

Design of Engine-Out Virtual NO_x Sensor Using Neural Networks and Dynamic System Identification

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ABSTRACT

Fuel economy improvement and stringent emission regulations worldwide require advanced air charging and combustion technologies, such as low temperature combustion, PCCI or HCCI combustion. Furthermore, NO_x aftertreatment systems, like Selective Catalyst Reduction (SCR) or lean NO_x trap (LNT), are needed to reduce vehicle tailpipe emissions. The information on engine-out NO_x emissions is essential for engine combustion optimization, for engine and aftertreatment system development, especially for those involving combustion optimization, system integration, control strategies, and for on-board diagnosis (OBD).

A physical NO_x sensor involves additional cost and requires on-board diagnostic algorithms to monitor the performance of the NO_x sensor. A control-oriented engine-out NO_x model that meets throughput constraints is desirable for on-board applications as a virtual NO_x sensor, which could be used in replacement of the physical sensor or run parallel as an analytical redundancy to detect potential in-range failure for the physical sensor.

This paper presents the design of a virtual NO_x sensor using neural networks combined with nonlinear dynamic system. NO_x emission estimation with or without cylinder pressure information is investigated, and a correction to a baseline NO_x model is proposed in order to compensate transient EGR responses. The developed virtual NO_x sensor demonstrates a higher level of fidelity estimation when compared with actual NO_x measurements.

INTRODUCTION

In an era of elevated competition in automotive industry and heightened concern over global warming, the technology development to improve fuel economy becomes increasingly critical. Diesel engines and lean-burn gasoline engines offer better fuel economy, but engine-out NO_x emissions are high during lean operations. As emission regulations are becoming more and more stringent worldwide, optimization and control of both in-cylinder combustion and exhaust aftertreatment systems become necessary in order to reduce tailpipe NO_x emissions. Computational modeling of engine-out NO_x emissions, with various levels of complexity and fidelity, have been extensively studied, with a wide range of applications such as engine combustion and aftertreatment system optimization, offline engine and aftertreatment control strategy development, online model-based engine and/or aftertreatment control, and on-board diagnosis (OBD).

Del Re *et al.* [1] suggested an approach to develop virtual NO_x sensor as an alternative to online measurement of NO_x emissions for diesel engine controls. In their approach, the experimental data were screened for hidden analytical structures, combining structural identification and evolutionary algorithms, and then these structures were used to develop the virtual NO_x sensor. The approach predicted NO_x emissions reasonably well over FTP cycle with and without EGR. NO_x emissions were identified as a nonlinear function of ECU parameters such as air mass flow, desired fuel amount, water temperature, and engine speed.

Lyons and Timoney [2] described a simplified semi-empirical method of estimating NO_x quantities for real-time onboard emission control system. Their method combined empirical NO_x estimation model with a zero-dimensional

thermodynamic model that uses in-cylinder pressure measurements for heat release calculation and adiabatic temperature prediction. The NO_x (in moles) was estimated using adiabatic temperature, fuel mass burned, engine speed, cylinder pressure, equilibrium nitrogen and oxygen concentrations, and activation energy of 46,851 J/mol from empirical regression analysis. The model correlates well with NO_x measurements at high engine load conditions with higher NO_x levels.

Andersson *et al.* [3] presented a fast NO_x model for diesel engines optimization, aftertreatment control, and virtual engine mapping. The NO_x model used in-cylinder pressure data to calculate heat release and combustion products, and Zeldovich mechanism for NO_x formation. Tables were used to calculate the equilibrium burned zone temperature and species concentrations by interpolation to achieve faster computation speed. The model accuracy was good when validated with single-cylinder data at higher NO_x level ($> 100\text{ppm}$), or the model was less accurate (contributing to Zeldovich mechanism's limitation at low temperature) and an empirical correction was proposed at low NO_x level.

Ericson *et al.* [4] developed diesel engine combustion and NO_x models for model-based control and simulation of the complete engine and aftertreatment system. A filling-and-emptying quasi-steady gas exchange model (including EGR and VGT) was used to estimate inlet manifold pressure and EGR rate, in junction with a two-zone zero-dimensional combustion model for in-cylinder pressure and temperature predictions and the Zeldovich mechanism for NO_x formation. The complete model was validated with 29 steady-state operating points. NO_x predication results were generally good except for an idle condition (500rpm, 0% load), which was attributed to Zeldovich mechanism's limitation at low cylinder pressures and temperatures. Black-box compensation was proposed for low load operating conditions.

Arsie *et al.* [5] described the development of a predictive multi-zone phenomenological model for the design and optimization of the multi-injection diesel engines control strategies. The model captures the spray penetration, the fuel evaporation and the air entrainment considering the jet core divided into a number of parcels with homogenous pressure and different temperature and chemical composition, the combustion based on the laminar and turbulent characteristics time, and NO formation using extended Zeldovich mechanism. This comprehensive model showed a very good agreement for measured engine cycles and NO emissions with minimal parameter tuning.

Arregle *et al.* [6] developed NO_x estimation models for engine control system and OBD, and studied the sensitivity of NO_x estimation to uncertainties in their model input

parameters. In this study, the NO_x estimation model consists of an in-cylinder thermodynamics model to predict the adiabatic flame temperature using air-fuel mixture temperature evolution (based on in-cylinder pressure measurement) and oxygen mass fraction at the end of the intake process, and NO_x formation model with Zeldovich mechanism. It was found that intake air/EGR mixture temperature and fresh air mass measurements are critical, much more than in-cylinder pressure measurements.

Atkinson *et al.* [8,9] applied recurrent Neural Network to model engine-out NO_x . The selected current inputs and the time histories of the past inputs are used to train a NO_x model. The advantage of this temporal model structure is the ability to capture both steady state and dynamic responses of a NNT model. It is known that the recurrent NNT takes quite time to train, and requires more neuron's to run, which adds more computational load.

This paper develops a virtual NO_x sensor using a new approach, which applies several key physical models as inputs to a neural network model. As the first step of modeling process, physical models are developed to estimate combustion parameters considered as main contributors to engine-out NO_x . These include peak cylinder temperature based on a two-zone combustion model, AFR, EGR rate, combustion phasing, etc. The next step in modeling uses a neural network (NNT) that is trained to model the NO_x formation during the combustion process. The NNT takes the estimated parameters from the first step, maps them directly to the engine out NO_x . This stage treats other unknown factors as a black box, including chemical reactions during combustion, and heat loss to cylinder wall; therefore, compensates unmodeled uncertainties through NNT. In the third step design, the NNT model is augmented with a dynamic model. The dynamic model captures fast transient responses where actual air mass flow or EGR could not track their commands during tip-in acceleration conditions. Experimental data from a diesel engine reveals that this NO_x virtual sensor can estimate engine out NO_x with good accuracy. Experimental data also shows that an available cylinder pressure sensor can further improve the accuracy of the NO_x estimation model.

METHODOLOGY

As described in the previous sections, a mixed approach that combines nonlinear system dynamic model with a neural network model is used for the development of the virtual NO_x sensor. A generic block diagram of the NNT model is shown in Fig. 1. For the modeling exercise, two cases are considered for the NNT input set. In the first case, cylinder pressure information is assumed to be available while in the second case, the set of inputs to the NNT are chosen to emulate an engine platform without cylinder pressure sensor.

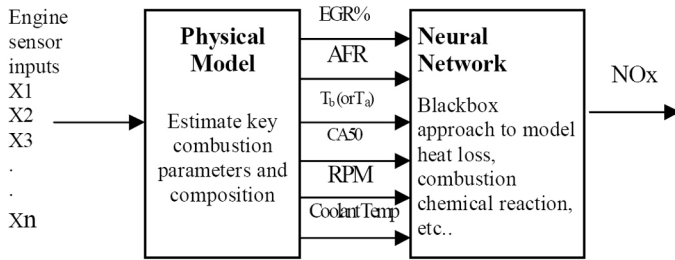


Figure 1. Generic engine-out NO_x modeling architecture (with cylinder pressure information)

In this model architecture, relevant engine sensor inputs are selected to build key physical models or combustion parameters, which contribute to NO_x formation during combustion process. As an example in Fig.1, the outputs of those key models include EGR%, AFR, combustion burned mixture temperature (T_b), or average combustion temperature (T_a), crank angle location of 50% mass fraction burn, measured engine speed and coolant temperature. Those physics model parameters feed into a neural network (NNT) model, which then estimates the engine out NO_x formation during the combustion process. The sensor inputs to the NNT model can be determined accordingly based on the available sensor measurements in an engine.

MODEL DESCRIPTION

The key inputs to the NNT model consists of the data set described below. One may also choose a subset as the inputs to the NNT model. The inputs considered include EGR rate, AFR, intake O₂%, fueling, SOI, intake manifold temperature, coolant temperature (CLT), engine speed (rpm), rail pressure (Prail), and relative humidity (RH). In case a cylinder pressure sensor be available, the input parameters can also include the crank angle at which 50% mass fraction is burnt (CA50), peak cylinder pressure (P_{max}), and estimated combustion flaming temperature, etc. The first physical model is described as EGR rate defined below.

$$egr\% = \left(1 - \frac{\dot{m}_a}{\dot{m}_c}\right) * 100\% \quad (1)$$

where $\dot{m}_a$, the fresh air mass flow is measured from a MAF sensor. The cylinder charge mass flow $\dot{m}_c$ is modeled from the speed density equation,

$$\dot{m}_c = \frac{P_{im} \cdot rpm \cdot D \cdot \eta}{2RT_{im}} \quad (2)$$

where D is the engine displacement, intake manifold pressure (P_{im}) is measured from a sensor, so are the intake manifold temperature (T_{im}) and engine speed (rpm). η represents the

volumetric efficiency. It can be modeled as a nonlinear function defined as

$$\eta = f(rpm, \frac{P_{im}}{T_{im}}, \Delta P, TP) \quad (3)$$

In Eqn(3), delta pressure is defined as the engine exhaust pressure divided by the intake manifold pressure. Estimating engine exhaust pressure is described in Wang et al.[7]. TP represents throttle position, which partitions the model into two individual models that depend on the throttle being open or close.

The next physical model is the combustion temperature of burned mixture. Modeling combustion flaming temperature is very challenging; instead we use a two-zone combustion model neglecting heat loss onto cylinder walls. Therefore, the burned (T_b) and the unburned combustion temperature (T_u) in each zone can be approximately modeled as

$$T_u = \frac{1.05 * \dot{m}_c}{1.05 * \dot{m}_c - \alpha(CA50) \cdot \dot{m}_f \lambda_s} [0.05\beta T_{ex} + 0.95T_{im}] \left(\frac{P_{max}}{P_{im}}\right)^{\frac{r-1}{r}} \quad (4)$$

$$T_b = \frac{T_a - (1 - x_b)T_u}{x_b} \quad (5)$$

where α , β are calibration constants, γ is the ratio of specific heats, P_{max} is the peak in-cylinder pressure, T_{ex} is the exhaust manifold temperature, λ_s is the stoichiometric air to fuel ratio, $\dot{m}_f$ is the fuel mass flow. The average temperature can be written as,

$$T_a = \frac{P_{max} \cdot V(PPL)}{1.05 * \dot{m}_c R} \quad (6)$$

where V(PPL) represents the cylinder volume at the cylinder peak pressure location, R is the gas constant. Also, the burnt mass fraction (x_b) is given by,

$$x_b = \frac{\alpha_b \cdot \dot{m}_f (1 + \lambda_s)}{1.05\dot{m}_c} \quad (7)$$

where α_b is a model constant, the scale 1.05 before the charge mass flow assumes 5% residual gas in cylinders. While a simple regression model