

Development and Validation of a New Zero-Dimensional Semi-Physical NO_x Emission Model for a D.I. Diesel Engine Using Simulated Combustion Process

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ABSTRACT

Reducing NO_x tailpipe emissions is one of the major challenges when developing automotive Diesel engines which must simultaneously face stricter emission norms and reduce their fuel consumption/CO₂ emission. In fact, the engine control system has to manage at the same time the multiple advanced combustion technologies such as high EGR rates, new injection strategies, complex after-treatment devices and sophisticated turbocharging systems implemented in recent diesel engines. In order to limit both the cost and duration of engine control system development, a virtual engine simulator has been developed in the last few years. The platform of this simulator is based on a 0D/1D approach, chosen for its low computational time. The existing simulation tools lead to satisfactory results concerning the combustion phase as well as the air supply system. In this context, the current paper describes the development of a new NO_x emission model which is coupled with the combustion model.

The proposed zero-dimensional, semi-physical, NO_x prediction model is based mainly on a high frequency combustion model (Barba's approach) coupled with a thermodynamic calculation of the temperature (adiabatic flame temperature) in the burned gas products from a stoichiometric mixture. Furthermore, a new empirical correlation is created to relate the corresponding physical components such as the highest local temperature and the available oxygen concentration, describing a uniform progression of NO_x emissions. The model was built and validated over a large range of operating points on a 1.6 liter Euro 5 diesel engine. The simulation results show that the model can predict the multiple effects of exhaust gas recirculation and of the various injection parameters for both single and multi-injection cases.

The model provides the required trade-off between predictability (pure physical models) and simplicity (empirical models) which are mostly incompatible. A major advantage of the final NO_x model is that it does not require any calibration process once the combustion model is identified.

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INTRODUCTION

Studying pollutant emission issues has already become a fundamental priority when developing automotive diesel engines. Due to rising environmental threats and thus emission legislations, industrial engine manufacturers attempt to integrate new emission reduction techniques. After-treatment systems can be considered as the most effective methods to respect strict emission regulations. Nevertheless, the highly expensive demands incite manufacturers to treat the original cause of emissions formation by sophisticated advanced technologies like EGR process, new injection strategies and turbocharging systems.

Current work is part of a simulator project which aims to simulate diesel engine performance and emissions using 0D/1D approaches. This simulator was basically built in order to minimize both cost and number of required experimental tests for development and control purposes.

All features that influence the formation of pollutant emissions in Diesel engine can be summarized as follows:

- Incomplete combustion
- Internal chemical reactions between the different components of the combustion mixture under high temperature and pressure.
- Combustion of the lubricating oil

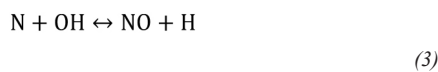
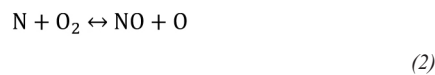
- Combustion of the non-hydrocarbons components such as sulfur and multiple other fuel additives.

The present work is only focusing on nitrogen oxides emission as it constitutes the most critical part of Diesel engine contaminants.

NO_x emissions consist of two essential elements: nitric oxide NO (70-90%) [1] and nitrogen dioxide NO_2 . In experimental work, these two elements are usually not measured separately, but grouped together in a unique engine-out NO_x value.

In Diesel engines, NO_x emission varies with opposite tendencies as compared with other pollutant emissions, as well as compared to the combustion performance and efficiency. The need for the corresponding trade-off is therefore growing more and more in the diesel engine manufacturing industry in order to both confront the environmental regulation norms and to maintain the optimum engine performance.

Many different mechanisms have been adopted to describe the NO formation process such as: thermal path, NO -prompt [2], NO -fuel, N_2O and NNH mechanisms. The first one is considered in the majority of previous researches as the main source of NO production. It is basically represented by the Zeldovich mechanism reactions [1] followed by some modifications in extended [3] and super extended Zeldovich mechanisms (SEZM & MSEZM) [4] [5]:



The application of the mass action law along with corresponding simplifications leads to the following overall expression for the rate of thermal NO formation [6]:

$$\frac{d[NO]}{dt} = \frac{6 \times 10^{16}}{T^{1/2}} \exp\left(-\frac{69,09}{T}\right) [O_2]_e^{1/2} [N_2]_e \quad (4)$$

T: In-cylinder temperature (Kelvin K)

[]_e: Equilibrium concentration (mole/cm³)

In the literature, Zeldovich mechanism widely dominates in most physical and semi-physical NO_x models [7] [8] [9] [10] [11]. The performances of these models depend on the approach and the physical regions in which the kinetic theory is applied.

The latter equation clearly indicates that NO_x formation rate is highly dependent on the formation temperature and the oxygen concentration. In other words, in order to model the engine-out NO_x emission, it should be sufficient to consider equilibrium oxygen concentration and the appropriate temperature. In order to calculate the concentration of various components under equilibrium

conditions, a chemical equilibrium scheme can be added describing the dissociation and the recombination that take place within the cylinder [7] [12] [13].

Various methods have been adopted for temperature calculation. First of all, it is worth to remember that most of NO_x emission forms in high-temperature and slightly lean regions in the cylinder [1]. The adiabatic flame temperature (or the burned gas temperature) has been therefore used in many semi-empirical models [12] [14] [15] [16] [17]. Such models depict the combustion chamber by dividing it into two distinct physical zones: burned and unburned zones. Ericson et al. [18] and Andersson et al. [19] account for the effect of heat losses due to the surrounding fresh unburned gases. While Hegarty et al. [20] proposed a combined temperature which is a function of the average in-cylinder temperature, the adiabatic flame temperature and the estimated heat release rate. Oppenauer et al. [21] and Querel et al. [22] [23] estimated the difference between the temperatures of the burned and unburned zones, which is described by Heider's equation [24] as a function of the in-cylinder pressure. Additionally, these models study the empirical sensitivity of NO_x emissions to EGR and swirl in dynamic engine state. The same approach is also presented by Finesso et al. [25] and Savva et al. [26] using Zeldovich mechanism. The difference in their study as compared to the previously mentioned models, is that each element of the injected fuel is individually modeled having its own path inside the combustion chamber. The instantaneous adiabatic temperature has been also maintained in others semi-empirical models such as those developed by Arrègle et al. [14] and Guardiola et al. [27] who proposed a similar exponential equation for the NO_x formation rate. This kind of models reveals a good estimation for the engine-out NO_x but with high dependence to input parameters, which measurement errors strongly affect the final estimated value. This hypothesis, which is suggested in most of NO_x models, that all components exist in the cylinder in their equilibrium state, is not maintained by Gong et al. [17]. Instead, they presented a characteristic time for the different species that interfere in the NO_x formation process.

Attempts were also made to predict NO_x emission developing correlations and maps based on experimental results obtained on diesel engines. Wang et al. [28] developed neural network models searching empirical correlations between different semi-physical parameters like EGR rate, equivalent air-fuel ratio, engine rotation speed, rail pressure and the estimated in-cylinder temperature. They also estimated the dynamic variation of NO_x emission during transients by adding an EGR correction to the input of the initial model. Similarly, Saravanan et al. [29] evaluated the effect of flame temperature, intake oxygen concentration, fuel density and auto-ignition delay. The temperature in this model is estimated by adding a mean value to the compression temperature (without combustion). They presented a polynomial relation between NO_x emission and the oxygen concentration considered as a surrogate for (the applied) load effect. This relation is also highlighted by Singh et al. [30] by a logarithmic correlation. In addition, they presented the effect of fuel injection pressure, start of injection and mass of injected fuel. Such models attempt to be directly applied in control strategies and for On Board Diagnostics as virtual engine-out NO_x estimators.

Based on this literature survey, it is apparent that in-cylinder NO_x production is basically attached to the burned gas zone. In addition, the kinetic Zeldovich mechanism can be considered as a confident approach to describe the physical NO_x formation. In contrast, the non-linearity of kinetic equations and the uncertainty in tabulated equilibrium concentrations complicate the construction of Zeldovich model. For this reason, semi-empirical models seem to be easier to build, but at the same time hard to be identified due to high number of calibration parameters. For overcoming these problems, present model will replace standard Zeldovich rates and equations by a new empirical correlation coupled with an extrapolated map model. The proposed model highlights the essential components that affect NO_x production operation in the cylinder like the highest local temperature and oxygen excess concentration. Following this approach, NO_x emissions will be attached to the main elements in Zeldovich mechanism by using a simple empirical model with minimum calibration parameters.

EXPERIMENTAL DATA

All pure empirical and semi-empirical prediction models are usually constructed on the basis of experimental data carried out on engine test bench. Current study is based on a large set of experimental data gathered on a 1.6 liter direct injection diesel engine and certified for Euro 5 emissions regulations. The details of the engine are given in Table (1):

Table1. Main specifications of the current diesel engine.

Injection	Direct
Turbocharger	1 stage (VGT)
EGR	HP & LP
Number of cylinders	4
Displacement	1598 cm ³
Compression ratio	15.5
Maximum Injection Pressure	1600 bars
Main Injection Timing (BTDC)	[-2.5;20] CAD

This study does not concern the experimental setup but only the analysis and exploitation of experimental results obtained from a large number of steady state operating points and some specific sweep tests (parametric variations). This data includes around 1400 different operating points distinguishing many different operating conditions: with and without EGR, single and multi-injection cases, cold engine and idle speed points. Some other instantaneous variables have been also given from the bench as in-cylinder pressure as well as inlet and exhaust air pressures serving to identify the basic combustion model.

As far as pollutant emissions are concerned, figures (1) and (2) show the profile of NO_x emissions in function of engine rotation speed N (rpm) and break mean effective pressure BMEP (bars) without and with EGR treatment, respectively.

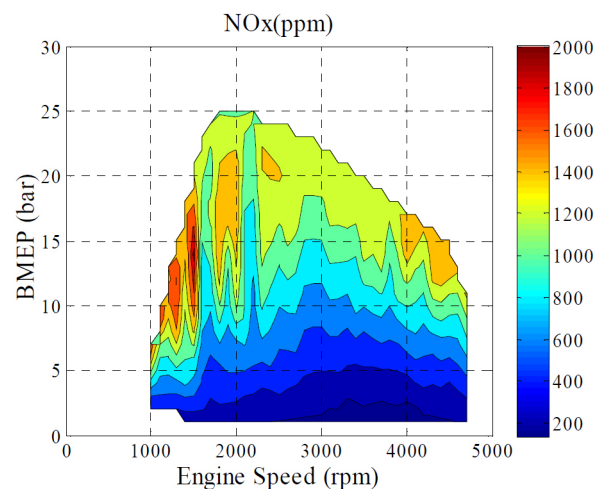


Figure 1. Measured NO_x emissions for steady state operating points without EGR.

From the plot in figure (1), high levels of NO_x emissions obviously occur in the absence of EGR process and especially for low rotational speed values and relatively high engine load cases. In these regions, local in-cylinder temperatures seem to be extremely higher with more homogenous local mixtures. figure (2) shows clearly the effect of EGR treatment over these elevated NO_x emissions reduced by up to half its initial values.

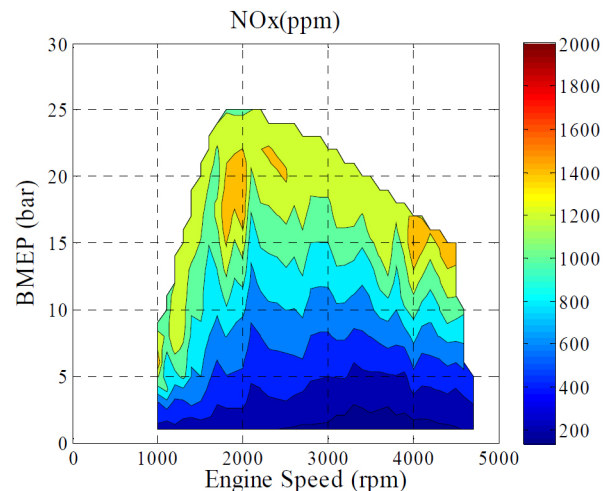


Figure 2. Measured NO_x emissions for steady state operating points with EGR treatment.

MODEL DESCRIPTION

As previously introduced, present model is a part of a long-term project that aims to construct a virtual diesel engine simulator based on zero and quasi-dimensional approaches and predicting both engine performance and pollutant emissions. As will be justified, the proposed NO_x model was developed on the basis of high frequency (cycle resolved) combustion model. In this context, two essential steps are needed to build the whole model. Firstly, it is necessary to identify the used combustion model in order to provide the intermediate high frequency information required by the NO_x model.

This physical combustion model that includes several sub-models to be calibrated has to be coupled with a thermodynamic model for adiabatic flame temperature calculation.

Secondly, based on the experimental data mentioned in the previous section, a specific empirical study has been applied using statistical and mapping methods. In the following, each step is described in details with the intermediate validation results.

Identification of Combustion Model

The main objective of this step is to determine the different parameters of combustion model in such a way that the final simulated pressure coincides as much as possible with the experimental one. The whole current model was built in AMESim environment including an isolated mono-cylinder simulator. Only the period between intake valve closure and exhaust valve opening was taken into account in this simulator.

Three main sub-models are needed in the present work: Fuel Injection sub-model, heat release rate calculation and the cylinder wall heat losses sub-model.

The injection sub-model (as presented in figure (3)) was designed to simulate the different possible split injection strategies using a 3D table to estimate the fuel injection rate.

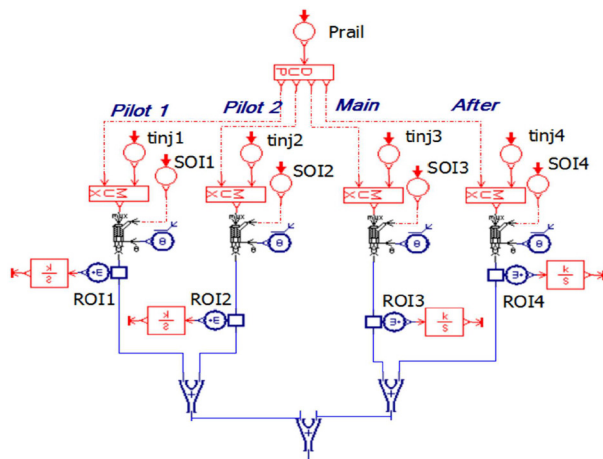


Figure 3. AMESim sketch of multi-injection sub-model enabling four injections per combustion cycle.

Three inputs are required for this table: injection pressure, injection duration and the simulation elapsed time. As a result, the simulated fuel injection rate reveals a good estimation compared to the experimental data with an average absolute error less than 0.3 mg in the final simulated mass of injected fuel.

As far as the heat exchanges are concerned, Woschni model was adopted in the current work to describe the wall heat exchange rate. This approach takes into account the convection heat transfer, while radiation effects are neglected.

As far as combustion model is concerned, many different approaches for the heat release rate prediction have been proposed in AMESim libraries. In this study, the attention is focused on two main criteria: the predictability and the economic issues. According to the literature [31], the mono-zone phenomenological model adopted by Barba et al. [32] represents a significant step forward in comparison to what has been done previously by Wiebe and Chmela [33] in terms of predictability, while maintaining its reduced computational time. More complicated models can obviously be more predictive but limited by the economic challenges due to higher CPU time cost [7] [34] [35] [36] [37] [38]. Given these points, Barba's approach was admitted in the current work. A high frequency sub-model constructed and implemented in the AMESim libraries by Lebas et al. [39] [40] describing Barba's model has been used. The reference single-cylinder model architecture is presented in figure (4).

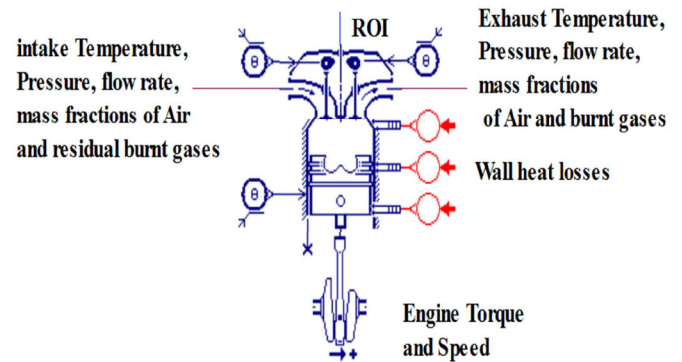


Figure 4. Single cylinder combustion sub-model sketch in AMESim environment.

In his study, Barba identifies three distinct gases: air, fuel and burned gases, and defines three main phases for the combustion process: the delay of auto-ignition, the pre-mixed and the diffusion phases as shown in figure (5).

One set of specific parameters (12 parameters) must be then determined in order to predict each phase by comparisons with experimental data for several engine operating points. In order to streamline this process and to optimize the required development time, a new automatic calibration method was developed using available statistical and mathematical tools in MATLAB environment. This method was successfully validated on two different diesel engines. These parameters are given in the figure (5) to allow the replication of current model. As shown in the mentioned figure, each parameter aims to describe a specific effect during all combustion phases. More details about the signification of these parameters are available in Barba's model [32]. Symbols used in this figure are extracted as they exist from AMESim libraries in order to facilitate their validation by AMESim users.

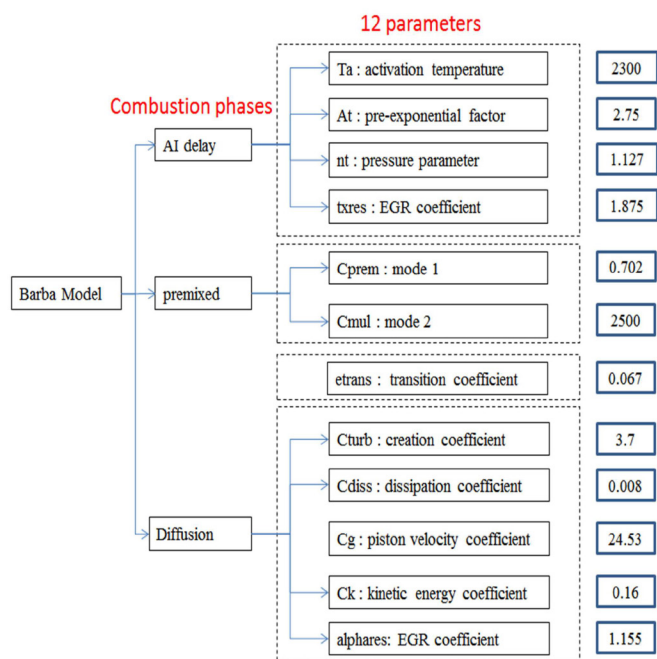


Figure 5. The identified parameters values for Barba's combustion model.

Figures (6) and (7) show the results for the present engine upon six validation criteria that represents the in-cylinder pressure and the fuel burning rate. CA05, CA10 and CA50, presented in figure (7) correspond respectively to the time during the combustion cycle when 5, 10 and 50% of the fuel mass is burnt. The first two figures (6-a) and (6-b) represent the pressure values. The indicated mean effective pressure is well predicted with a required accuracy of ± 1 bar. The simulated maximum in-cylinder pressure plays a key role in the proposed model through its effect on the highest in-cylinder temperatures. As illustrated in figure (6-b), the maximum in-cylinder pressure is well estimated by ensuring the required trade-off between all operating points. The same result is almost observed for the location of the maximum pressure, which is outlined by the crankshaft angle. It is worth to note that the blue bars in figures (6) and (7) represent the tolerable marge error regarding the tests over each of the four cylinders error margin, due to cylinder-to-cylinder variations.

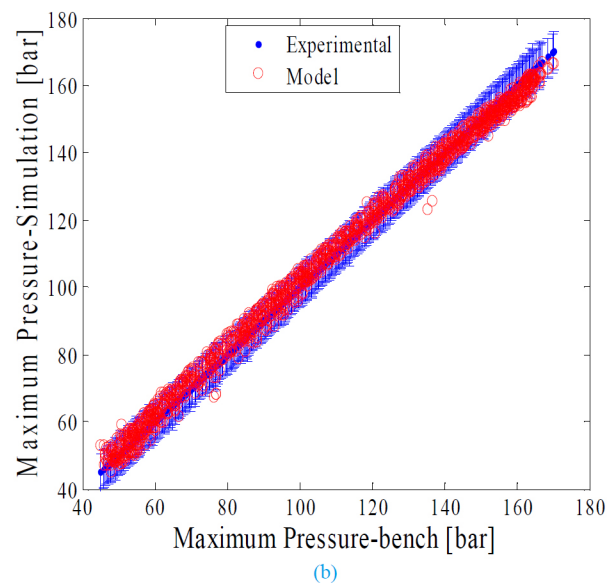
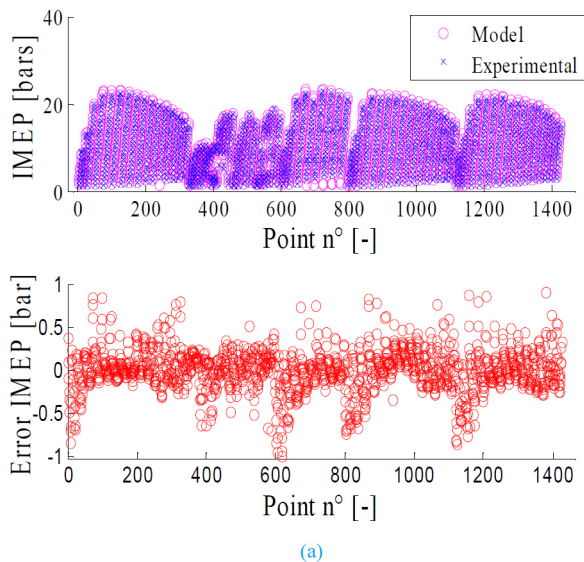


Figure 6. Validation of identification results concerning the indicated mean effective pressure (a) and the maximum in-cylinder pressure (b).

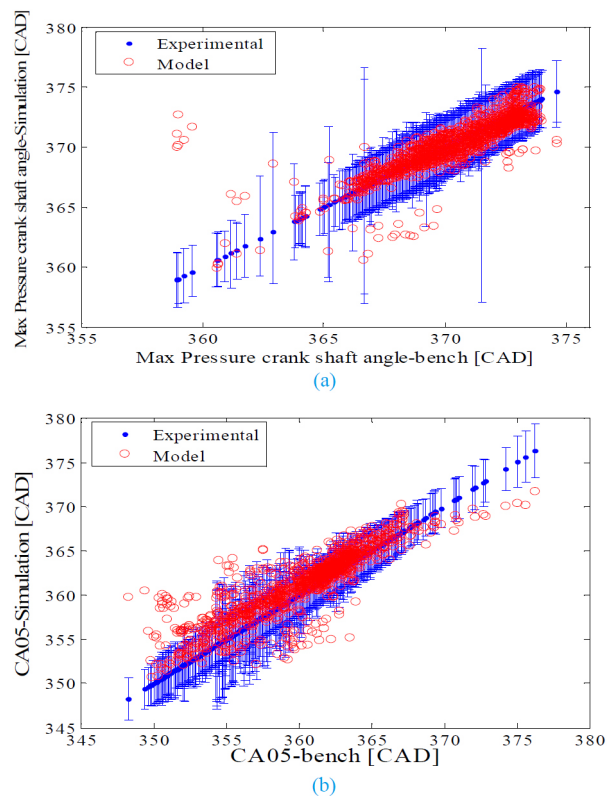


Figure 7. Validation of the combustion phases by comparing measured and simulated maximum pressure crankshaft angle-bench (a), CA05 (b), CA10 (c) and CA50 (d).