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Prediction of NOx emissions for high speed DI Diesel engines using a semi-empirical, two-zone model

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ABSTRACT

In the present paper, the authors have applied a newly developed semi-empirical, zero-dimensional, two-zone model on two automotive DI Diesel engines: a heavy (truck) and a light-duty (passenger car) engine. The aim of the study is to examine model's ability to predict NO_x trends with the variation of engine load/speed, fuel injection timing, EGR rate, boost pressure and fuel injection pressure.

The model makes use of cylinder geometrical data, basis engine operating data and the experimental combustion rate, as deduced from heat release analysis, to calculate engine tailpipe exhaust NO emissions and their formation history inside the combustion chamber. Apparently, combustion and hence NO_x formation, occurs inside the burnt zone. The required air for the combustion is provided from the unburnt zone. The entrained air mass, at each time step, is calculated using a mean equivalence ratio value and the corresponding fuel mass burnt during the calculation time step (as defined by the experimental combustion rate). The mean equivalence ratio value, at each operating point, is obtained using a new correlation which makes use of parameters derived from the processing of the measured pressure trace, as well as typical engine operating parameters. NO (the predominant part of total NO_x) is calculated using the extended Zeldovich mechanism at each time step (during combustion and expansion). Thus, the NO formation history inside the cylinder is provided, considering the two-zone approach. The specific concept of the two-zone approach combined with the utilization of engine's measured parameters, the empirical correlation for the mean equivalent ratio and the simplicity of the model's calculations, provide a robust and time efficient tool for NO prediction which can be applied on various engine configurations and operating conditions without extended calibration.

The derived results reveal model's ability to predict exhaust NO emissions and trends satisfactorily at a variety of engine settings. Considering its low computational cost, it can serve as a useful tool for emissions trade-off optimization studies, as well as for real-time model based NO_x control applications.

1. Introduction

A large number of vastly populated cities worldwide face the important issue of pollution, which takes a toll in human health and diminishes life quality standards [1]. Today it is well accepted that a significant part of pollution is attributed to vehicle exhaust emissions. The strong demand to reduce this form of pollution led to the implementation of rigid regulations [2], forcing the internal combustion engine (*ICE*) industry to adopt measures for the reduction of these harmful emissions. As a result, manufacturers concentrate on developing technologies, aiming to reduce exhaust emissions and meet with strict emissions regulations.

Up to now, a series of methodologies has been proposed to serve the purpose of reduced exhaust emissions [1,3] focusing either on low-emission engine development (in-cylinder emission control-primary measures) or use of after-treatment technologies (secondary measures) or even a combination of the above. Towards this effort, simulation models are intensely used to develop and implement these methodologies, based on their ability to predict exhaust emissions and mainly trends at a low expense in comparison with experimental tests. Since NO_x is a major Diesel engine pollutant, authors were motivated to further develop and apply a formerly introduced simplified model [4] for *NO* emissions prediction on various engine configurations at a variety of engine operating conditions and settings.

The related, up to date literature records a significant variety of models that can predict exhaust emissions. A model configuration, common for NO_x prediction, is the multi-zone phenomenological one [5–9], which considers the local mechanisms that drive mixture formation and combustion. The latter is achieved using phenomenological/semi-empirical relations for spray penetration, air fuel mixing

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Nomenclature

ABDC	After Bottom Dead Center
ATDC	After Top Dead Center
bara	absolute pressure measured in bar
CA	Crank Angle
CAD	Crank Angle Degrees
CFD	Computational Flow Dynamics
COC	Center Of Combustion
cp	constant pressure specific heat capacity [J/kmol/K]
dH_{sens}	sensible enthalpy difference between reactants and combustion products
DI	Direct Injection
dQ	energy (heat) differential [J]
ECU	Engine Control Unit
EESC	Extended European Stationary Cycle
EGR	Exhaust Gas Recirculation
EVO	Exhaust Valve Open
h	specific enthalpy [J/kmol] or [J/kg]
H	total enthalpy [J]
H_{sens}	sensible enthalpy ($H_{sens}(T) = H(T) - H(25\ ^\circ C)$) [J]
HRR	Heat Release Rate
ICE	Internal Combustion Engine
IVC	Intake Valve Closure [°CA ATDC]
LHV	Lower Heating Value [J/kg]
m	Mass [kg]
MARE	Mean Absolute Relative Error [%]
MW	*M*olecular *W*eight [kg/kmol]
N	engine speed [rpm]
n	number of moles [kmole]
n_{cyl}	number of cylinders [–]
P	power [kW]
p	pressure [Pa]
R	reaction rates [kmol/m^3/s]
RG	Residual Gas
RMSE	Root Mean Square Error
SOC	Start Of Combustion
SOI	Start Of Injection
T	temperature [K]
TDC	Top Dead Center
V	volume [m^3]
x	charge mole fraction [ ]

Greek symbols

ΔCA	Crank Angle step [°]
Φ	equivalence ratio [–]

Subscripts

b	burnt
cyl	cylinder
e	equilibrium
f	fuel
i	*i*th crank angle, *i*th operating point
IA	*I*ntake *A*ir
IM	*I*ntake *M*anifold
k	*k*th iteration
p	products
r	reactants
tr	trapped
ub	unburnt
z	zone order number

and combustion. *CFD* models [10,11] are also used for NO_x prediction because they describe the in-cylinder phenomena fundamentally. Although these models are proven able to calculate local temperatures and chemical compositions and hence estimate NO_x reliably and accurately [10,12,13], they present a significant disadvantage: increased computational cost (computational time and computing power). This is a preventing factor for their use in real-time applications (e.g. model-based/closed loop control). In addition, their significantly complex structure and high calibration demands are also factors which limit their application. On the other hand, the use of single-zone models appears to be a suitable solution to this problem [14–16] due to their simplicity. Their ability to provide information only for the average cylinder temperature (and conditions), makes direct NO_x formation calculation impossible. Zero-dimensional two-zone models [4,17,18] or multi-zone models [19–21] can be applied to overcome this difficulty, along with fully empirical/statistical/mean-value [22–25], semi-empirical models [26–31] or even neural network-based models [32] presenting very low computational cost. The latter require significant calibration effort, so a comprehensive experimental database is required. Even in this case, acceptable accuracy can be achieved only inside the calibration range, mainly because of their physical base deficiency.

The aforementioned difficulties, combined with the trending internal combustion engine industry requirement for NO_x prediction models that will have acceptable accuracy, low calibration cost and at the same time be simple and easy to handle, motivated the authors to develop a simplified, zero-dimensional *NO* prediction model based on a two-zone approach. The proposed model offers a compromise between single- and multi-zone phenomenological combustion models. For this reason, a recently developed model has been applied on two different Diesel engine configurations (a heavy-duty truck engine and a light-duty car engine) at various operating conditions and engine settings [33,34]. The present paper records the significant work that has been conducted to strengthen the model's predictive ability. This has been accomplished by introducing a new empirical/statistical approach into the existing physical model [4], to expand its implementation range. To further fulfill this target, additional operating points of the aforementioned engines were used to expand its range of validation. Specifically the effect of the following parameters has been examined: injection timing, injection pressure, *EGR* rate and boost pressure. The validation range considers various engine loads and operating speeds.

The model makes use of the measured cylinder pressure trace as input, as well as the combustion rate derived from it using a well-validated model integrated into an in-house diagnosis software [35,7,36,37]. A two-zone approach is then used to predict *NO* emissions. The model concept is based on the increase of the burnt zone mass, due to the entrainment of the burnt fuel mass and the corresponding oxidizer charge (air, *EGR* and residual gases) acquired from the unburnt zone at each time-step. These are then used to calculate the thermodynamic properties of the burnt zone and finally the *NO* formation rate. The burnt and unburnt zones are considered as autonomous and evolve inside the combustion chamber, where the first law of thermodynamics abides. *NO* formation is calculated via the extended Zeldovich mechanism.

Models of similar philosophy have been already presented in the literature [38–40] adopting a completely different approach for NO_x estimation. The combustion rate is estimated using phenomenological/semi-empirical formulas for air entrainment, fuel/air mixing, heat and mass transfer etc. These introduce higher computational cost, but most important, uncertainties concerning the accuracy of the predicted combustion rate which affects local temperature and hence *NO* formation. In the proposed model, this issue is fronted by using the actual