}{\bar{Q}}(k_5\Omega(1-\theta_{est})C_{\mathrm{NH_3},est} \\ & - k_6\Omega\theta_{est}) + \frac{1}{\lambda\bar{Q}}(\dot{\bar{p}}_{des} + 2\Omega\theta_{est}k_1 C_{\mathrm{NO},est}C_{\mathrm{NO_2},est} \\ & + \Omega\theta_{est}k_2 C_{\mathrm{NO},est}C_{\mathrm{O_2}} + \Omega\theta_{est}k_3 C_{\mathrm{NO_2},est}) \end{aligned}$$

The complete control law is created by appending a correction term that penalizes deviations from the objective of $e_{\bar{p}} = 0$,

$$C_{NH_3,in} = C_{NH_3,in,dyn} - \Gamma sgn(e_{\bar{p}})$$

The complete control law is created by appending a correction term that penalizes deviations from the objective of $e_{\bar{p}} = 0$,

$$C_{NH_3,in} = C_{NH_3,in,dyn} - \Gamma sgn(e_{\bar{p}})$$

Ensuring stability in the presence of model, measurement and disturbance uncertainty places constraints on the design parameter Γ. These constraints are developed using Lyapunov's Direct Method illustrated below.

Create a candidate Lyapunov function: $V = \frac{1}{2} e_{\bar{p}}^2$

If $\dot{V} < 0$ for the 4 state model dynamics, then the closed loop system is asymptotically stable.

$$\dot{V} = e_{\bar{p}} \dot{e}_{\bar{p}} = -\Gamma |e_{\bar{p}}|$$

Thus, $\Gamma > 0$ guarantees closed loop stability.

Brief Introduction to Urea-SCR Modeling

Model Based Estimator and Control System Design

- ***Development of Sensor Models***
- Simulation Based Analysis of NH3 Sensor Feedback
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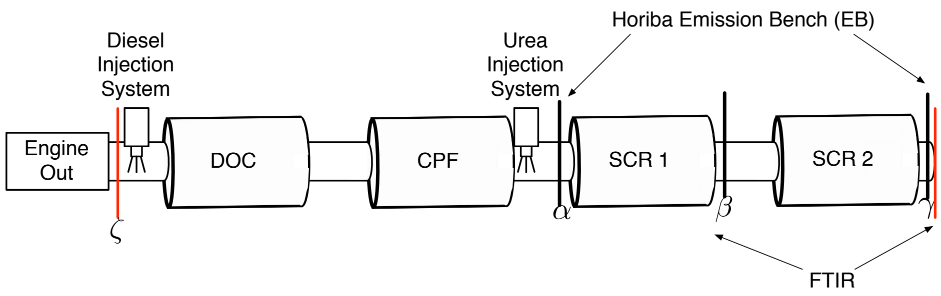
Problem Description

- NOx sensors are placed downstream of the catalyst to provide NOx feedback to the closed loop control system which determines the urea injection rate.
- State-of-the-art NOx sensors have cross-sensitivity towards NH3 which is a limitation for accurate NOx feedback.
- This limitation can be overcome through a NOx sensor model which determines the individual components of the sensor signal.
- One other approach is to use an NH3 sensor which from the literature does not possess any cross-sensitivity.



Approach Followed

- A NOx sensor model is developed based on the test data and is experimentally validated.
- The linear system based on NH3 sensor feedback is analyzed for state estimation design.
- Using a two catalyst model in series and further reducing the 4 state model to a single state model for real-time implementation, the sensor models are validated.
- The control systems based on their respective sensor models are compared and analyzed.

The NOx sensor model is designed based on the NOx sensor signal and the concentrations from the FTIR analyzer downstream of the SCR catalyst. As the state-of-the art NOx sensor is cross-sensitive to NH_3, A_3 is calculated as a function of α which is the ratio of ammonia (from the urea injection flow rate) injected (NH_3, in) in PPM to the engine out NOx from the engine out NOx sensor/virtual NOx sensor (NO_x, in) in PPM (Ref: Schar, 2003)

$$\alpha = \frac{NH_3, in}{NO_x, in}$$

$$NH_3, in = 2.0 * \frac{\dot{m}_{urea}}{\dot{m}_{exh}} \frac{MW_{exh}}{MW_{urea}} * 1E6$$

$\dot{m}_{urea}$ is the mass flow rate of urea injected and $\dot{m}_{exh}$ is the mass flow rate of exhaust gas. MW_{urea} is the molecular weight of urea (60 grams/gram-mole)

MW_{exh} is the molecular weight of exhaust gas (28.8 grams/gram-mole)

NOx sensor signal can be represented as

$$S = A_1 C_{\mathrm{NO}} + A_2 C_{\mathrm{NO_2}} + A_3(\alpha) C_{\mathrm{NH_3}}$$

where S is the sensor signal in PPM.

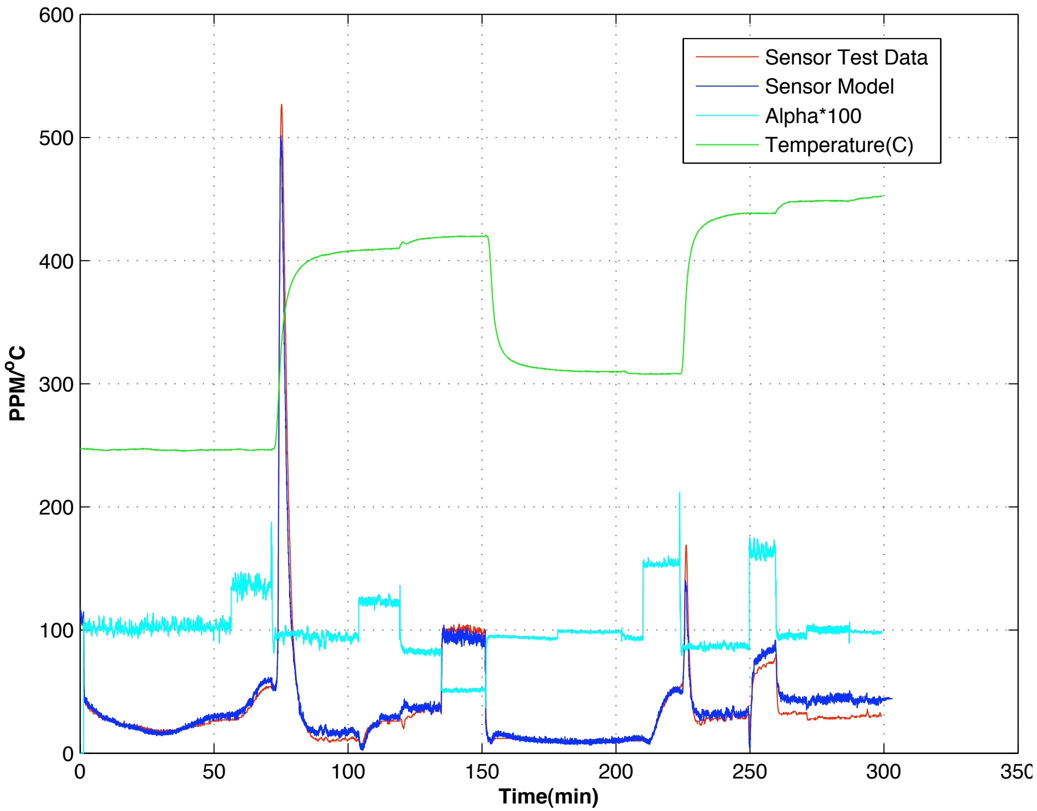
$C_{NO}, C_{NO_2}\, and\, C_{NH_3}$ are the concentrations from the FTIR analyzer at the tail pipe.

There is significant scatter in the data related to;

- accuracy of measurements both by NOx sensor and FTIR, especially at low concentrations
- signal delay and dispersion in FTIR due to relatively long sampling pipes, different for each individual component due to differences in their interaction with the walls

Alternatively at low concentrations, it can be assumed that the coefficients A_i are constants as given below
A_1 = 1.0
A_2 = 0.95
A_3 = 1.0

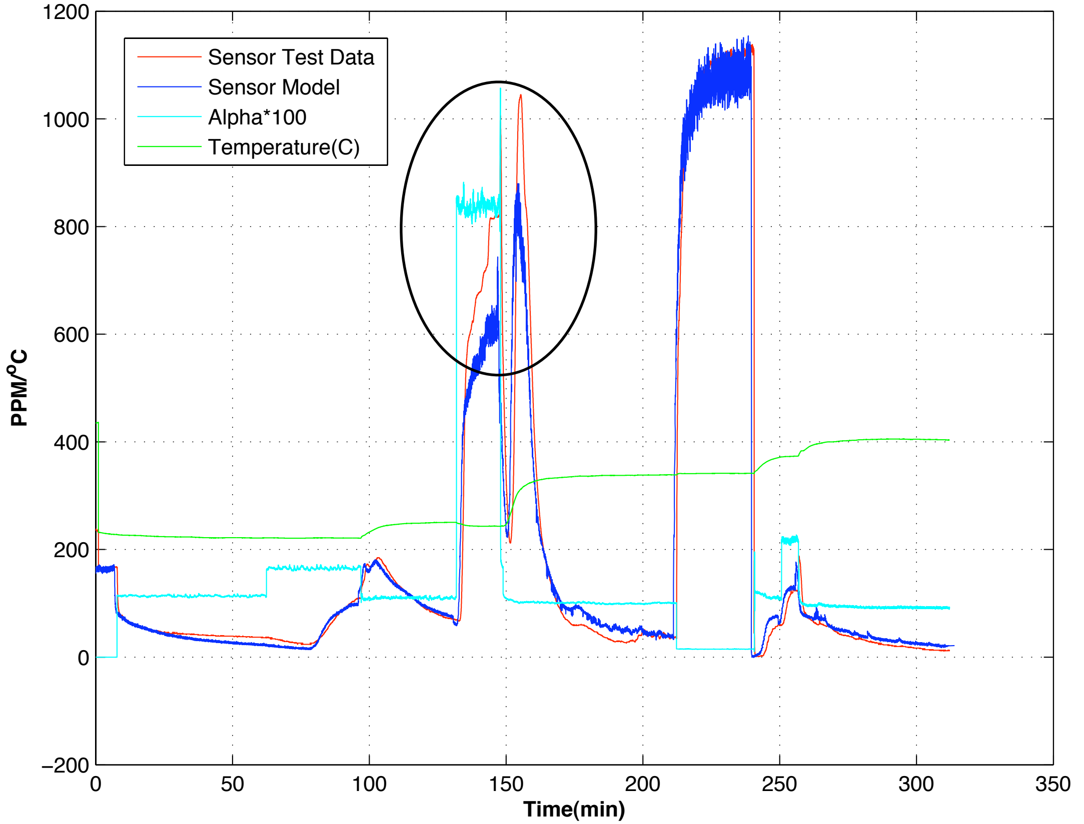
Experimental Validation of NOx Sensor Model



Experimental validation of the sensor model using test data

✓ Needs more work on understanding the impact of alpha on the sensor model

✓ Alternatively any other formulation of the sensor model as a function of individual species concentrations and other factors need to be explored.



Experimental validation of the sensor model using test data

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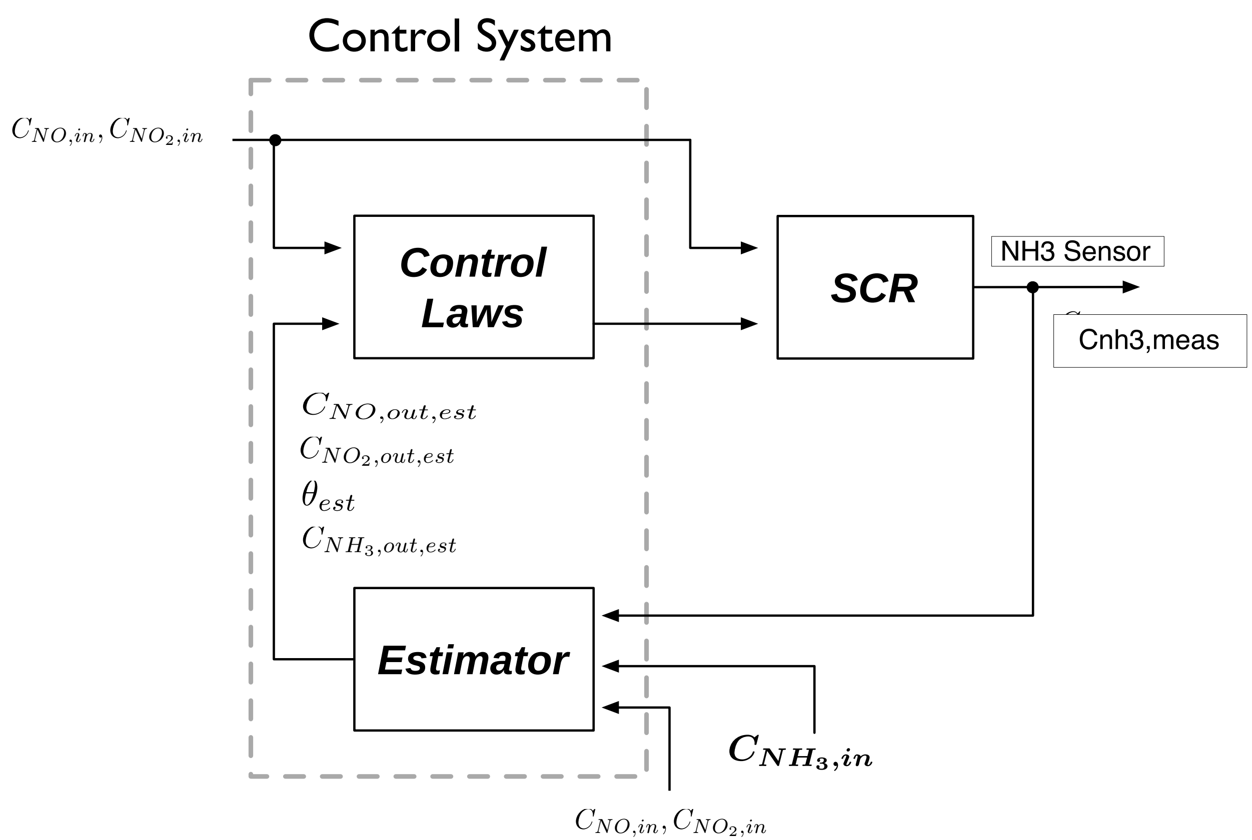
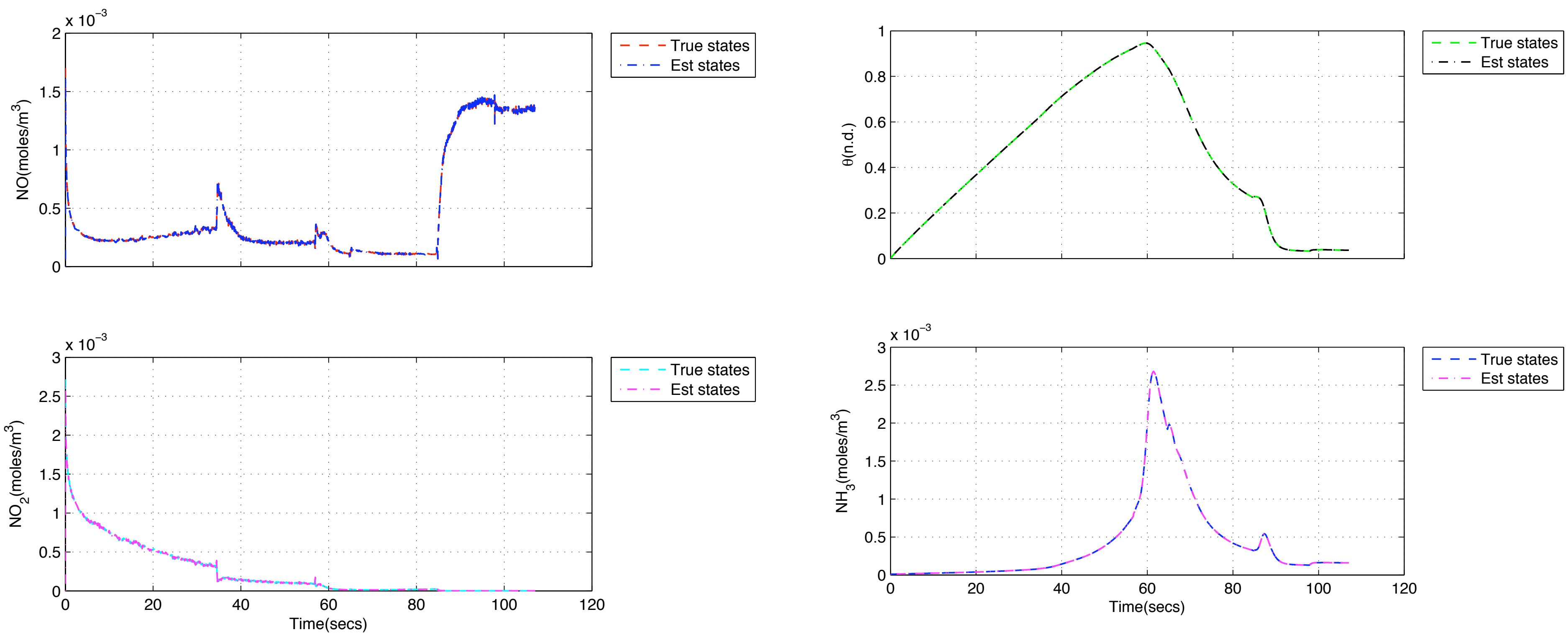
- Model-based state estimator
- Full state feedback, nonlinear control law

Both the estimator and the control strategy are based on a 4-state, reduced order model.



- NH3 concentration from the FTIR analyzer is assumed as the NH3 sensor signal.
- NH3 sensor is assumed to have no cross-sensitivity towards NO and NO2 species as reported in the literature.
- Using the 4 state model, the linear system based on NH3 sensor feedback is observable and controllable under all engine operating conditions.

A model estimator of the form $\dot{\vec{x}}_{est} = \vec{f}(\vec{x}_{est}, u, t) + \vec{L}(C_{NH_3} - C_{NH_3,est})$ is designed. $\bar{L} = [-5; -5; -1; -5]^T$



Estimator Design for the 4 State Model Based on NH3 Sensor Feedback

The time constants associated with the species concentrations ($C_{NO}, C_{NO_2}\, and\, C_{NH_3}$) in the 4 state model are of the order of magnitude of micro-seconds and therefore for real time control strategy implementation, the 4 state model has been reduced to a single state model by solving ($\dot{C}_{NO}\,, \dot{C}_{NO_2}\,, \dot{C}_{NH_3}$) as steady state expressions.

Solving for $\dot{C}_{NO}\, and\, \dot{C}_{NO_2}$ results in a quadratic equation in C_{NO_2} written as

$$aC_{NO_2}^2 + bC_{NO_2} + c = 0 \qquad \text{where}$$

$$a = k_1\Omega\theta\bar{Q} + k_1k_3\Omega^2\theta^2$$

$$b = \bar{Q}^2 + k_2\Omega\theta\bar{Q}C_{O_2} + k_1\Omega\theta\bar{Q}C_{NO,in} + k_3\Omega\theta\bar{Q} + k_2k_3\Omega^2\theta^2C_{O_2} - k_1\Omega\theta\bar{Q}C_{NO_2,in} \quad \text{and}$$

$$c = -\bar{Q}^2C_{NO_2,in} - k_2\Omega\theta\bar{Q}C_{NO_2,in}C_{O_2}$$

which is solved to obtain C_{NO_2}

C_{NO} is then solved by using the expression

$$C_{NO} = \frac{\bar{Q}C_{NO,in}}{\bar{Q} + k_1\Omega\theta C_{NO_2} + k_2\Omega\theta C_{O_2}}$$

C_{NH_3} is solved by in steady state by setting $\dot{C}_{NH_3} = 0$

$$C_{NH_3} = \frac{\bar{Q}C_{NH_3,in} + k_6\Omega\theta}{k_5(1-\theta)\Omega + \bar{Q}}$$

The only state in the single state model is the ammonia storage given by

$$\dot{\theta} = -(k_6+k_4)\theta + k_5C_{NH_3} - k_1C_{NO}C_{NO_2}\theta - k_2C_{NO}C_{O_2}\theta - k_3C_{NO_2}\theta - k_5\theta C_{NH_3}$$

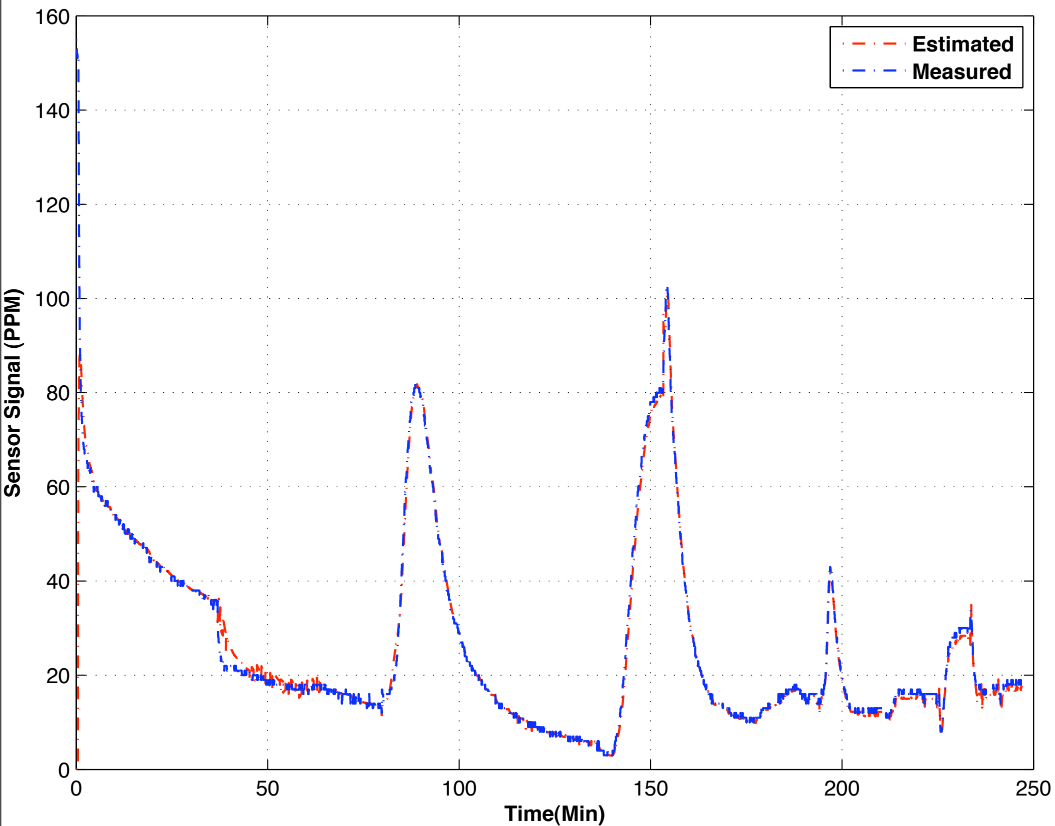
which is a function of $C_{NO}, C_{NO_2}\, and\, C_{NH_3}$

A linear state estimator for the single state model based on NOx sensor feedback is then written as

$$\dot{\theta}_{est} = \vec{f}(C_{NO}, C_{NO_2}, \theta, C_{NH_3}, C_{NO,in}, C_{NO_2,in}, C_{NH_3,in}) + \vec{L}(C_{NO_x,meas} - C_{NO_x,est})$$

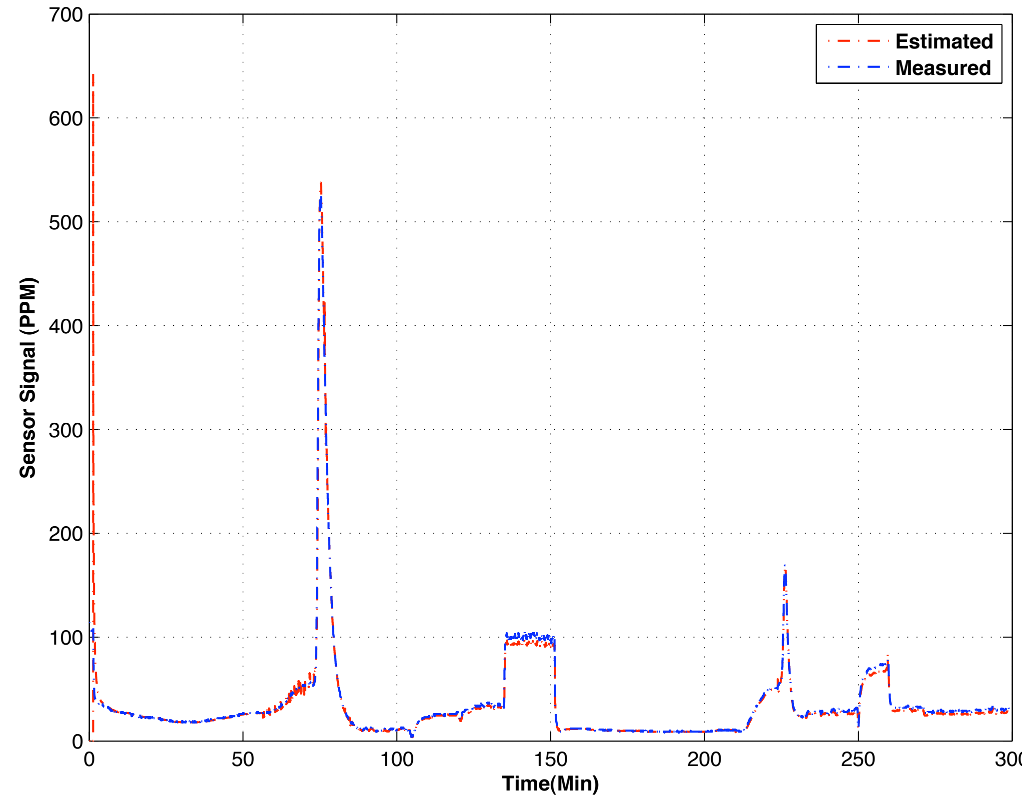
Here $C_{NO_x,meas}$ is the signal from the downstream NO_x sensor

Single State Estimator Validation with NOx Sensor Model



Estimator with NOx Sensor Model Validation Using Test Data

Using two catalysts in series, the estimator with the NOx sensor model is validated against the measured NOx sensor signal.



Estimator with NOx Sensor Model Validation Using Test Data

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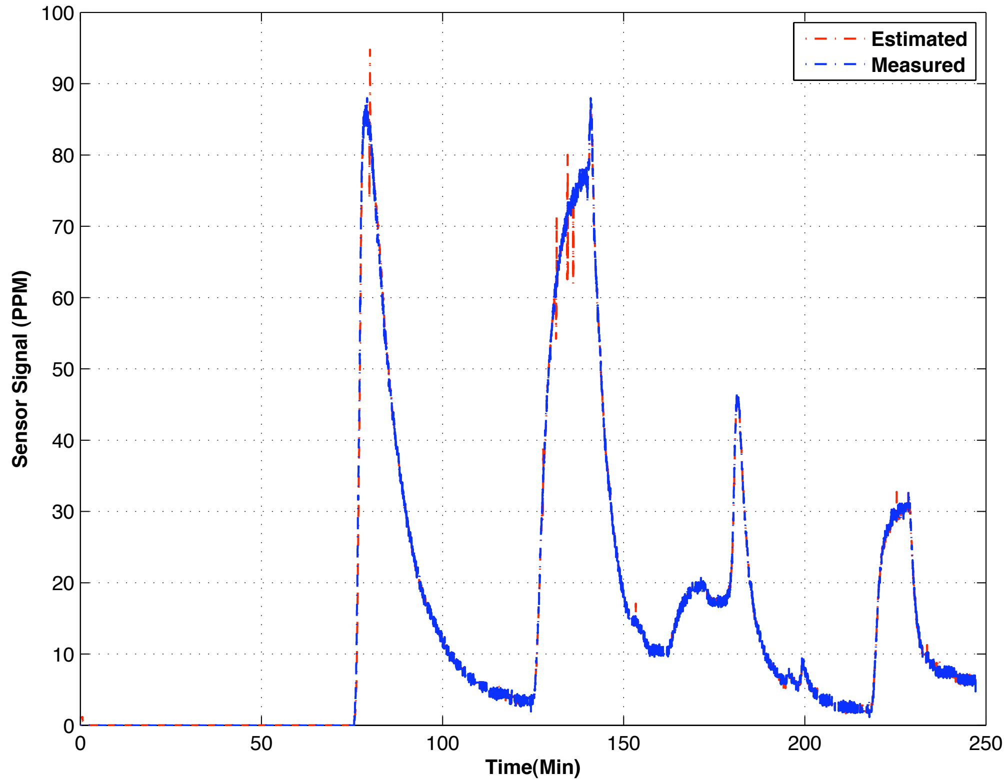
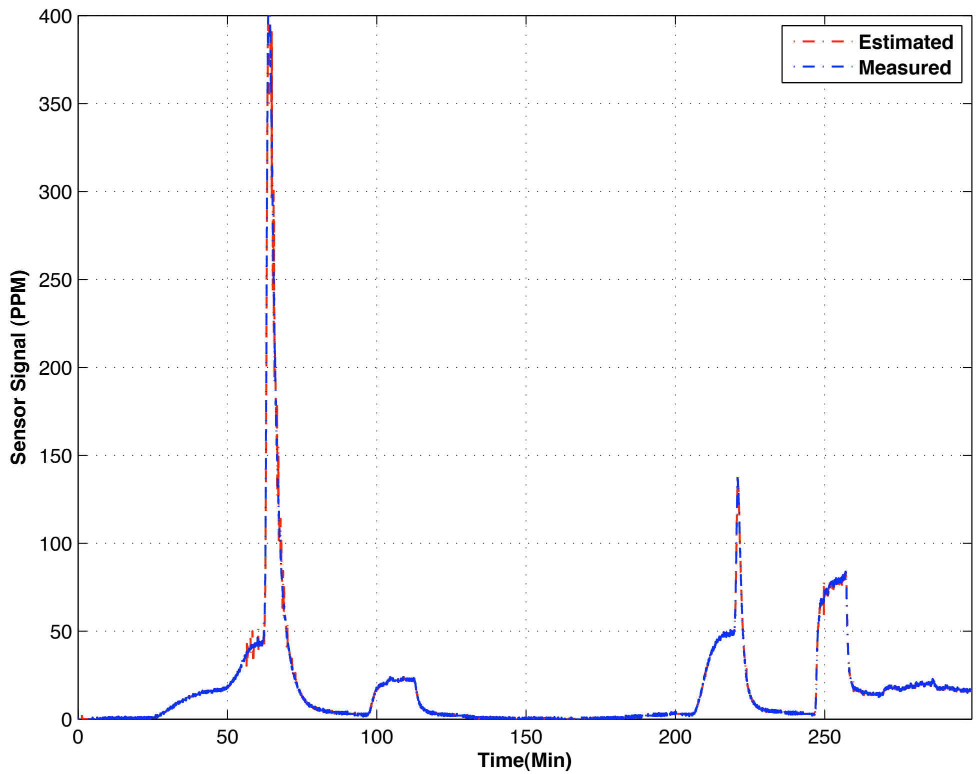


Using two catalysts in series, the estimator with the NH3 sensor model is validated against the measured NH3 sensor signal.



The NH3 sensor model is formulated as a function of alpha. $S_1 = A_3(\alpha) C_{\mathrm{NH_3}}$

A linear state estimator for the single state model based on NH3 sensor feedback is then written as

$$\dot{\theta}_{est} = \vec{f}(C_{\mathrm{NO}}, C_{\mathrm{NO_2}}, \theta_{est}, C_{\mathrm{NH_3}}, C_{\mathrm{NO},in}, C_{\mathrm{NO_2},in}, C_{\mathrm{NH_3},in}) + \vec{L}(C_{\mathrm{NH_3},meas} - C_{\mathrm{NH_3},est})$$

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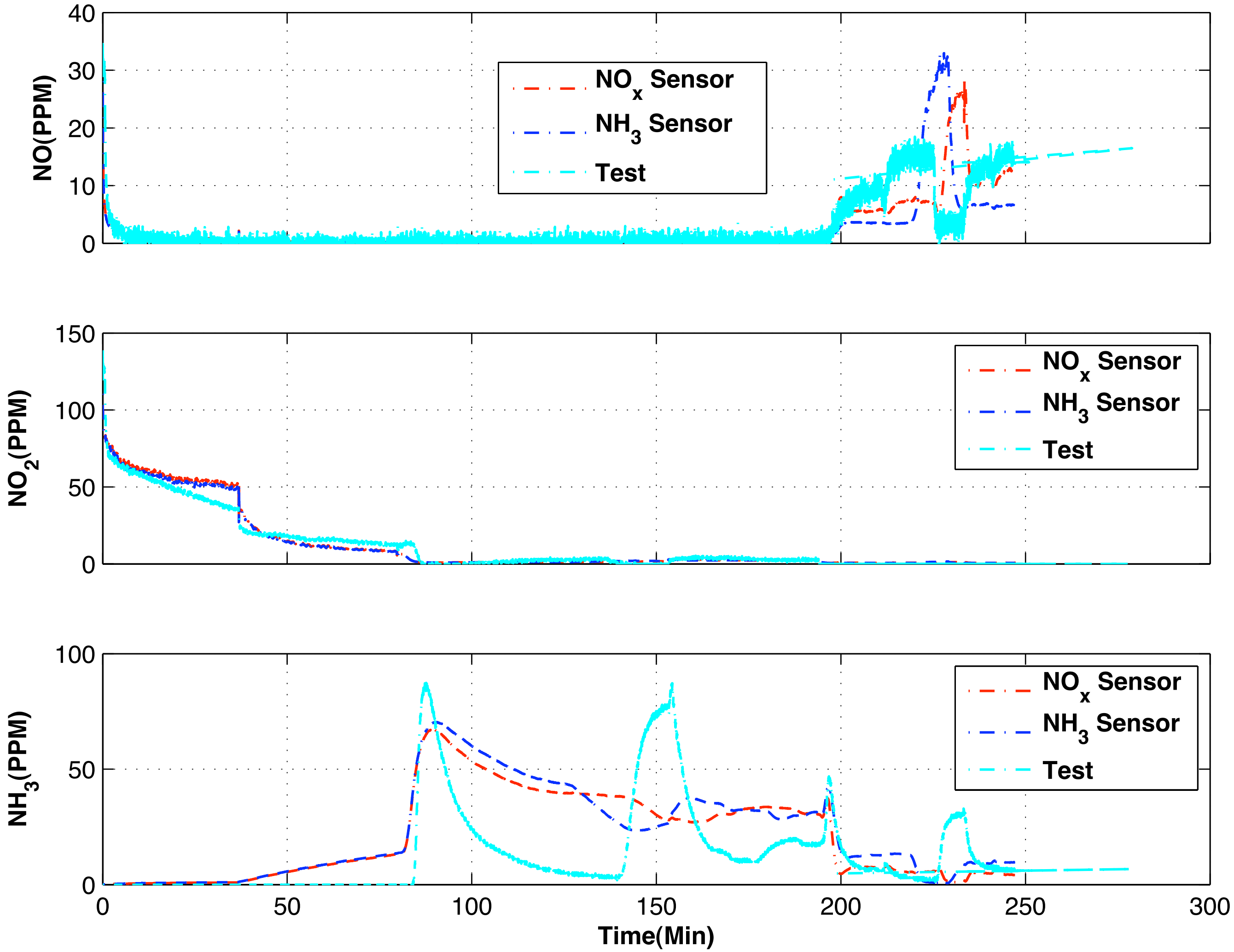


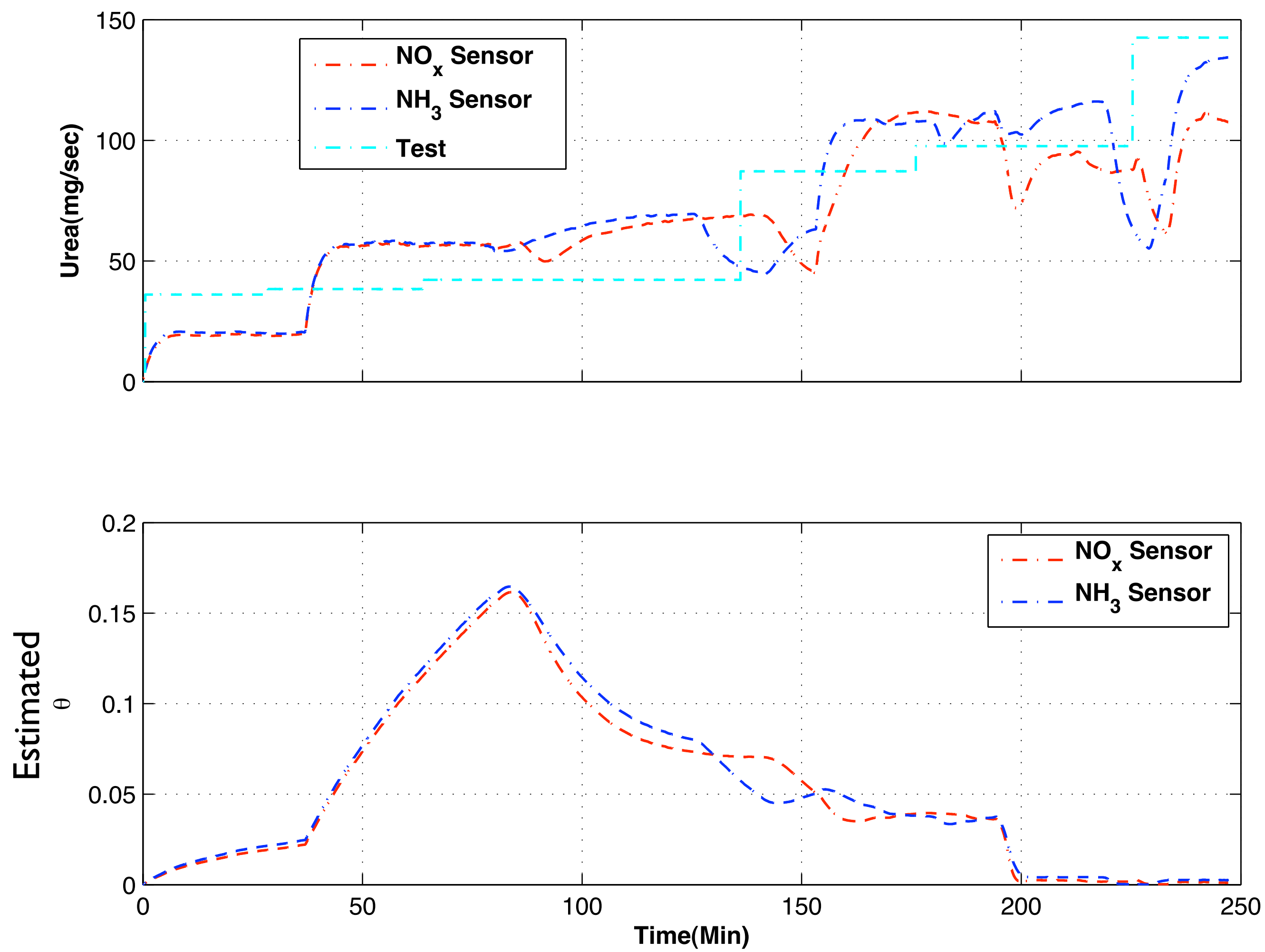
The control systems with the NOx and NH3 sensor models are compared.

Performance metrics in NOx index, urea index, urea usage and NH3 slip are defined and compared.

Strategy	NO_x Index	Urea Index	Urea	Total NH_3 Slip
Units	$\frac{gm\ of\ NO_x\ reacted}{gm\ of\ urea\ injected}$	$\frac{gm\ of\ urea\ reacted}{gm\ of\ urea\ injected}$	kg	kg
NO_x sensor based	0.42	0.27	0.99	0.0289
NH_3 sensor based	0.40	0.26	1.04	0.0315
% Change	4.7 ↑	4.7 ↑	5.3 ↓	9.1 ↓

Control Strategy Comparison Using Test Data

Control System Comparison Based on Sensor Models



Strategy	NO_x Index	Urea Index	Urea	Total NH_3 Slip
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NO_x sensor based	0.42	0.27	0.99	0.0289
NH_3 sensor based	0.40	0.26	1.04	0.0315
Test data	0.43	0.28	1.01	0.0162

- A simple NOx sensor model based on experimental data is developed and validated using various sets of test data. The sensor model is then tested in simulation using a single state model by considering two catalysts in series.
- An NH3 sensor assuming no cross-sensitivity towards NO and NO2 species is analyzed using linear systems theory for observability and controllability and analysis shows that the system based on NH3 sensor feedback is controllable and observable (proof not shown for conciseness, See reference)
- An interesting observation from the analysis is that the NH3 storage and urea injection flow rate from the strategy based on NH3 sensor match within 2-5% of those obtained from a strategy based on NOx sensor.
- One important conclusion from the analysis is that the NH3 sensor, from its simulation based performance, can be regarded as a potential candidate for SCR control applications in the absence of an accurate NOx sensor model.
- One interesting area for future research will be enhancement of sensor model performance at high urea injection rates and understanding the impact of other system variables on the sensor signal scattering and delays.

Ref: Devarakonda, Parker, Johnson, Strots and Santhanam., ASME Journal of Dynamic Systems, Measurement and Control (Submitted)

Questions