Axially Distributed NH3 Storage Estimation for a Control-Oriented SCR Model

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Control-Oriented Models

Why use real-time models?

- Control – Performance and robustness improvements
- On-Board Diagnostics (OBD) – Restrict diagnostics to run under desired system states
- Cost – sensor deletion → save money and OBD
- e.g. SCR
  - Control to an NH3 storage setpoint, not ANR
  - NH3 storage used as an entry condition
  - Feedgas NOx model for sensor deletion

Tradeoffs

- Models must be computationally efficient for real-time implementation while retaining a desired level of model fidelity
- Calibration complexity should be constrained and scalable to different applications with limited re-tuning
- Increased model complexity can provide new opportunities and/or additional challenges for control and diagnostics
- Models and/or the control system that employs them should be robust to sensor and actuator biases

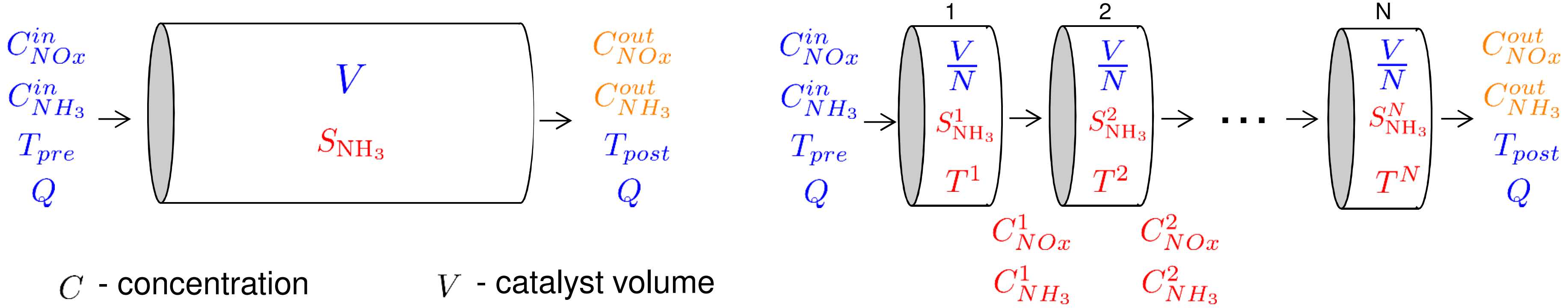
Control-Oriented SCR Model

Lumped parameter vs distributed model

- Lumped parameter model has been the standard but new requirements and system configurations may demand extensions. e.g. regulation, split brick system

Cost/Benefit considerations of an axially distributed control-oriented SCR model

- Improved model accuracy, particularly during periods with large temperature gradients. How much?
- Opportunity for axially distributed NH3 storage control
- Additional computational burden
- Thermal model required
- Robustness to sensor & actuator biases and mis-estimated NH3 storage distribution
    - Implications for NH3 storage observer?



Lumped Parameter (0D)

Axially Distributed (1D)

C - concentration
T - temperature
Q - volumetric flowrate

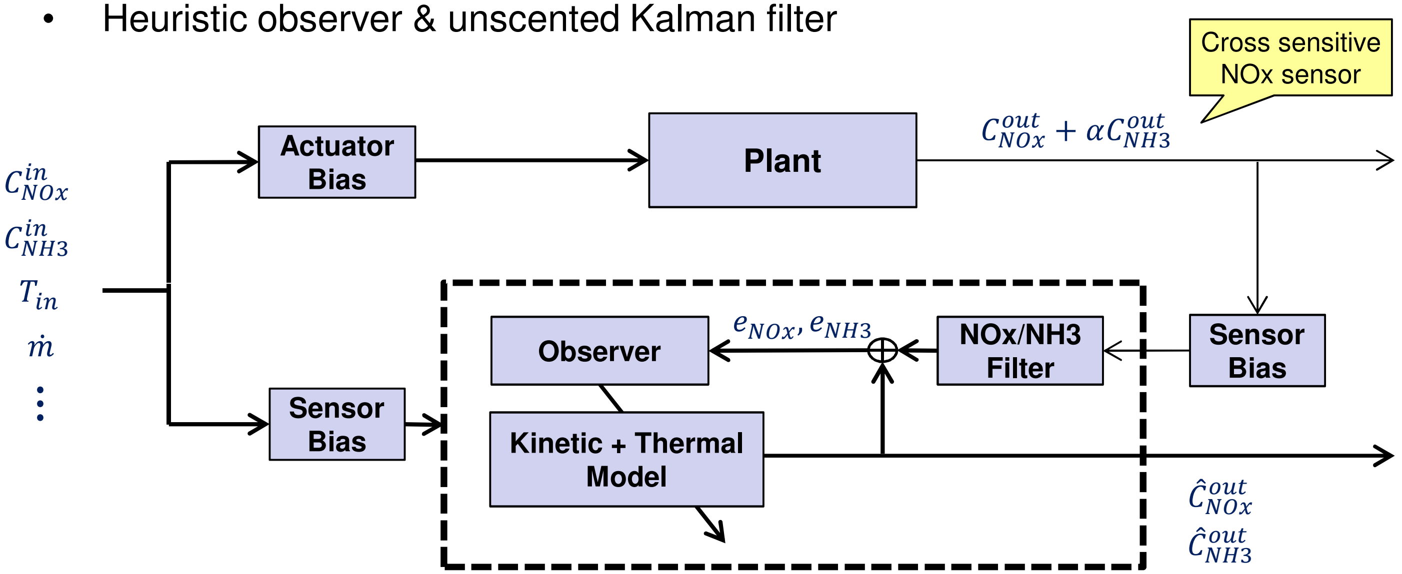
V - catalyst volume
S - stored species

🟦 Sensor / Actuator / Geometry
🟥 Model
🟨 Cross-sensitive sensor / Model

Distributed Storage Observer Study

Axially Distributed NH3 Storage Observer Summary:

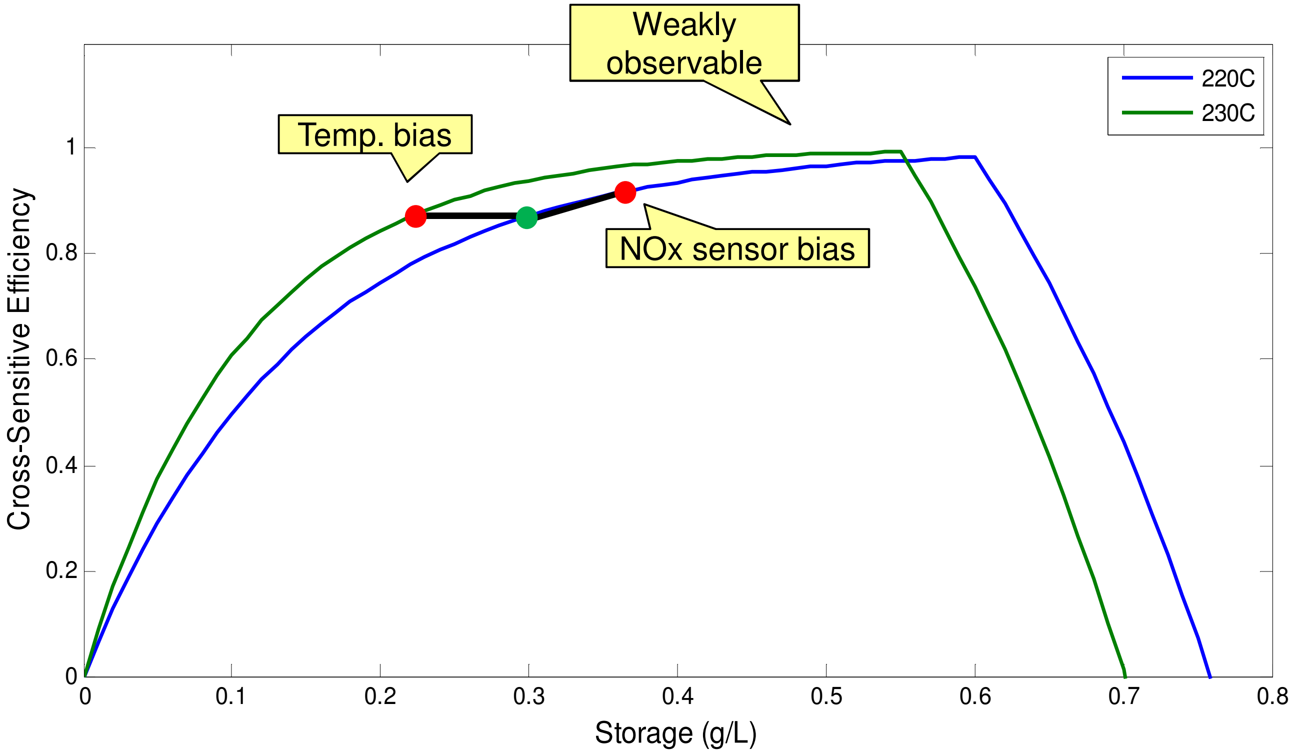
- Problem Definition
  - Correct the SCR control oriented model's distributed NH3 storage state based on NOx and NH3 slip errors
  - Error sources: Sensors/actuator biases, initial conditions, plant/model mismatch
- Simulation study
  - Comparison of plant and control models with actuator/sensor biases and initial condition errors imposed on the control model
  - Evaluation of the total and sub-element storage error with various observer designs
- Observer Design
  - Heuristic observer & unscented Kalman filter



Distributed Storage Observer Study

Note on observability:

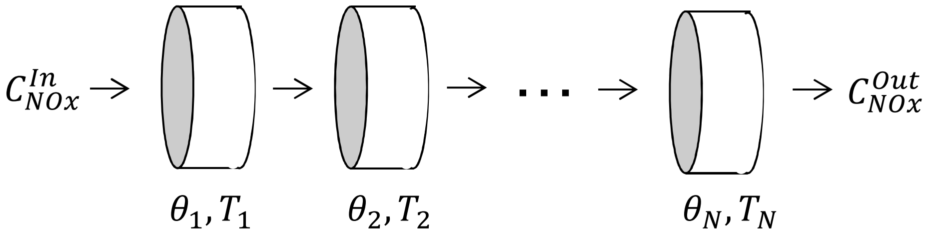
- The SCR often reaches unobservable or weakly observable states
- Small differences in the measured efficiency may indicate significantly different NH3 storage quantities
- → NH3 storage observer is sensitive to sensor and actuator biases



Distributed Observer Study – NOx Slip

What can be said about the NH3 storage distribution for a given NOx conversion efficiency?

- Modeled NOx reduction – standard SCR reaction, plug flow assumptions



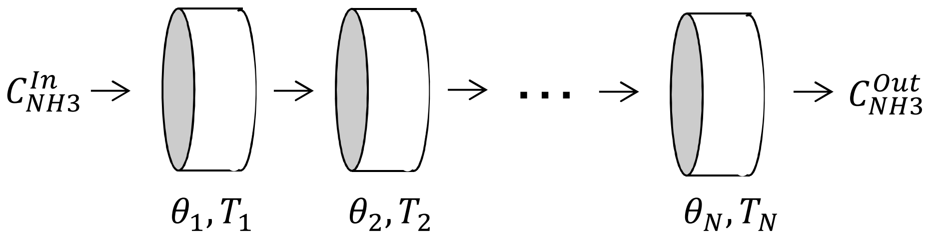
$$C_{NOx}^{Out} = C_{NOx}^{In} e^{-k_{red}\frac{1}{SV}\left(e^{\frac{-E_{red}}{RT_1}}\theta_1 + e^{\frac{-E_{red}}{RT_2}}\theta_2 + \cdots + e^{\frac{-E_{red}}{RT_N}}\theta_N\right)}$$

- NOx efficiency is underdetermined → Different storage distributions can yield the same efficiency
  - Isothermal case: The total NH3 storage determines efficiency, distribution is irrelevant
  - Some distribution information can be obtained in the non-isothermal case
    - e.g. Split brick system configuration
      - Brick 1 lights-off before brick 2 → measured NOx error isolated to brick 1

Distributed Observer Study – NH3 Slip

What can be said about the NH3 storage distribution given a certain level of NH3 slip?

- Modeled NH3 slip



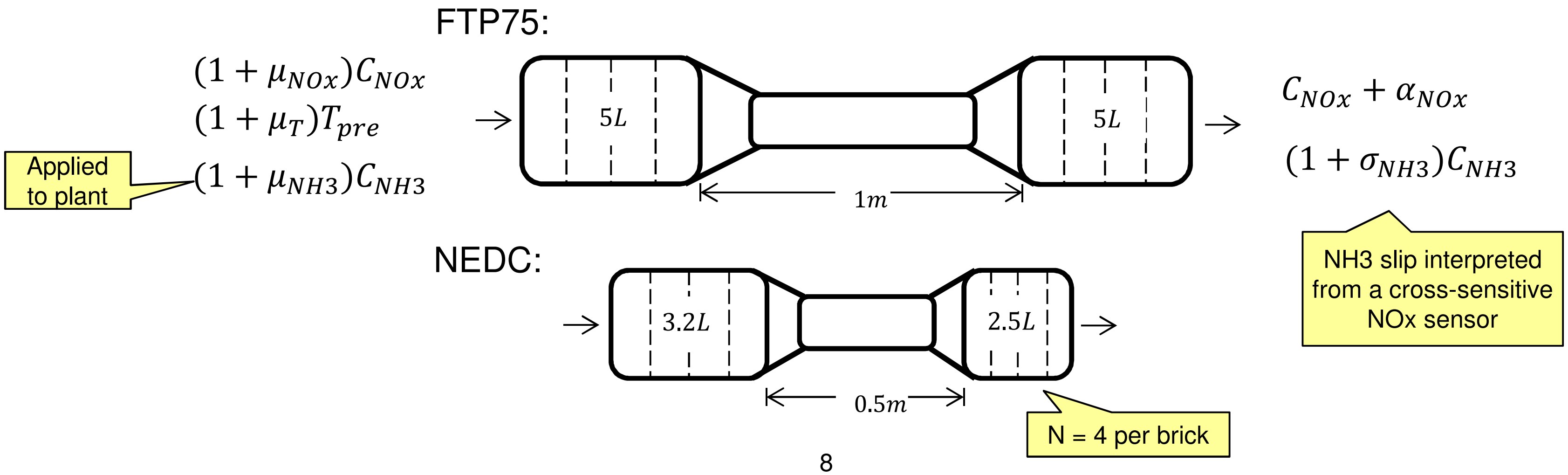
Single slice:

$$C_{NH3}^{i} = C_{NH3}^{i-1} e^{-k_{ads}(1-\theta_i)\frac{1}{SV}} + \frac{k_{des} e^{\frac{-E_{des}(1+\alpha\theta_i)}{RT_i}} \theta_i}{k_{ads}(1-\theta_i)} \left(1 - e^{-k_{ads}(1-\theta_i)\frac{1}{SV}}\right)$$

- For a multi-slice model, NH3 slip is a function of the storage location
  - Can show greater NH3 slip occurs from a back loaded model as compared to a front loaded model.
    - Isothermal with the same total storage
  - → Suggests back weighted observer gains

Simulation Setup

- Simulated plant and control model
  - Control model sees sensor biases (FG NOx mult., FG Temp mult., TP NOx add, TP NOx NH3 sensitivity)
  - Plant model sees actuator biases (FG NH3 mult.)
- FTP75 & NEDC drive cycles
  - Simulation inputs taken from vehicle data. NH3 input unchanged except by actuator bias
- Split brick system configuration
  - FTP75: 5L brick 1, Pipe = 1m, 5L brick 2
  - NEDC: 3.3L brick 1, Pipe = .5m, 2.5L brick 2
- Repeated cycles to see long term error propagation and observer effects
  - 8x starting from 0g initial storage
  - 2x starting from high initial storage



Applied to plant

NH3 slip interpreted from a cross-sensitive NOx sensor

N = 4 per brick

NH3 Storage Estimation Details

Two Approaches:

- Heuristic Observer
  - The observer gains are designed based on insights into the system dynamics

Plant

$$\dot{x} = f(x,u) + d$$
$$y = h(x,u) + n$$

Control Model

$$\dot{\hat{x}} = f(\hat{x},u) - L(\hat{x},u)(\tilde{y} - \hat{y})$$
$$\hat{y} = h(\hat{x},u)$$

$$x = \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_N \end{bmatrix} \qquad u = \begin{bmatrix} C_{NOx}^{In} \\ C_{NH3}^{In} \\ T_{in} \\ \vdots \end{bmatrix} \qquad y = \begin{bmatrix} C_{NOx}^{Out} \\ C_{NH3}^{Out} \end{bmatrix}$$

$\tilde{y} =$ Filtered from NOx sensor

$$L(\hat{x},u) = \begin{bmatrix} g_1 & g_2 & \cdots & g_N \\ k_1 & k_2 & \cdots & k_N \end{bmatrix}^T$$

NOx gains

NH3 gains

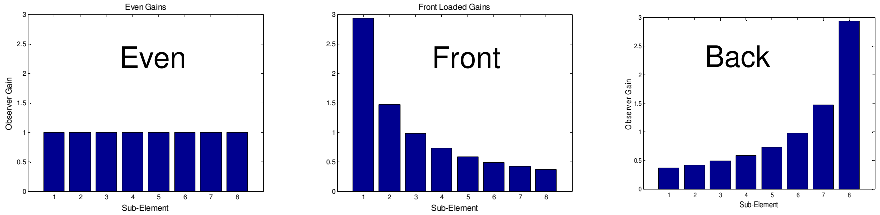
- Unscented Kalman Filter
  - Kalman filter for nonlinear systems, 2 stages at every time step
    1. State and state covariance propagation through the nonlinear model (2N+1 points)
    2. State and state covariance update with a new measurement
  - Temperature and biases added to state estimation

$$x_{aug} = \begin{bmatrix} m_1 \\ T_1 \\ \vdots \\ m_N \\ T_N \\ \beta \end{bmatrix} \qquad \beta = \begin{bmatrix} \mu_{NOx} \\ \mu_{NH3} \\ \mu_T \\ \alpha_{NOx} \\ \sigma_{NH3} \end{bmatrix}$$

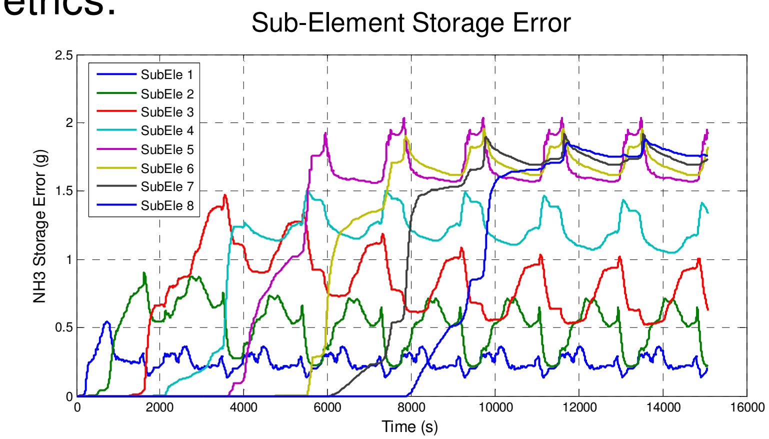
Observer Study

Investigated parameters:

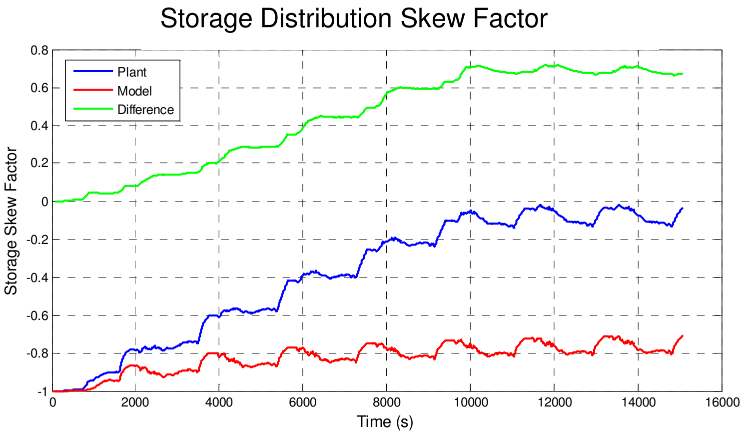
- Overall NOx and NH3 gains
- Sub-element gain distributions
    - e.g. front vs. back weighting
    - Heuristic observer vs. Kalman filter
- Static vs. dynamic gains
    - NOx gains mainly a function of temperature
- Entry conditions
    - NOx/NH3 filter confidence, temperature range etc.



Metrics:



Sub-element RMS error = 1.0 g



$$Skew = 2\frac{[0\!:N-1].*\,[\,m_2\ \ldots\ m_N]}{m_{Tot} * (N-1)} - 1$$

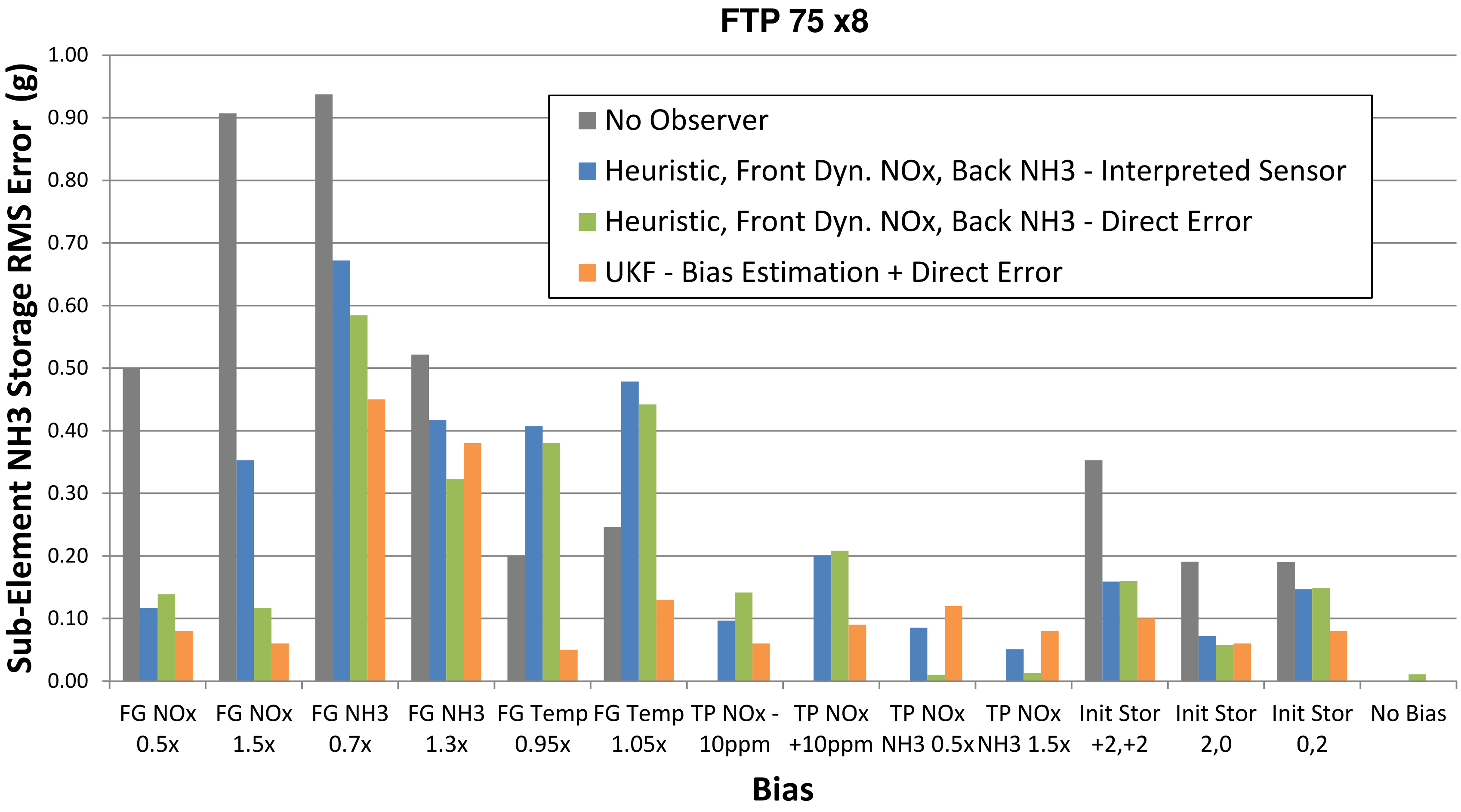
All NH3 stored on first sub-element

$$-1 \le Skew \le 1$$

All NH3 stored on last sub-element

Results

- **Heuristic Observer**
  - Front weighted, dynamic NOx gains
  - Back weighted NH3 gains



Bias Estimation

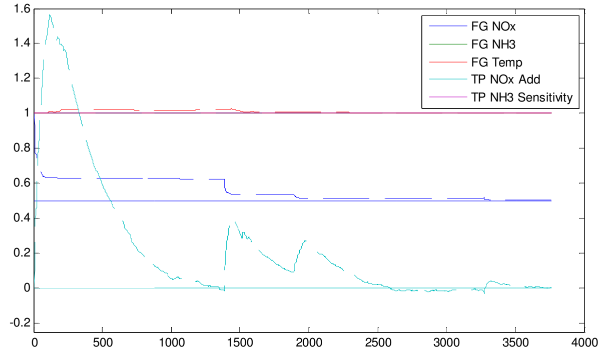
Ex) Bias Estimation w/ Kalman Filter

- FTP75 x2
- NOx and NH3 outputs directly from plant (no interpreted species)
- White noise added to the output

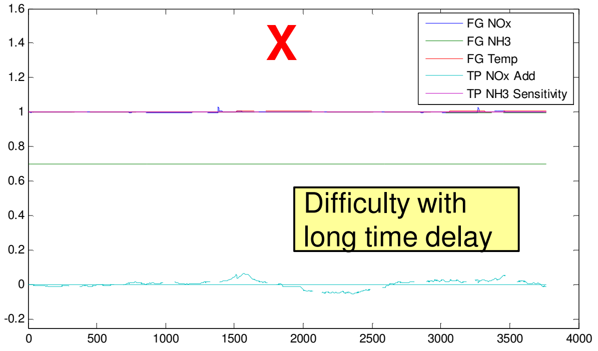
Solid line – Actual Bias
Dashed line – Estimated Bias

Bias Estimation

0.5x FG NOx

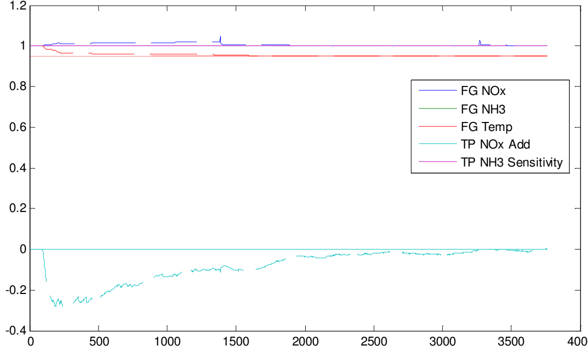


0.7x FG NH3

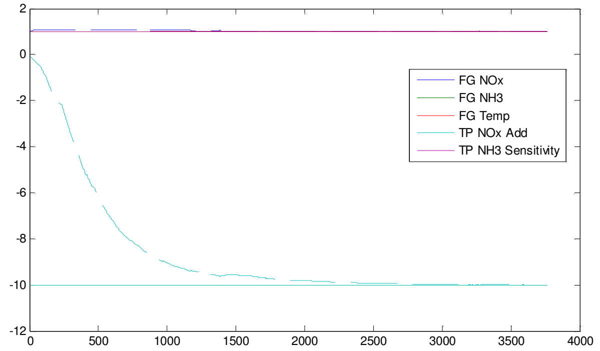


Difficulty with long time delay

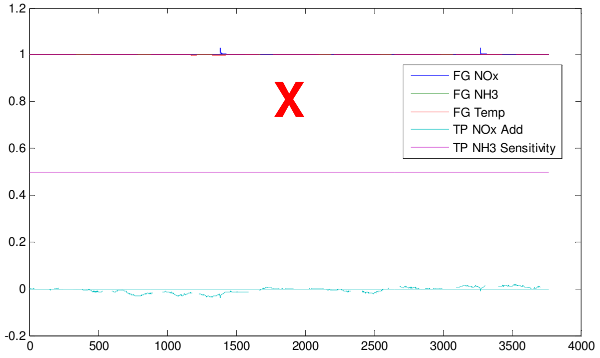
0.95x FG Temp



-10 PPM TP NOx



0.5x TP NH3 Sensitivity



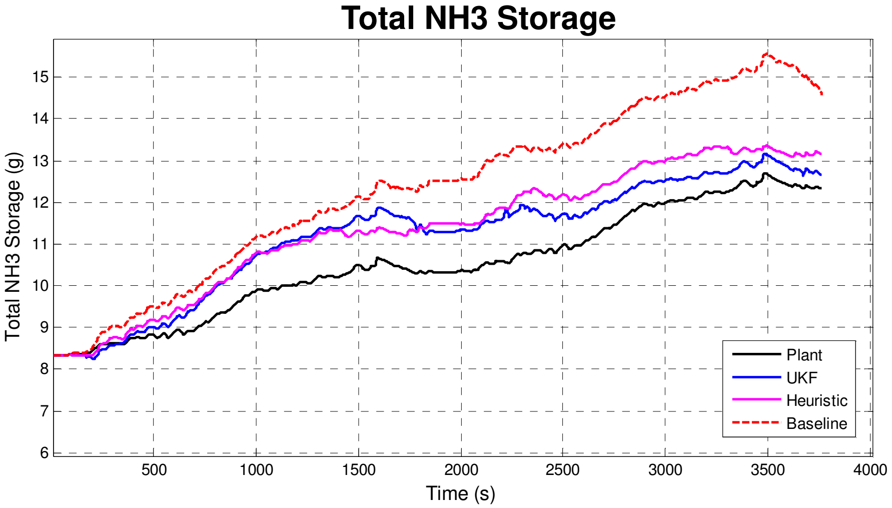
FG NH3 and TP NH3 biases do not converge. TP NH3 bias gain is artificially reduced due to unstable behavior

Observer Gain Distribution

Ex) **0.5x FG NOx Bias**

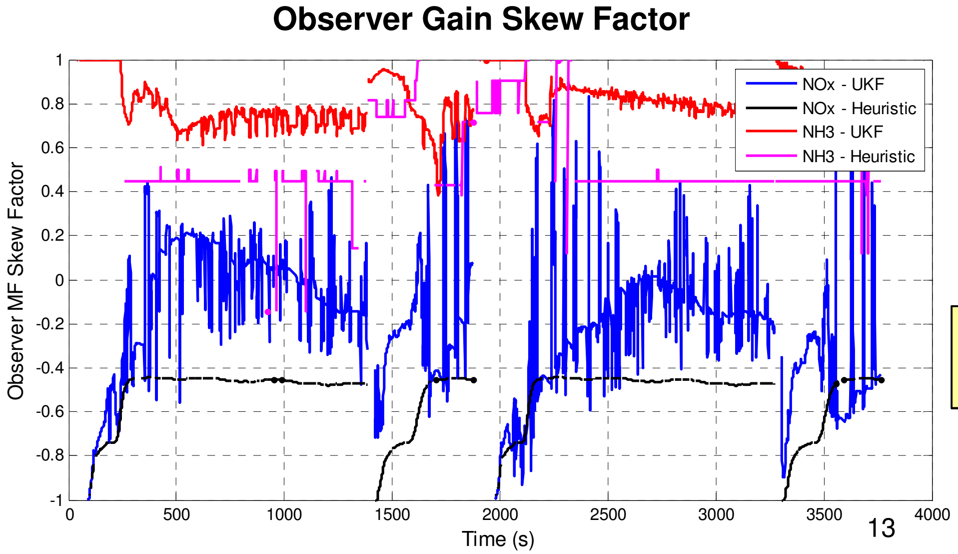
- FTP75 x2
- NOx and NH3 outputs directly from plant (no interpreted species)

Total NH3 Storage



Similar gain distributions for the best heuristic observer and UKF

Observer Gain Skew Factor



$$Skew = 2\frac{[0:N-1]*[|g_1| \ \ldots \ |g_N|]'}{\sum|g|*(N-1)} - 1$$

Gain on first sub-element only

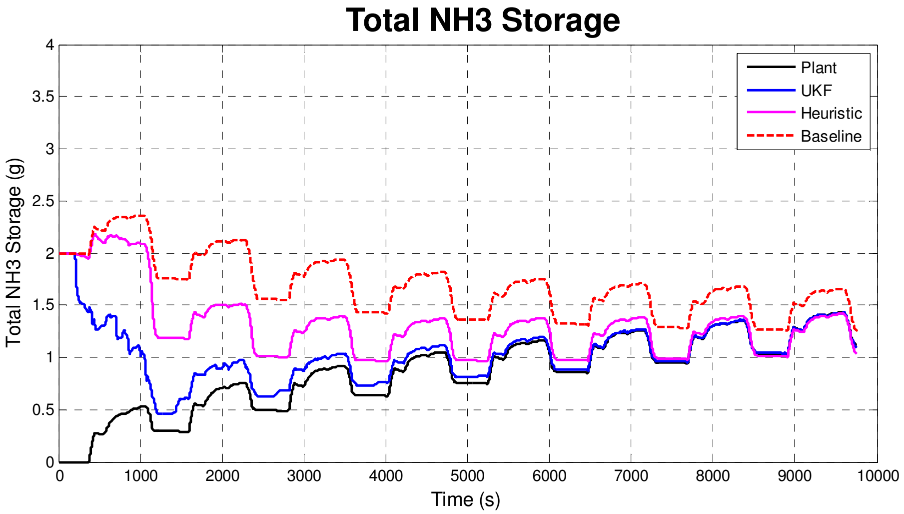
$$-1 \leq Skew \leq 1$$

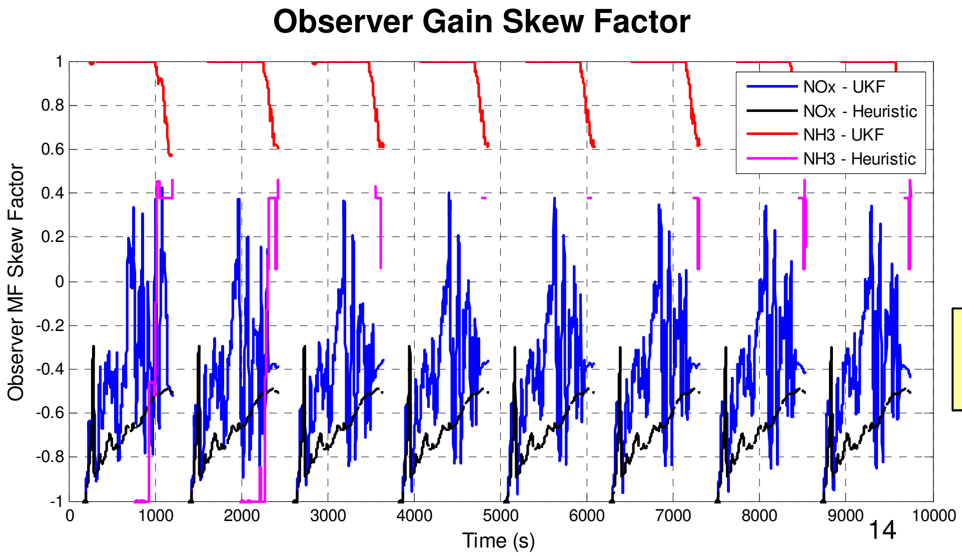
Gain on last sub-element only

Observer Gain Distribution

Ex) **+1g, +1g Initial Storage Bias**

- NEDC x8
- NOx and NH3 outputs directly from plant (no interpreted species)





$$Skew = 2\frac{[0\!:N-1] * [|g_1| \; \dots \; |g_N|]'}{\sum |g| * (N-1)} - 1$$

$$-1 \le Skew \le 1$$

Gain on first sub-element only

Gain on last sub-element only

Conclusions

- Many factors must be considered when designing control-oriented models
  - A new NH3 storage observer must be designed for the axially distributed SCR model. Carry over of the lumped parameter observer can do more harm than good (increase NH3 storage estimation errors) when considering biases and sensor limitations
  - Plant/model mismatch (piece to piece variation and aging) should be considered in addition to sensor & actuator biases

- Simplified approaches should be used wherever possible due to the computational and memory constraints of a real-time model
  - The heuristic observer can achieve comparable performance to the more complex unscented Kalman filter
  - Combining bias estimation with the heuristic observer may lead to further improvements