Modelling and simulation of virtual $NO_x$ sensor for diesel engine using thermodynamic model

Shoaib Ahmed$^1$, Halesh M R$^2$, Narasimha kollaparti$^3$, Aman P V$^4$, Satish V T$^5$

1 PG Research Student, Department of Electronics and Communication, SJCE Mysore.
2 Assistant Professor, Department of Electronics and Communication, SJCE Mysore.
3 Subject Matter Expert, KPIT Technologies, Bangalore.
4 Subject Matter Expert, KPIT Technologies, Bangalore.
5 Assistant Professor, Department of Mechanical Engineering, MCE Hassan.

Abstract: This paper presents a thermodynamic model for virtual $NO_x$ sensor which is capable of predicting nitrogen oxides ($NO_x$) emissions in diesel engines. In-cylinder volume and pressure are the inputs from estimator. The proposed method is based on a two-zone thermodynamic model which divides the combustion chamber into burned and unburned gas zone. The contribution of proposed method arises from: In-cylinder volume and pressure are the inputs from estimator using slider crank mechanism. And the two-zone thermodynamic modeling framework is applied in a way that the thermodynamic equations can be solved in a closed form, which provides the basis for achieving high level of predictiveness using MATLAB which uses ADVISOR as prerequisite for the project. The model is validated using real data values. The model is suitable for two different direct injection diesel engines, i.e. a light and a heavy-duty engine. Also, it maintains a low pipe emission which minimizes fuel consumption.

Keywords: Thermodynamics, $NO_x$ (Nitrogen Oxide), Burnt zone, Unburnt zone, Estimator, MATLAB and ADVISOR (Advanced Vehicle Simulator).

1. Introduction

DieSEL engine powered automobiles are increasing in recent years, due to high thermal efficiency of diesel engines. These engines have become an environmental issue since it represents a major source of $NO_x$ emissions [1]. The ADVISOR is used as prerequisite for understanding the exhaust gas temperature, exhaust catalyst efficiency and emissions for a selected vehicle. ADVISOR package developed by national renewable energy laboratory is being utilized for rapid analysis of performance and fuel economy of mentioned vehicles such as conventional, electric and hybrid vehicles. ADVISOR package runs in background of MATLAB environment, which provides a backbone for simulation and analysis for the defined drivetrain components. Based on survey carried, the well-known deficiencies always found with emissions [2]. To overcome these increasingly stringent emissions in diesel engine adoption of control strategies based on models is required. A real time-based $NO_x$ model can be able to estimate engine out $NO_x$ in diesel engines. The accurate measurement of in-cylinder $NO_x$ being an input parameter for active control methods (like control closed loop combustion) and also for the control of exhaust treatment systems. Real time models for ignition delay and emission formation combined with closed-loop control and optimization of injection timing might be a powerful tool to control these future engines and to bring out the full potential of the emerging technologies. Another application of fast emission model is for engines fitted with a $NO_x$ after treatment system that adds a reduction agent to the exhaust stream. In that case it is essential to know engine out $NO_x$ level in order to control the reduction agent flow into the catalytic converter [3]. Some of the modern diesel engines are equipped with pressure sensors (Transducer), which gives input to combustion related data [4, 5]. The importance of measuring in-cylinder pressure used for obtaining information related to aging of engine components as well as adaption of the injection strategy with respect to the variation in the fuel quality [6]. Thus, focusing on this importance of pressure estimator, it can be useful for emerging a pressure estimator model. The research uses input for the combustion modelling and input for calculation of thermodynamic parameters inside the cylinder which enables virtual $NO_x$ sensor with higher level of predictiveness. Over the past decade, diesel engine technology
has increasing rapidly and evolved to the point where control solutions for obtaining high fuel efficiency and low NO$_x$ emissions are possible. The strategies are being implemented to manage fueling system and air handling system. Also, this will be relying on sensor replacement and limitations of costs. A space of special interest is considered for this type of analysis inside the cylinder volume. The laws of thermodynamics are being an application for solving this kind of equations [7]. According to piston-cylinder geometry it is seen that straight-line motion can be converted into rotary motion. Hence the slider crank model has led to derive in-cylinder volume. The available piezoelectric transducer will lose its sensibility due to aging factor. Hence this allows for development in grey area of an automobile [8]. The model accuracy largely depends on tuning parameter. Hence, advanced virtual NO$_x$ sensor models have general applicability for NO$_x$ estimation [3]. The Estimation of NO$_x$ at upstream and downstream opens a capability for getting SCR efficiency for further urea dosing strategy. As per the research, the main thermodynamic parameters require for NO$_x$ prediction are rate of heat release (ROHR) and consequently the temperatures and concentrations in the combustion chamber. The properties of thermodynamic model can be assessed by physical depth in models which also reflects computational complexity of models [9]. On the system level, 0-D combustion models, [10,11], are often used as models that are effectively combine the requirements on multi-zone spatial resolution and much shorter computational times compared to the 3D CFD models.

2. Specifications of the work
The specifications used for modelling is given below. The simulation is carried on light duty vehicle and heavy-duty vehicle. Table 1 provides specification of light-duty vehicle. Similarly, Table 2 provides specification of heavy-duty vehicle.

### Table 1: Light duty vehicle specification

| Specification             | Value                      |
|---------------------------|----------------------------|
| Cylinders                 | 4 inline                   |
| Displacement              | 1560Cms                    |
| Bore x Stroke             | 75mm x 88.3mm              |
| Compression               | 18:1                       |
| Fuel injection system     | CRDI                       |
| Connecting rod length     | 136.8mm                    |
| Maximum power             | 66.2kW @ 4000 rpm         |
| Maximum Torque            | 215Nm @ 1750 rpm          |

### Table 2: Heavy duty vehicle specification

| Specification             | Value                      |
|---------------------------|----------------------------|
| Cylinders                 | 6 inline                   |
| Displacement              | 6870cm$^3$                 |
| Bore x Stroke             | 108mm x 125mm              |
| Compression               | 18:1                       |
| Fuel injection system     | DI                         |
| Connecting rod length     | 182.5mm                    |
| Maximum power             | 162kW @ 2400 rpm          |
| Maximum Torque            | 825Nm @ 1400-1700 rpm      |

3. Workflow of modelling and methodology
The modelling framework starts with estimation of in-cylinder volume which is obtained using slider crank mechanism. The instantaneous volume can be obtained by applying derivative. The estimation of in-cylinder volume is further used for instantaneous pressure estimation. The instantaneous values are inputs from estimator. Till the end of injection, the in-cylinder gas mixture is modelled as single zone. The measurement of temperature for considered ideal and non-perfect gas is followed. The main concentration is given for deducting temperature out of mass of fuel, heat addition terms using thermodynamic modeling for thermal NO$_x$ calculation. After the combustion begins and burns the
The proposed methodology is shown in figure 2, which indicates the Overall view of models used for modelling the NO\textsubscript{x} estimator. The following are the models which are modelled as per the engine specification: Volume Estimator model, Pressure estimator model, Fuel rate model, Model for conserved mass in two-zones, Heat release model, Heat transfer model, Temperature model for thermal NO\textsubscript{x} calculation, and NO\textsubscript{x} estimator model.
4. Simulation of NO\textsubscript{x} sensor

4.1 Volume model

It is assumed that volume can be derived using slider crank model from the compression ratio, bore, connecting rod and stroke. The energy equations are applied to the volume and crank-angle domain and the volume estimator obtained as given in equation 1:

\[
\frac{dV}{d\theta} = A_p \left[ (-r \sin \theta) \frac{1}{1} + \cos \frac{1}{h} \sqrt{\left( \frac{r}{r} \right)^2 - \sin^2 \theta} \right]
\] (1)

4.2 Pressure estimator model

The energy equations are applied to the pressure and crank-angle domain and the pressure estimator derived as follows:

\[
\frac{dP}{d\theta} = -\frac{\gamma}{V_{cyl}} \frac{dV}{d\theta} + \frac{\gamma - 1}{V_{cyl}} \left[ (1 - \alpha)m_{fuel} Q_{LHV} \frac{dx_k}{d\theta} \right]
\] (2)

4.3 Model of conserved mass in two zone

The Conservation of mass is applied to the control volume and conservation of mass of burnt is equal to the mass transfer from unburnt to burnt zone, accord into this assumption it is given as:

\[
\frac{dm_{u-b}}{d\theta} = \frac{dm_{fuel}}{d\theta} (\lambda_{comb} L_{st} + 1) (1 + \lambda L_{st})
\] (3)

Thus, the conservation of mass of burnt zone is obtained as:

\[
\frac{dm_b}{d\theta} = \frac{dm_{u-b}}{d\theta}
\] (4)

Assuming the unburned zone usually consists of trapped air, unburnt fuel and its equation is given as:

\[
\frac{dm_u}{d\theta} = \frac{dm_{ini}}{d\theta} - \frac{dm_{u-b}}{d\theta}
\] (5)

4.4 Heat release model

It is assumed that the rate of heat release occurs in burned zone only and can be obtained by heat addition parameter as follows:

\[
\frac{dQ_{b,b}}{d\theta} = \frac{dm_{fuel}}{d\theta} Q_{LHV}
\] (6)

4.5 Temperature model for thermal NO\textsubscript{x} calculation

The temperature responsible for thermal NO\textsubscript{x} is calculated using following equations and separate equations are written for burnt and unburnt zones as given below:

\[
\frac{dT_b}{d\theta} = \frac{dQ_{b,b}}{d\theta} + \frac{dQ_{b,b}}{d\theta} + h_a \frac{dm_b}{d\theta} - h_b \frac{dm_b}{d\theta} + \frac{m_R T_b dP}{P} \frac{d\theta}{d\theta}
\] (7)

\[
\frac{dT_u}{d\theta} = \frac{dQ_{ini}}{d\theta} + h_{ini} \frac{dm_{ini}}{d\theta} + \frac{m_R T_u dP}{P} \frac{d\theta}{d\theta}
\] (8)
4.6 NOx estimator model

The equilibrium species calculation is being performed using Gibbs free energy equation. To reduce the complexity for computation, the pre-calculated values are being used as stored look-up table. The calculation of equilibrium species can be performed for many sets of reactions using extended zeldovich mechanism. Here the case of one reaction is considered for modelling basic NOx estimator.

\[ N_2 + O \rightarrow NO + N \]

The extended zeldovich mechanism [12] is obtained for the above reaction and initial NO formation rate is given as:

\[ \frac{d[NO]}{d\theta} = 6 \times 10^{16} e^{-\frac{69,090}{T_b^{1/2}}} \left[ O \right]^{2.5} \left[ N_2 \right]^{0.5} \]  \hspace{1cm} (9)

5. Results

The simulation of NOx estimator is done for light-duty vehicle and heavy-duty vehicle. The mass of air, mass of fuel, engine specifications are different to simulate on two different engines. Considering these factors, the simulation is carried in MATLAB platform.
Figure 3: Simulation result of Light-duty engine operating point at N=3000rpm
(a) Volume estimator, (b) Pressure estimator, (c) Mass of burnt, (d) Mass of unburnt, (e) Burnt zone temperature, (f) Unburnt zone temperature, (g) NOx estimator.
Figure 4: Simulation result of Heavy-duty engine operating point at N=3000rpm
(a) Volume estimator, (b) Pressure estimator, (c) Mass of burnt, (d) Mass of unburnt, (e) Burnt zone temperature, (f) Unburnt zone temperature, (g) NOx estimator.

**LD ENGINE:** The light-duty engine is equipped with common rail direct injection system. The build in pressure for the light-duty engine is less comparative to heavy-duty engine. Sensible check is carried and analyzed the plots of mass of burnt zone which is getting increased as combustion begins with respect to provided combustion angle. Also, the unburnt mass getting decrease at the same angle.
since unburnt zone is supplying amount of charge. The combustion temperature starts increasing rapidly at same instant, it also considers heat transfer. Thus, the NO formation starts at same angle for the cycle.

**HD ENGINE:** The heavy-duty engine is equipped with direct injection fuel injection system for validation purpose which influences the air and fuel preparation, also the HD-engine operates with leaner mixture compare to LD-engine. Thus, it impacts on start of combustion temperature and concentration. The build in pressure for the heavy-duty engine is very high. Sensible check is carried and analyzed the plots of mass of burnt zone which is getting increased as combustion begins with respect to provided combustion angle. Also, the unburnt mass getting decrease at the same angle since unburnt zone is supplying amount of charge. The combustion temperature starts increasing rapidly at same instant, also it considers heat transfer. Thus, the NO formation starts at same angle for the cycle.

6. **Conclusion**
The analysis is carried using ADVISOR package. A NO\textsubscript{x} sensor estimator is modelled for diesel engine which is able to measure engine out NO\textsubscript{x} using thermodynamic modelling framework which is usually measured to maintain low tail pipe emissions. In-cylinder pressure and volume are obtained successfully using slider crank mechanism, and input from pressure and volume estimator is used for calculating fuel rate. Finally, the temperature is obtained which estimates engine out thermal NO\textsubscript{x}. A two-zone thermodynamic modelling is carried in such a way that, it gives the mass of burnt and its temperature which signifies the amount of thermal NO\textsubscript{x} produced in diesel engine using MATLAB. The application of model on two different injection engines is validated, which allows to obtain NO\textsubscript{x} in heavy-duty engine which produces slightly higher amount of NO\textsubscript{x} emission compare to light-duty engine as mentioned in equation (9). The reason for NO\textsubscript{x} production is due to higher inlet temperature for this purpose equation (7) is modelled. The pressure estimator is modelled to correct the inlet pressure. Thus, by increasing inlet pressure the lower NO\textsubscript{x} can be obtained. It also seen that increase in compression ratio increases pressure which effects the combustion temperature to a higher value which produces higher NO\textsubscript{x}. The future work needs to be carried out to maintain low emissions while minimizing fuel consumption. Thus, it limits harmful gases from internal combustion engine.

7. **References**
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8. Abbreviations

\[ \text{Ap} = \text{Area of piston} \]
\[ \text{Lc} = \text{Connecting rod length} \]
\[ \text{R} = \text{Crank radius} \]
\[ \theta = \text{Crank angle} \]
\[ \gamma = \text{Ratio of specific heats} \]
\[ \text{Vcyl} = \text{Cylinder volume} \]
\[ \text{Pcyl} = \text{Cylinder pressure} \]
\[ \alpha = \text{Calibration parameter} \]
\[ \text{mfuel} = \text{Mass of fuel} \]
\[ \text{Q_{LHV}} = \text{Lower heating value} \]
\[ x_b = \text{Burn rate} \]
\[ m_b = \text{Mass of burnt zone} \]
\[ m_u = \text{Mass of unburnt zone} \]
\[ m_{u,inj} = \text{Mass of unburnt fuel due to injection} \]
\[ m_{u\rightarrow b} = \text{Mass transfer from unburnt to burnt zone} \]
\[ \text{L}_{\text{st}} = \text{Stiochiometric ratio} \]
\[ \lambda = \text{Relative air fuel ratio} \]
\[ \lambda_u = \text{Relative air – fuel of unburnt} \]
\[ \lambda_{\text{comb}} = \text{Relative air – fuel of combustion} \]

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