

Integration of Reformer Model Based Estimation, Control, and Diagnostics for Diesel LNT Based Aftertreatment Systems

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ABSTRACT

Future government emission regulations have lead to the development and implementation of advanced aftertreatment systems to meet stringent emission standards for both on-road and off-road vehicles [1, 2, 3, 4]. These aftertreatment systems require sophisticated control and diagnostic strategies to ensure proper system functionality while minimizing tailpipe NO_x and PM emissions across all engine operating conditions. In this paper, an integrated algorithm design approach with controls and diagnostics for an aftertreatment system consisting of a fuel doser, fuel reformer, LNT, DPF, and SCR is discussed.

From a high level advanced algorithm design perspective, the aftertreatment strategies are categorized into four areas: 1) model-based temperature controls with fuel reformer H₂ and CO yield consideration, 2) estimation of non-immediately available signals, 3) evaluation of system performance for long term and short term compensation, and 4) diagnostics for the purpose of safety and tolerant controls. Advanced methodologies, such as optimal cascade control, Kalman filtering, nonlinear system identification and (sliding-mode) observer design are integrated to optimize and enhance the overall system performance and reliability. Vehicle and engine testing as well as simulation results are shown.

KEYWORDS

Modeling, Simulation, Reformer, LNT, DPF, SCR, Diesel Aftertreatment Controls, PM, NO_x, Observer design, Diagnostics

I. INTRODUCTION

In the past several years, Eaton has developed an LNT and SCR based diesel aftertreatment system to meet the 2010 US HD EPA on-road and tier 4 US HD EPA off-road emission standards. The aftertreatment system consists of a fuel dosing system, a fuel reformer (REF), a lean NO_x trap (LNT), a catalyzed diesel particulate filter (cDPF), and a selective catalytic reduction (SCR) catalyst arranged in series to reduce tailpipe nitrogen oxides (NO_x) and particular matter (PM). [Figure 1](#) illustrates the aftertreatment system configuration used herein.

A REF catalyst is used to generate hydrogen (H₂) and carbon monoxide (CO) from injected diesel fuel to effectively desulfate and regenerate the LNT. The LNT traps NO_x under lean conditions and subsequently reduces it to nitrogen (N₂) and ammonia (NH₃) using rich REF operation. The ammonia (NH₃) produced by the LNT is utilized by the SCR to reduce NO_x that slips past the LNT to improve the overall system NO_x conversion.

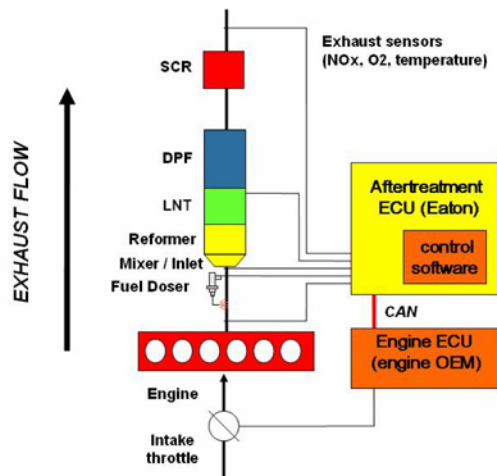


Figure 1. Aftertreatment system layout

Aftertreatment systems require comprehensive controls to perform deSulfation (deSO_x), LNT regeneration (de-NO_x) and DPF regeneration (deSoot) under a wide range of operating conditions. To ensure proper system functionality, estimation and diagnostic techniques are also required during operation to: monitor the system aging, detect system faults, and compensate for sensor drift.

In this paper, several portions of the integrated controls are discussed along with testing and simulation results. In section II, a simplified REF model that can be used for real-time controls is discussed. In section III, a cascade control algorithm using the model from section II along with an extended Kalman filter is proposed, implemented, and tested. In section IV, real-time temperature estimation and compensation for a production type temperature sensor (RTD) is discussed. In section V, fault diagnostics using sensor offsets and REF aging characteristics are discussed along with simulation results. Finally, section VI concludes with a discussion on integration of the above mentioned model based estimation, control, and diagnostics.

II. REFORMER MODELING

MODELING APPROACH

To control the REF catalyst, a simple model was derived to estimate the catalyst temperature and reformate production in real-time during operation. The overall modeling approach is illustrated in Figure 2. To derive the REF model, the catalyst is first split into two control volumes: one representing the solid phase, and one representing the gas phase. After the ordinary differential equations (ODEs) for each phase were derived, the reactor was discretized into i subsections along the axial length of the catalyst. Two separate ODEs are used to represent each subsection of the REF catalyst (one solid phase ODE, and one gas phase ODE); therefore, the overall

order of the model is equal to $2i$. Spatial temperature estimation across the axial length of the catalyst is required due to the non-uniformity in axial temperature during operation. If a simple lumped parameter approach was used, catalyst over-tempering may occur in the inlet zone of the REF due to the higher fuel oxidation rate in the front of the reactor. Finally the equations are implemented in a state space format so that an observer can be added to improve the accuracy of the model by utilizing the measured REF outlet gas temperature as feedback.

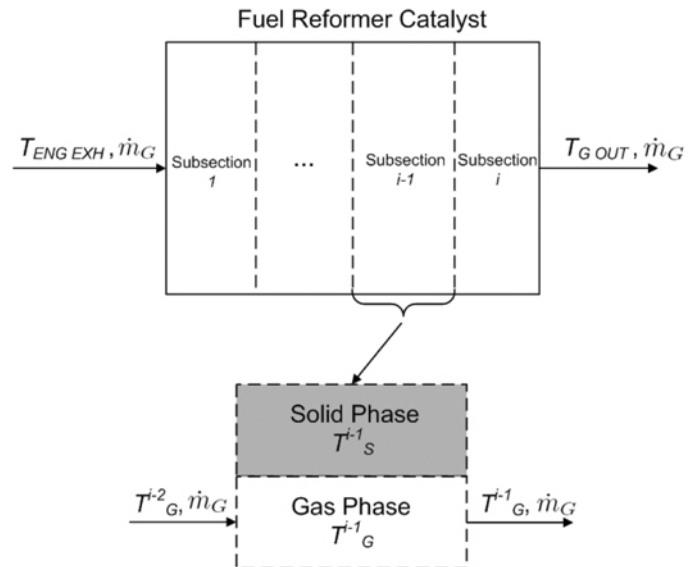
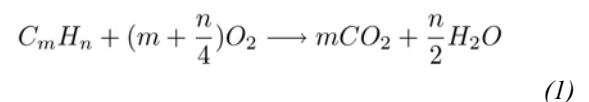


Figure 2. Discretized REF modeling approach

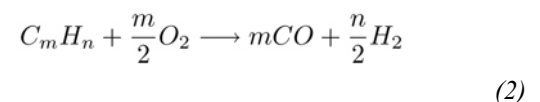
REFORMER REACTION KINETICS

The REF chemistry can be represented using the following four chemical reactions [5, 6]:

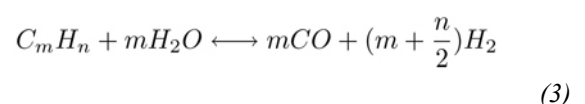
Combustion



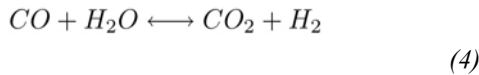
Catalytic Partial Oxidation



Steam Reforming



Water Gas Shift



The first two reactions represent the exothermic fuel oxidation within the REF, while the second two reactions are used to represent the endothermic fuel reforming within the REF. To simplify the model, the catalytic partial oxidation reaction is ignored and only complete fuel combustion is considered. Also rather than trying to predict the individual concentrations of H_2 and CO , they are lumped together in the model output as total reductant ($H_2 + CO$) which allows reactions 3 and 4 to be combined into one single reforming reaction. For LNT regeneration control, an estimation of the total reductant is sufficient to optimize the deNO_x performance.

The mass balance of the injected fuel within the REF is given by:

$$\dot{m}_{HC\ IN} - \dot{m}_{HC\ OUT} = \frac{dm_{HC}}{dt} \quad (5)$$

where $\frac{dm_{HC}}{dt}$ is the fuel converted within the REF catalyst, which is defined as the summation of the oxidation and reforming reaction rates (Eqn. 6).

$$\frac{dm_{HC}}{dt} = \dot{r}_{OX} + \dot{r}_{REF} \quad (6)$$

Rather than using detailed reaction kinetics and mass transfer, the reaction rates for the oxidation and reforming reactions are mapped over the range of standard REF operating conditions, and an efficiency factor for each reaction is determined under each specific operating condition. The conversion efficiency maps are generated offline using a least squares optimization routine. The optimized maps can then be implemented as 2D lookup tables within the controller. This approach enables simple control of the REF temperature since the plant model is linear with respect to the input HC flow. If Arrhenius equations were instead used to model the reaction rates, the temperature control would become more complicated due to the nonlinear relationships (temperature and concentration) of the resulting kinetic equations. Therefore, the fuel oxidation and reforming reaction rates are calculated using the following two empirical relationships:

$$\dot{r}_{OX} = \dot{m}_{HC}\eta_{OX}(F_{EXH}, T_{IN}) \quad (7)$$

$$\dot{r}_{REF} = \dot{m}_{HC}(1 - \dot{r}_{OX})\eta_{REF}(F_{EXH}, x_{HC\ RICH}) \quad (8)$$

where $\dot{m}_{HC}$ is the inlet HC flow rate, $x_{HC\ RICH}$ is the mole fraction of the HC remaining after all of the exhaust O_2 is depleted, η_{OX} is the REF fuel oxidation efficiency factor, η_{REF} is the REF fuel reforming efficiency factor, and F_{EXH} is the exhaust flow rate.

REFORMER THERMAL MODEL

SUBSTRATE TEMPERATURE

The substrate temperature is derived starting with the energy balance given below in Equation 9:

$$m_S c_{v,S} \frac{dT_S}{dt} = \dot{Q}_{CONV} + \dot{Q}_{RXN} \quad (9)$$

where m_S is the mass of the REF substrate, and $c_{v,S}$ is the REF substrate specific heat capacity. $\dot{Q}_{CONV}$ is the convective energy transfer between the gas and solid phase, and $\dot{Q}_{RXN}$ is total heat generation from the combined exothermic oxidation reaction and the endothermic reforming reactions which are given below as Equations 10 and 11:

$$\dot{Q}_{CONV} = hA(T_G - T_S) \quad (10)$$

$$\dot{Q}_{RXN} = - \sum_{j=1}^n \Delta H_j \dot{r}_j \quad (11)$$

where h is the convective heat transfer coefficient, A is the surface area of the REF substrate, ΔH_j is the change of enthalpy for each reaction, and $\dot{r}_j$ is the reaction rate of each reaction. In this model the conductive heating along the axial length of the REF catalyst is assumed to be much smaller the energy transfer from the convective heating and chemical reactions; therefore, it is neglected in this analysis. This is consistent with other approaches in the literature [7]. By substituting Equations 10 and 11 into 9 and discretizing into i subsections along the axial length of the catalyst, the final ODE for the solid phase is obtained:

$$\frac{dT_S^i}{dt} = \frac{h\hat{A}}{\hat{m}_S c_{v,S}} (T_G^i - T_S^i) - \frac{1}{\hat{m}_S c_{v,S}} \sum_{j=1}^n \Delta H_j^i \dot{r}_j^i \quad (12)$$

where $\hat{m}$ and $\hat{A}$ denote m/i and A/i respectively.

GAS TEMPERATURE

The gas temperature is derived in the same manner as the solid phase yielding the following ODE for the gas temperature:

$$\frac{dT_G^i}{dt} = \frac{h\hat{A}}{\hat{m}_G c_{v,G}} (T_S^i - T_G^i) + \frac{\dot{m}_G c_{p,G}}{\hat{m}_G c_{v,G}} (T_G^{i-1} - T_G^i) \quad (13)$$

where $\dot{m}_G$ is the exhaust flow rate entering each subsection, and $\hat{m}_G$ is the mass of the exhaust gas within each subsection. Finally all of the ODEs (12-13) are represented using the following state space form:

$$\begin{aligned} \dot{x}(t) &= A(t)x(t) + B(t)u(t), \\ y(t) &= Cx(t) \end{aligned} \quad (14)$$

$$\text{where } x = \begin{bmatrix} T_S^1 \\ \vdots \\ T_S^i \\ T_G^1 \\ \vdots \\ T_G^i \end{bmatrix} \text{ and } u = \begin{bmatrix} T_{IN} \\ \sum_{j=1}^n \Delta H_j^1 \dot{r}_j^1 \\ \vdots \\ \sum_{j=1}^n \Delta H_j^i \dot{r}_j^i \end{bmatrix}$$

Note that the matrices A and B are time variant due to the changing exhaust flow rate entering the REF catalyst, and the varying REF fuel oxidation and reforming efficiencies.

The REF model prediction and measured REF Out HC, CO, and H_2 are shown in Figure 3 for three LNT deNOx regenerations. These results were collected during testing in an engine dynamometer test cell under quasi steady state engine conditions. The HC and CO measurements were obtained using a Horiba MEXA 7100D emission bench, while the H_2 measurements were obtained with an H-Sense H_2 mass spectrometer. Due to the measurement time delay and signal filtering of the exhaust species analyzers, the total integrated HC, CO, and H_2 are used for comparison rather than instantaneous flow rates.

Each fuel pulse is divided into two phases: a lean warm-up phase with a target warm-up temperature of 600°C, and a 4 sec rich phase at a target equivalence ratio ϕ of 1.3. Detailed deNOx operation information has been published in previous work [8]. From the results it was observed that the model was able to accurately estimate the REF HC, and $H_2 + CO$ production for each cycle. For this test run, the model was able to predict the REF out HC with an average error of 7.7%, and the REF out $H_2 + CO$ with an average error of 4.6%.

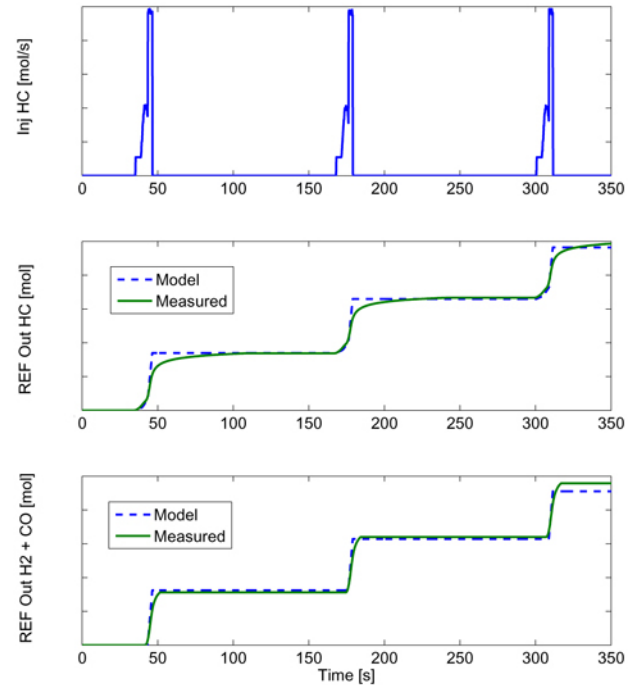


Figure 3. REF HC and $H_2 + CO$ estimation results during LNT deNOx regeneration

The REF model temperature prediction and measured REF temperature are shown in Figure 4 for the same three LNT deNOx regenerations. Prior to testing, K-type thermocouples were inserted into the REF catalyst substrate to measure the REF substrate temperatures at the outlet of each modeled zone. The model is divided into 3 catalyst subsections; therefore, the overall model is 6th order. With 3 subsections, the REF temperatures can be accurately estimated within a microcontroller without consuming a large amount of computational resources. From the results, it was observed that the REF model was able to accurately estimate the temperature in each of the REF catalyst zones with a maximum error of 15°C.

Based on the results that were obtained during testing it was determined that accuracy of this model was sufficient for model based control under most conditions; however, under some testing conditions system disturbances could cause significant error. To improve the modeling accuracy and robustness, an observer was added to the model.

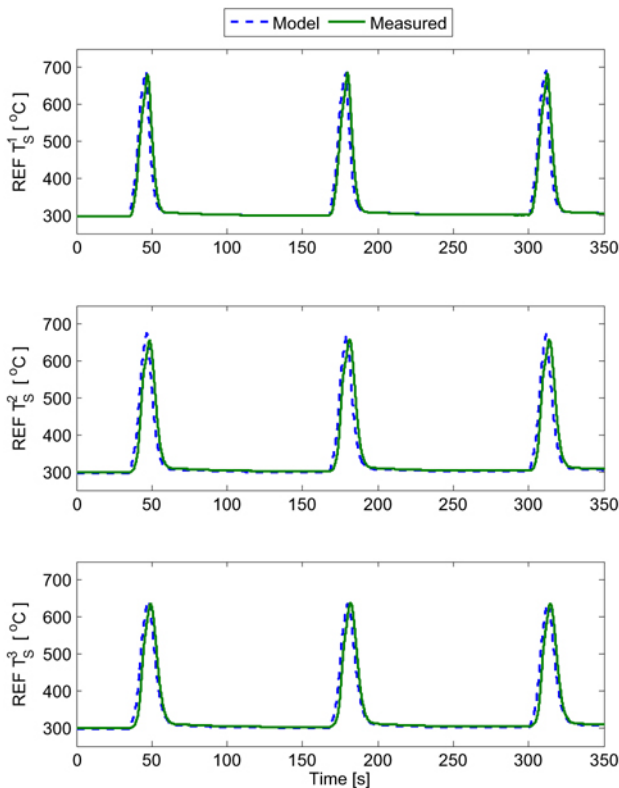


Figure 4. REF temperature estimation results during LNT deNOx regeneration

OBSERVER DESIGN

During REF operation there are many measurement, system, and input disturbances that can lead to inaccuracies in the REF temperature estimation. Possible disturbances during operation include: inlet fuel flow and exhaust flow non-uniformity, fuel doser calibration drift, REF part to part variation, REF performance degradation from aging, and sensor (MAF, UEGO, and temperature) drift. To correct the model for these disturbances, an extended Kalman filter is added to the model. Kalman filters are commonly used in control systems to improve the estimation of unmeasurable states [9, 10, 11]. To implement the extended Kalman filter, a temperature sensor is installed directly downstream of the REF catalyst to measure the REF gas outlet temperature, and the measured REF gas outlet temperature is used as feedback to correct the model. To account for the temperature sensor dynamics, an additional state is added to the model (see Section III) which is used to estimate the temperature of the sensor using the predicted REF gas outlet temperature. The estimated sensor temperature and the measured sensor temperature are compared to calculate the error of the model. The error is used to correct the estimation using a Luenberger observer [9]:

$$\dot{\hat{x}}(t) = A(t)\hat{x}(t) + B(t)u(t) + L(t)(y - C\hat{x}) \quad (15)$$

where $\hat{x}(t)$ is the observer estimate of the actual state $x(t)$. The gain matrix L is chosen such that the eigenvalues of the closed loop matrix $A - LC$ have only negative real parts which ensures that $e(t) = (\hat{x}(t) - x(t)) \rightarrow 0$ as $t \rightarrow \infty$. Since the matrix A is time-variant, L is generated offline for all possible values of A . Gain scheduling is then used online to select L based on the engine exhaust flow. By utilizing gain scheduling, the desired eigenvalues, and thus the closed loop response of the estimation, can be optimized across the full range of operating conditions.

The REF model temperature prediction and measured REF temperature are shown in Figure 5 for two short thermal management cycles. Two separate REF temperature estimations are shown in the figure; the first using the REF model with no disturbance correction, and the second with the addition of an observer to correct the error. A K-type thermocouple was used for the observer feedback during this experiment; however, a production type sensor could be utilized for error feedback by simply adjusting the sensor dynamics within the model (see Section III). For this experiment the open loop model gave a good approximation of the first REF zone; however, the model did not accurately predict the temperature of zones 2 and 3 due to an over-prediction of the REF HC oxidation within these two zones. Without the observer the steady state error of zone 2 was approximately 30°C, and the steady state error of zone 3 was approximately 50°C. With the addition of an observer to correct the model prediction, the steady state error is reduced to within 5°C for all three zones. This improvement in temperature estimation greatly improves the accuracy of the REF control during LNT regenerations, DPF regenerations, and LNT desulfations where very tight REF temperature control is required to minimize the catalyst aging over time.

III. REFORMER TEMPERATURE CONTROL

REFORMER WARM-UP TRAJECTORY

During REF thermal management, a target warm-up trajectory is generated to schedule the in-pipe fuel injection. When generating the target trajectory, constraints must be placed on the fuel injection rate so that the REF can be protected from thermal damage, and the aftertreatment fuel consumption can be minimized. If the REF is heated too quickly, radial and axial temperature gradients across the REF may cause deformation within the metallic REF substrate. To avoid damage, a maximum warm-up rate is defined and all warm-up trajectories are generated such that the target warm-up rate is always less than the maximum. If the warm-up fuel injection rate produces an equivalence ratio greater than 1, the net heat generation rate will be reduced due to the endothermic reforming reactions that occur on the REF catalyst under rich conditions.