Note on SCR-OBD algorithm developement

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October 11, 2023

Contents

1 Introduction

Goal:

"Developing model-based non-introsive 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, NO_2
6. Tail-pipe NO_x, 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 Reactions and Dynamics

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

2.1 SCR 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: $R_{4R} = \underbrace{k_{4R} \exp\left(-\frac{E_{4R}}{RT}\right)}_{r_{4R}} \theta \Theta V$
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 – efficiency factor

2.3.3 Dynamic model

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

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

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