Notes on SCR-OBD algorithm developement

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October 18, 2023

Contents

1 Introduction

Goal:

"Developing model-based non-intrusive diagnostics for SCR-ASC that can work with commercial NO-x sensors and demonstrate the results on a real-world on-road truck data."

Kaushal's work:

- Diagonstic-oriented aging models for SCR-ASC.
  - Chemical Kinetics based model for SCR
  - Non-linear look-up table for ASC
- Term-by-term observer design for SCR Ammonia adsorption.
- Diagnosis algorithm
  - Sequence of filters
  - Residual generation for fault detection using the stochastic version of the models.

1.1 Available measurements

1. Engine Torque
2. Engine Speed
3. Diesel exhaust fluid (DEF) injection
4. Engine-out NO_x.
5. Diesel oxidation catalyst (DOC)-out NO_x.
6. Tail-pipe NO_x. (Test cell: NH_3 and N_2O)
7. DOC-in, DOC-out, SCR-in, SCR-out and ASC-out temperatures.
8. Exhaust flow rate.

1.2 Available data

1. Road data
   - Cold FTP (Federal Test Procedure)
   - Hot FTP
   - RMC (Ramped mode cycle)
2. Test Cell data
   - Cold FTP (Federal Test Procedure)
   - Hot FTP
   - RMC (Ramped mode cycle)

2 SCR-ASC Reactions and Dynamics

The SCR reactions involve reduction of NO_x into N_2 and H_2O [1].

2.1 SCR-ASC Reactions

Eley Rideal reaction mechanism [2] [3], [4] is considered for the interpreting the SCR reactions. The mechanism involves the following reactions:

$$NH_2 - CO - NH_2(liquid) \longrightarrow NH_2 - CO - NH_2^* + xH_2O \quad \text{[AdBlue evaporation]} \quad (1)$$

$$NH_2 - CO - NH_2^* \longrightarrow HNCO + NH_3 \quad \text{[Urea decomposition]} \quad (2)$$

$$HNCO + H_2O \longrightarrow NH_3 + CO_2 \quad \text{[Isocynic acid hydrolysis]} \quad (3)$$

$$NH_3 + \theta_{free} \longleftrightarrow NH_3(ads) \quad \text{[Adsorption/Desorption]} \quad (4)$$

$$4NH_3(ads) + 4NO + O_2 \longrightarrow 4N_2 + 6H_2O \quad \text{[Standard SCR reaction]} \quad (5)$$

$$2NH_3(ads) + NO + NO_2 \longrightarrow 2N_2 + 3H_2O \quad \text{[Fast SCR reaction]} \quad (6)$$

$$4NH_3(ads) + 3NO_2 \longrightarrow 3.5N_2 + 6H_2O \quad \text{[Slow SCR reaction]} \quad (7)$$

$$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O \quad \text{[AMOX with/without ASC]} \quad (8)$$

$$4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O \quad \text{[AMOX with/without ASC]} \quad (9)$$

$$2NH_3 + 2O_2 \longrightarrow N_2O + 3H_2O \quad \text{[AMOX with/without ASC]} \quad (10)$$

$$2NO + O_2 \longrightarrow 2NO_2 \quad \text{[NO oxidation]} \quad (11)$$

The PDE model for SCR reaction kinematics [4] is reduced to ODE model [5] using by assuming "continuous stirred tank reactor (CSTR)" model (Control volume approach).

2.2 Ammonia input (Urea Dosing) dynamics

The actual input to the system is urea from AdBlue (32.5% aqueous urea solution) injection that converted to ammonia (through reactions: (1), (2) and (3)). This can be modelled by the following eqation [4]:

$$\dot{C}_{NH_3,in} = -\frac{1}{\tau} C_{NH_3,in} + 2\frac{1}{\tau}\frac{\eta u_{Adblue}}{N_{urea} F}$$

where,

τ – Time constant

u_{AdBlue} – Mass injection rate of the AdBlue solution

η – Mass fraction of urea in the solution

N_{urea} – Atomic number of urea

F – Exhaust flow rate of the catalyst m^3/s

The above model is re-parametrized as follows:

$$\dot{C}_{NH_3,in} = \frac{1}{\tau}\left(-C_{NH_3,in} + \eta_{urea} C_{NH_3,ideal}\right)$$

where,

η_{urea} – urea $\rightarrow NH_3$ conversion efficiency

τ – urea $\rightarrow NH_3$ time-constant

$C_{NH_3,ideal}$ – ideal $C_{NH_3,in}$ if $\eta_{urea} = 1$ (constant parameter obtained through calibration)

In the present work, $C_{NH_3,in}$ is considered as the input instead of AdBlue injection as its dynamics are completely decoupled from that of other states. Further, it is observed that AdBlue is completely converted to Ammonia at the very upstream part of the SCR catalyst [2].

2.3 4 State Dynamic Model

A four state nonlinear model for the above reactions can be developed using Arrhenius equations, CSTR assumption and further simplification based on the following assumptions:

2.3.1 Assumptions

1. Slow SCR reaction is neglected.
   - The flow rate of the exhaust would ensure that the not a significant concentration of tail-pipe exhaust components are due to the slow SCR reaction [4].
2. Mass transfer is neglected. That means the chemical kinetics in the catalyst are reaction controlled.
   - The standard SCR reaction rate is faster than the flow rate of the exhaust fluids.
3. Nitrogen selectivity for ammonia oxidation is 100%.
   - This assumption is relaxed by including algebraic relationship between selectivity and the temperature (ASC model [1]).
4. Reaction rates are assumed to be a function of the gas phase concentration of NO_x and ammonia storage.

2.3.2 Reaction Rates

The reaction rates for the processes being considered are modelled using Arrhenius equations as follows:

1. Standard SCR Reaction (5): $R_1 = \underbrace{k_1 \exp\left(-\frac{E_1}{RT}\right)}_{r_1} C_{NO} C_{O_2} \theta \Theta V^2$
2. Fast SCR Reaction (6): $R_2 = k_2 \exp\left(-\frac{E_2}{RT}\right) C_{NO} C_{N_2O} \theta \Theta V^2$
3. Ammonia Oxidation (8): $R_3 = \underbrace{k_3 \exp\left(-\frac{E_3}{RT}\right)}_{r_3} C_{O_2} \theta \Theta V$
4. Ammonia Adsorption/Desorption (4):
   (a) Forward: $R_{4F} = \underbrace{k_{4F} \exp\left(-\frac{E_{4F}}{RT}\right)}_{r_{4F}} C_{NH_3} (1-\theta) \Theta V$
   (b) Reverse: $R_{4R} = \underbrace{k_{4R} \exp\left(-\frac{E_{4R}}{RT}\right)}_{r_{4R}} \Theta V$
5. NO oxidation (11): $R_5 = \underbrace{k_5 \exp\left(-\frac{E_5}{RT}\right)}_{r_5} C_{NO} C_{O_2} V^2$

Where,

$\theta -$ NH_3 storage capacity fraction in SCR $= \dfrac{\text{Moles of } NH_3 \text{ adsorbed}}{\text{Total moles of } NH_3 \text{ that can be adsorbed}}$

$\Theta -$ Ammonia storage capacity$(moles)$

$\Theta = S_1 e^{S_2 T}$ $\quad S_1, S_2$ $-$ Aging parameters of the catalyst (positve constants)

$E_i -$ Activation Energy of i^{th} reaction

$k_i -$ Pre-exponential factor

$R -$ Universal gas constant

$T -$ Temperature

$C_{\{\bullet\}} -$ Concentration $\left(mol/m^3\right)$

$V -$ Volume of the exhaust gas in the substrate[6] $\left(m^3\right)$

$V_e = \epsilon A_c L_{cat}$

A_c – Open frontal area of the catalyst
L_{cat} – Length of the catalyst
ϵ – Void fraction

2.3.3 Dynamic model

Using above assumptions and definitions, we have the dynamic model [4]:

$$\begin{bmatrix} \dot{C}_{NO} \\ \dot{C}_{NO_2} \\ \dot{C}_{NH_3} \\ \dot{\theta}_{NH_3} \end{bmatrix} = \begin{bmatrix} -r_1 C_{NO} C_{O_2} \theta_{NH_3} \Theta V - 0.5 r_2 C_{NO} C_{NO_2} \theta_{NH_3} \Theta V - r_5 C_{NO} C_{O_2} V - b C_{NO} \\ -0.5 r_2 C_{NO} C_{NO_2} \theta_{NH_3} \Theta V + r_5 C_{NO} C_{O_2} V - b C_{NO_2} \\ -C_{NH_3} \left[\Theta r_{rF} \left(1 - \theta_{NH_3}\right) + b\right] + V^{-1} r_{4R} \Theta \theta_{NH_3} \\ -\theta_{NH_3} \left(r_{4F} C_{NH_3} V + r_3 C_{O_2} V + r_{4R} + r_1 C_{NO} C_{O_2} V^2 + r_2 C_{NO} C_{NO_2} V^2\right) + r_{4F} C_{NH_3} V \end{bmatrix} + b \begin{bmatrix} C_{NO,in} \\ C_{NO_2,in} \\ C_{NH_3} \\ 0 \end{bmatrix} \tag{12}$$

Where,

$$b = \frac{F}{V}$$

2.4 3 state dynamic model

2.4.1 Assumptions

The following are the additional assumptions along with the assumptions of 4-state model that are used to arrive at the three-state dynamic model[6]:

1. Only the standard SCR reaction is considered.
2. All NO_x in the exhaust gas is assumed to be NO.
   - The commercially available NO_x sensor (Horiba gas analyzer [4]) cannot differentiate between NO and NO_2.

The above two assumptions result in the following:

$$C_{NO_2} = 0 \qquad C_{NO_2,in} = 0$$
$$r_5 = 0$$

2.4.2 Dynamic Model

Including the above assumptions in the 4-state dynamic model (12):

$$\begin{bmatrix}\dot{C}_{NO}\\ \dot{C}_{NH_3}\\ \dot{\theta}_{NH_3}\end{bmatrix} = \begin{bmatrix}-r_1 C_{NO} C_{O_2} \theta_{NH_3} \Theta V - b C_{NO}\\ -C_{NH_3}\left[\Theta r_{rF}\left(1-\theta_{NH_3}\right)+b\right] + V^{-1} r_{4R} \Theta \theta_{NH_3}\\ -\theta_{NH_3}\left(r_{4F} C_{NH_3} V + r_3 C_{O_2} V + r_{4R} + r_1 C_{NO} C_{O_2} V^2\right) + r_{4F} C_{NH_3} V\end{bmatrix} + b\begin{bmatrix}C_{NO,in}\\ C_{NH_3,in}\\ 0\end{bmatrix} \quad (13)$$

The following parameters are defined for convenience:

$$p_1 = r_1 C_{O_2} V \quad p_2 = \tfrac{r_{4R}}{V} \quad p_3 = r_{4F} V \quad p_4 = r_3 C_{O_2} V \quad p_5 = r_1 C_{O_2} V^2$$

$$\begin{bmatrix}\dot{C}_{NO}\\ \dot{C}_{NH_3}\\ \dot{\theta}_{NH_3}\end{bmatrix} = \begin{bmatrix}-p_1 C_{NO} \theta_{NH_3} \Theta - b C_{NO}\\ -C_{NH_3}\left(\Theta r_{4F} + b\right) + r_{4F} \Theta C_{NH_3} \theta_{NH_3} + p_2 \Theta \theta_{NH_3}\\ -p_3 C_{NH_3} \theta_{NH_3} - \left(p_4 + r_{4R}\right)\theta_{NH_3} - p_5 C_{NO} \theta_{NH_3} + p_3 C_{NH_3}\end{bmatrix} + b\begin{bmatrix}C_{NO,in}\\ C_{NH_3,in}\\ 0\end{bmatrix}$$

Defining the following coefficients of product of states and states:

Coefficients of product of states:

	C_{NO}	C_{NH_3}	θ_{NH_3}
C_{NO}		f_{12}	
C_{NH_3}			f_{23}
θ_{NH_3}	f_{31}	f_{32}	

Coefficients of states:

	C_{NO}	C_{NH_3}	θ_{NH_3}
C_{NO}	g_1		
C_{NH_3}		g_2	g_{23}
θ_{NH_3}		g_{32}	g_3

$$\begin{aligned} f_{12} &= p_1\Theta = r_1 C_{O_2} V \Theta \\ f_{23} &= r_{4F}\Theta \\ f_{32} &= p_3 = r_{4F} V \\ f_{31} &= p_5 = r_1 C_{O_2} V^2 \end{aligned} \qquad \begin{aligned} g_1 &= b \\ g_2 &= (\Theta r_{4F} + b) \\ g_3 &= p_4 + r_{4R} = r_3 C_{O_2} V + r_{4R} \\ g_{23} &= p_2\Theta = \tfrac{r_{4R}}{V}\Theta \\ g_{32} &= p_3 = r_{4F} V \end{aligned}$$

$$\begin{bmatrix}\dot{C}_{NO}\\ \dot{C}_{NH_3}\\ \dot{\theta}_{NH_3}\end{bmatrix} = \begin{bmatrix}-f_{12} C_{NO} \theta_{NH_3} - g_1 C_{NO}\\ -g_2 C_{NH_3} + f_{23} C_{NH_3} \theta_{NH_3} + g_{23} \theta_{NH_3}\\ -f_{32} C_{NH_3} \theta_{NH_3} - g_3 \theta_{NH_3} - f_{31} C_{NO} \theta_{NH_3} + g_{32} C_{NH_3}\end{bmatrix} + b\begin{bmatrix}C_{NO,in}\\ C_{NH_3,in}\\ 0\end{bmatrix}$$

Let,

$$\begin{aligned} x_1 &= C_{NO} & u_1 &= C_{NO,in} \\ x_2 &= C_{NH_3} & u_2 &= C_{NH_3,in} \\ x_3 &= \theta_{NH_3} \end{aligned}$$

$$\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\\ \dot{x}_3\end{bmatrix} = \begin{bmatrix}-f_{12} x_1 x_3 - g_1 x_1\\ -g_2 x_2 + f_{23} x_2 x_3 + g_{23} x_3\\ -f_{32} x_2 x_3 - g_3 x_3 - f_{31} x_1 x_3 + g_{32} x_2\end{bmatrix} + b\begin{bmatrix}u_1\\ u_2\\ 0\end{bmatrix} \quad (14)$$

2.4.3 Small Perturbation model

We have the small-perturbation model from eqn. 14:

$$\begin{bmatrix}\delta\dot{x}_1\\ \delta\dot{x}_2\\ \delta\dot{x}_3\end{bmatrix} = \begin{bmatrix}-\left(g_1 + f_{12} x_{30}\right) & 0 & -f_{12} x_{10}\\ 0 & -\left(g_2 - f_{23} x_{30}\right) & \left(f_{23} x_{20} + g_{23}\right)\\ -f_{31} x_{30} & g_{32} - f_{32} x_{30} & -f_{32} x_{20} - g_3 - f_{31} x_{10}\end{bmatrix}\begin{bmatrix}\delta x_1\\ \delta x_2\\ \delta x_3\end{bmatrix} + b\begin{bmatrix}\delta u_1\\ \delta u_2\\ 0\end{bmatrix} \quad (15)$$

3 Sensor corss-sensitivity and non-linear control from of the model

The NO_x sensor is cross-sensitive to ammonia, resulting in the following measurement model (output) of the system:

$$y = C_{NO} + \chi C_{NH_3}$$

We have the non-linear state-space model form eqn. (14):

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -f_{12}x_1x_3 - g_1x_1 \\ -g_2x_2 + f_{23}x_2x_3 + g_{23}x_3 \\ -f_{32}x_2x_3 - g_3x_3 - f_{31}x_1x_3 + g_{32}x_2 \end{bmatrix} + b \begin{bmatrix} u_1 \\ u_2 \\ 0 \end{bmatrix} \tag{16}$$

$$y = x_1 + \chi x_2 \tag{17}$$

4 Timescale separation

$$r_{rF} << r_i \implies r_{4F} = \varepsilon r_0$$

$$\implies \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} f_1(x_1, x_3) \\ f_2(x_2, x_3, \varepsilon) \\ \varepsilon f_3(x_1, x_2, x_3, \varepsilon) \end{bmatrix} + b \begin{bmatrix} u_1 \\ u_2 \\ 0 \end{bmatrix}$$

Using Averaging method:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} f_1(x_1, x_2, M_{NH_3^*}) \\ f_2(x_1, x_2, M_{NH_3^*}) \end{bmatrix} + b \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

5 Catalyst aging factor

We have the ammonia storage capacity of the catalyst:

$$\Theta = S_1 e^{-S_2 T}$$

The parameters S_1 and S_2 change with age effecting the storage capacity at a given temperature.

Assumption: The aged catalyst results in small changes in S_1, S_2.

The above assumption is valid if the catalyst's operating range is limited to a small range of storage capacity.

Using small perturbation,

$$\delta\Theta = \left(\frac{\delta S_1}{S_1} - \delta S_2 T\right) S_1 e^{-S_2 T}$$

$$\implies \Theta_{aged} = \Theta + \delta\Theta = \left(1 + \frac{\delta S_1}{S_1} - \delta S_2 T\right) S_1 e^{-S_2 T}$$

Let,

$$a(T) = 1 + \frac{\delta S_1}{S_1} - \delta S_2 T = a_1 + a_2 T$$

Thus, a is the factor by which the storage capacity is reduced due to the catalyst's aging. Hence, for optimal performance:

$$a > a_{min} \quad \forall T \in [T_{min}, T_{max}]$$

Note: The above definition is consistent with that of the literature [7]. The major difference lies in its derivation and assumptions. Also, [7] considers aging factor as temperature independent fraction and has no minimum value for classifying the catalyst as aged.

Consequently, ***the catalyst aging detection problem becomes estimating the aging factor and testing if it is bellow*** a_{min} ***in presence of uncertainties***.

5.1 Aging factor estimation problem formulation

Given the simplified non-linear concentration dynamics for SCR-ASC reactions with internal dynamics and sensor corss-sensitivity 16. Estimate the total molar Ammonia storage capacity of the catalyst $[\Theta(t, T)]$. Then,

$$\implies a(t, T) = \frac{\Theta(t, T)}{\Theta(0, T)}$$

No fault condition:

$$a(t, T) > a_{min} \quad \forall T \in [T_{min}, T_{max}],\ t > 0$$

We have the following high-level steps in fault-diagnosis:

1. Estimate cross-sensitivity factor χ.
2. Estimate the lumped model parameters $f_\bullet, g_\bullet$.
   - This requires an observer for ammonia storage fraction θ.
3. Using $f_\bullet, g_\bullet$, estimate $\Theta(t, T)$.
4. Estimate $a(t, T)$ and propagate all the uncertainties down to δ_a, the uncertainty in $\hat{a}$.
5. Check for no-fault condition:

$$\hat{a}(t, T) \pm \delta_a > a_{min} \quad \forall T \in [T_{min}, T_{max}]$$

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