A Parametric Analysis of Exhaust Emissions Prediction during Transient Turbocharged Diesel Engine Operation

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ABSTRACT: The modeling of turbocharged diesel engine transient operation appeared in the early 1970s and continues to be in the focal point of research due to the importance of transient response in the everyday operating conditions of engines. Simulations of various levels of complexity have been used so far to study engine performance during transients. On the other hand, the very important issue of exhaust emissions has been studied mainly on an experimental rather than simulation basis, owing to the high computational time required for the analysis of many cycles. The study of transient emissions from turbocharged diesel engines is extremely important for the manufacturers, since newly produced engines must meet the stringent regulations concerning exhaust emissions levels. In the present work, a comprehensive two-zone transient diesel combustion model is used for a parametric analysis of exhaust emissions prediction during load changes. The parameters studied are the load characteristics (magnitude and change schedule), the exhaust manifold volume, the geometric turbine inlet area as well as the exhaust valve opening timing. Also, the very interesting case of insulated cylinder walls is investigated. Analytical diagrams are provided for the time histories of nitric oxide (NO) and soot emissions, which depict the effect of each parameter considered. Moreover, the peculiarities of each case are discussed mainly in relation to turbocharger lag effects.

Keywords: turbocharged diesel engine, transient operation, exhaust emissions, parametric study

NOMENCLATURE

A	Soot formation model constant
E	Activation energy [J/kmol]
k_f	Forward reaction rate constant [m^3/kmol/s]
m	Mass [kg]
n	Soot formation model exponent
p	Pressure [N/m^2]
R_i	One-way equilibrium constant for reaction i
R_{mol}	Universal gas constant, 8314.3 J/kmol/K
t	Time [sec]
T	Temperature [K]
V	Volume [m^3]

Subscripts

e	Equilibrium
f	Fuel
sc	Soot oxidized
sf	Soot formed
sn	Soot net

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Abbreviations

°CA	Degrees crank angle
EVO	Exhaust valve opening
NO	Nitric oxide
PSZ	Plasma spray zirconia
rpm	Revolutions per minute
SN	Silicon nitride
TDC	Top dead center

1. INTRODUCTION

The turbocharged diesel engine is nowadays the most preferred prime mover in medium and medium-large units application. Moreover, it continuously increases its share in the highly competitive automotive market, owing to its reliability that is combined with excellent fuel efficiency.

During the last decades, diesel engine modeling has greatly supported the study of transient operation. Particularly, simulations of various levels of complexity have been used to study engine performance during transients and extended analyses have been conducted [1-5]. On the other hand, the vital issue of exhaust emissions, which is of primary concern to engine manufacturers, has been studied mainly on an experimental rather than simulation basis [6,7]. The latter is the result of a compromise which has to be made, since transient simulations require high computational times, which would be prohibitive if exhaust emissions prediction was also included. Thus, transient codes incorporating a multi- or even a two-zone combustion model are scarce [2].

As it has long been established, turbocharger lag is the most notable effect related to turbocharged diesel engine transient response [2]. As a result, off-design operation and increased exhaust emissions are observed under such conditions. In both major cases of transient operation, i.e. load acceptance with constant governor setting and acceleration under constant load, the air supply to the engine during the early cycles of the transient event is not sufficient, since the turbocharger needs more time to accelerate and produce higher boost pressure, compared to fuelling response. Thus, fuel-air equivalence ratio assumes higher than normal values, favoring soot formation, which is noticed as black smoke coming out of the exhaust pipe. Moreover, higher combustion temperatures occur resulting in elevated nitric oxide (NO) concentrations in the exhaust.

The aim of this paper is to evaluate the effect of various parameters on NO and soot exhaust emissions during transient turbocharged diesel engine operation. To this target, a two-zone transient diesel combustion model developed in-house is used, having the added advantage of limited requirement in terms of execution time and computer memory. Analytical modeling of fuel spray and in-cylinder processes is included, while detailed equations concerning all engine sub-systems, describe the peculiarities of transient operation. The parameters considered are the magnitude of the applied load, the load-time schedule, the exhaust manifold volume, the geometric turbine inlet area and the exhaust valve opening timing. Also, the interesting case of insulated cylinder walls is investigated. The results of the study are given in a series of analytical diagrams, which depict the effect of each parameter considered on transient exhaust emissions of diesel engine.

2. SIMULATION ANALYSIS

2.1 Thermodynamic Modeling

The evaluation of the thermodynamic processes is based on the first law of thermodynamics and the perfect gas state equation, combined with the various sub-models incorporated into the simulation code. The chemical species considered are N_2, O_2, CO_2, H_2O, CO, H_2, NO, OH, N, H and O. The complete chemical equilibrium scheme proposed by Way [8] is applied for the calculation of each species concentration at each time step. Polynomial expressions are used for the species considered, concerning the evaluation of internal energy, enthalpy and specific heat capacities [9].

The model separates cylinder contents in two zones: the air (unburned) zone, consisting of pure air, and the fuel spray (burned) zone, consisting of the combustion products, injected fuel and the incoming air from the air zone. During compression only one zone (that of pure air) exists. As soon as combustion begins, all equations are solved separately for each zone, providing the zonal volume, temperature and species concentration, with the pressure assumed the same in both zones. Also, a mean state of the cylinder contents at each time step is calculated, assuming isenthalpic mixing between the two zones [10].

For heat release rate predictions, the fundamental model proposed by Whitehouse and Way [11] is applied.

Heat loss to the cylinder walls is simulated using the model of Annand [12]. During transient operation, the thermal inertia of the cylinder wall is taken into account, using a detailed heat transfer scheme [13].

2.2 Nitric Oxide (NO) Formation Model

Since it is well established that NO formation cannot be predicted accurately by chemical equilibrium considerations, the chemical kinetics model proposed by Lavoie *et al.* [14] is used; it describes the extended Zeldovich kinetics scheme. The following three chemical equations apply, together with the respective forward reaction rate constants

$$\begin{aligned} &N+NO \rightleftharpoons N_2+O, \quad k_{f1}=3.1\times10^{10}\, e^{(-160/T)} \\ &N+O_2 \rightleftharpoons NO+O, \quad k_{f2}=6.4\times10^{6}\, T\, e^{(-3125/T)} \\ &N+OH \rightleftharpoons NO+H, \quad k_{f3}=4.2\times10^{10} \end{aligned} \qquad (1)$$

The change of NO concentration is given by

$$\frac{1}{V}\frac{d((NO)V)}{dt}=2(1-\alpha^2)\frac{R_1}{1+\alpha R_1/(R_2+R_3)} \qquad (2)$$

where $\alpha=(NO)/(NO)_e$ and R_i is the one-way equilibrium rate for reaction i, which is defined as

$$\begin{aligned} R_1&=k_{f1}(N)_e(NO)_e \\ R_2&=k_{f2}(N)_e(O_2)_e \\ R_3&=k_{f3}(N)_e(OH)_e \end{aligned} \qquad (3)$$

2.3 Soot Formation Model

Soot is modeled as particulates consisting of carbon atoms. The model proposed by Hiroyasu *et al.* [15], as modified by Lipkea and DeJoode [16], is used for the calculation of the net soot rate, which is defined as the difference between formation and oxidation rates. The former is given by

$$\frac{dm_{sf}}{dt}=A_{sf}\, dm_f^{0.8}\, p^{0.5}\, e^{(-E_{sf}/(R_{mol}\,T))} \qquad (4)$$

while the latter is defined as

$$\frac{dm_{sc}}{dt}=A_{sc}\, m_{sn}\, (p_{O_2}/p)\, p^{n}\, e^{(-E_{sc}/(R_{mol}\,T))} \qquad (5)$$

Finally, the net soot formation rate is expressed as follows

$$\frac{dm_{sn}}{dt}=\frac{dm_{sf}}{dt}-\frac{dm_{sc}}{dt} \qquad (6)$$

2.4 Dynamic Analysis

Various detailed sub-models are incorporated into the simulation code, which provide an in-depth analysis of important engine features during transient operation. These refer to ‘true’ multi-cylinder engine modeling, fuel pump operation under dynamic conditions, friction modeling at each °CA, detailed connecting rod modeling and crankshaft torque balance [4,17].

3. RESULTS AND DISCUSSION

Prior to the parametric study, a detailed experimental investigation, concerning engine performance, was carried out on a 6-cylinder, 4-stroke, turbocharged and aftercooled, diesel engine of 16.62 lt. total displacement volume and rated power 236 kW at 1500 rpm operating under steady-state and transient conditions [4]. After gaining confidence in the model predictive capabilities, an extensive parametric study was conducted in order to investigate the effect of various parameters on NO and soot emissions. An important feature of the engine under study is its very high mass moment of inertia (3-4 times greater than in similar configuration), which tends to limit the differences between the cases examined.

Figure 1 illustrates a typical load increase transient event of 10-80% commencing from an engine speed of 1180 rpm; this forms the baseline for the parametric study that follows. The upper sub-diagram in Fig. 1 shows the NO and soot (exhaust) emissions development during the nominal transient event, while in the lower sub-diagram the engine speed response together with the fuel-air equivalence ratio development are illustrated. Also, the maximum value of the mean (comprising of both burned and unburned zones contribution) temperature in each transient cycle is provided.

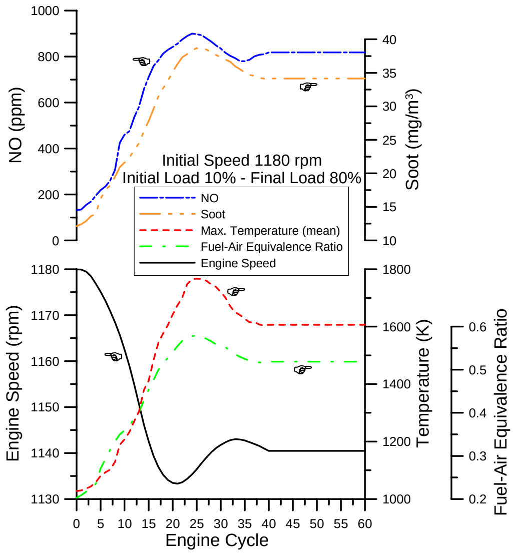

Figure 1: Development of NO and soot emissions, mean temperature, fuel-air equivalence ratio and engine speed response during the nominal transient event.

During the first cycles of the transient event, NO and soot emissions are low, due to the low values of fuel-air equivalence ratio and, thus, temperature, resulting from low engine load. As the load increases, emissions increase too. NO exhaust emission development follows closely the temperature profile; this was expected due to the well known strong dependence of NO formation on temperature. Soot emission increases too, owing to the increase of fuel-air equivalence ratio (i.e. greater amount of fuel burned, as the result of the governor response to engine speed drop), as well as, due to the higher temperature levels, which nonetheless affect both soot formation and oxidation rates. Also, the turbocharger lag effect is evident during the early cycles (up to cycle No. 20, which is indeed an early cycle owing to the high total mass moment of inertia of the engine in hand) of the transient event, favoring higher emissions (especially black smoke) due to the higher fuel-air equivalence ratios experienced.

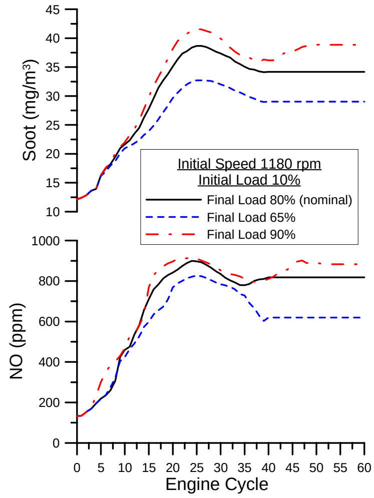

Figure 2: Effect of load change magnitude on NO and soot emissions during transient operation after a load increase.

The effect of the load change magnitude is demonstrated in Fig. 2. Engine operation at higher loads practically means higher values of fuel-air equivalence ratio, approaching stoichiometric ones. As a result, higher in-cycle pressures and temperatures occur and, thus, NO and soot emissions are greater. Moreover, turbocharger lag effect is more prominent in the case of higher load changes, leading to greater peak values of these emissions during the transient event.

Figure 3 presents the development of NO and soot emissions during transient operation for various realistic load-time schedules. As was expected this parameter affects only the profile of emissions and not their final steady-state values. The worse case for both emissions is the instantaneous load application (Δt_{load}=0 sec). Here, the final load torque is applied during the first transient cycle, leading to a more abrupt governor response, resulting in higher fuellings (middle sub-diagram of Fig. 3). At the same time, turbocharger lag causes a delay in boost pressure build-up. As a result, higher values of fuel-air equivalence ratio are observed (not shown in Fig. 3) and, thus, higher in-cycle temperatures, which favor both NO and soot formation. A pulsating recovery is also observed (intensified for higher load changes), which is unacceptable. On the contrary, a longer load change duration causes smoother response of the engine and exhaust emissions.

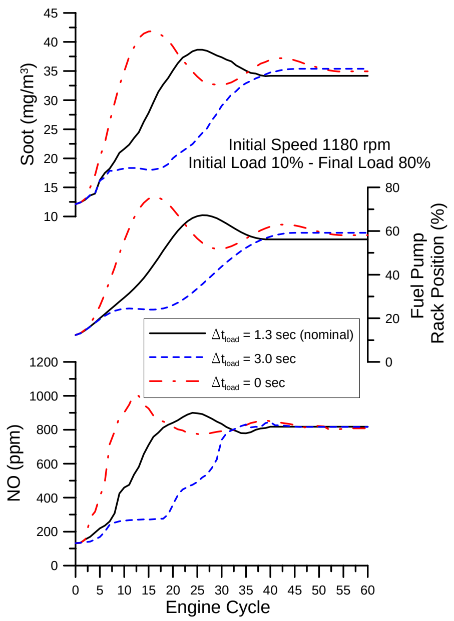

Figure 3: Development of NO and soot emissions and fuel pump rack position response during transient operation after a load increase, for various load-time schedules.

The effect of the exhaust manifold volume on exhaust emissions is illustrated in Fig. 4, together with the mean exhaust manifold pressure development during transient operation. A ten times larger exhaust manifold volume (resembling a constant pressure turbocharging system) causes a significant decrease in mean exhaust manifold pressure. As a result, turbocharger compressor produces low boost pressure, which combined with the increased fuelling, results in higher values of fuel-air equivalence ratio, worsening accordingly the exhaust emissions. On the other hand, a five times smaller exhaust manifold improves slightly engine response and exhaust emissions.

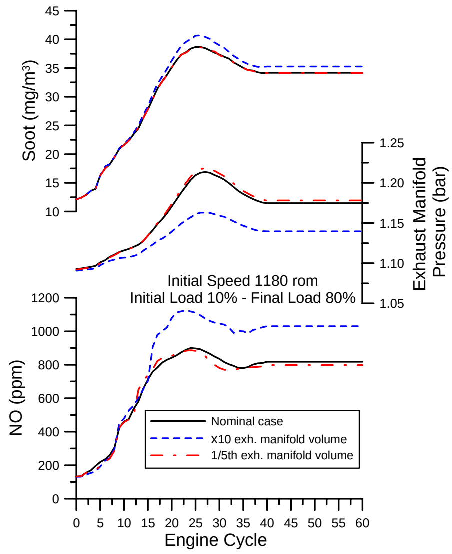

Figure 4: Effect of exhaust manifold volume on NO and soot emissions and mean exhaust manifold pressure response during transient operation after a load increase.

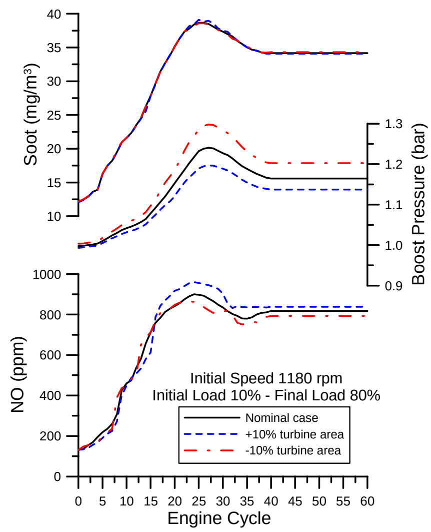

Figure 5: Effect of geometric turbine inlet area on NO and soot emissions and boost pressure response during transient operation after a load increase.

Figure 5 depicts the effect of the geometric turbine inlet area (a feature of variable geometry turbine (VGT) operation), which is a measure of turbine size, on exhaust emissions and boost pressure response during transient operation. Consistent with previous research [3], a smaller turbine inlet area improves engine response; this is documented in Fig. 6 by the higher values of boost pressure. Consequently, lower values of fuel-air equivalence ratio are to be expected (fuelling is not affected) reducing NO and soot exhaust emissions. However, the effect seems to be rather weak, especially as regards soot emission.

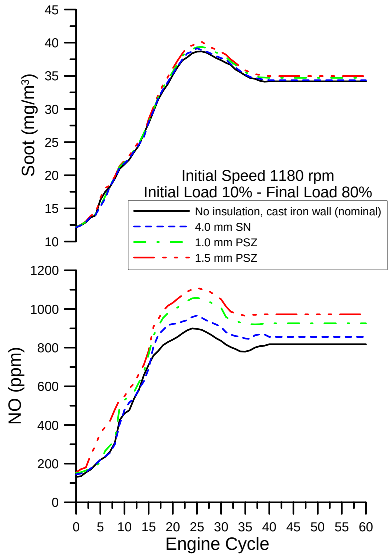

Figure 6: Effect of insulated cylinder walls on NO and soot emissions during transient operation after a load increase.

The very interesting case of insulated cylinder walls is investigated in Fig. 6. Two different insulators, i.e. plasma spray zirconia (PSZ) and silicon nitride (SN) are examined [13]. Clearly a higher degree of insulation increases NO emission, whereas it only slightly influences soot emission. The main impact of insulation is the increase of cylinder gas temperature, due to lower heat loss to the walls. At the same time it has been found to affect engine and turbocharger response only moderately [13]. As a result, NO emission is higher, owing to its direct dependence on gas temperature. On the other hand, the effect of temperature on both soot formation and oxidation processes (see Eqs. (4) and (5)), increase soot emission only moderately.

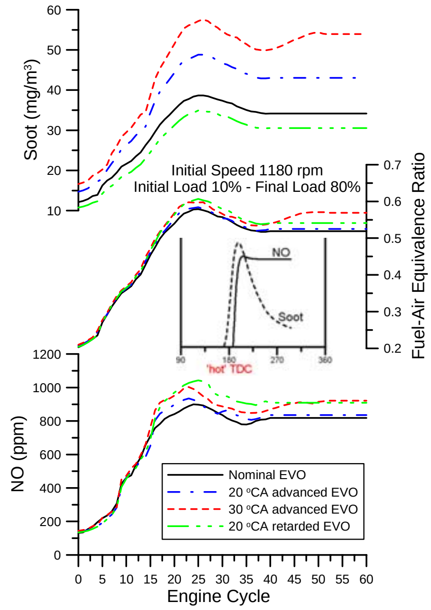

Figure 7: Development of NO and soot emissions and fuel-air equivalence ratio during transient operation after a load increase, for various exhaust valve opening timings.

Finally, Figure 7 illustrates the effect of exhaust valve opening (EVO) timing on NO and soot emissions. Advancing the EVO timing results in higher values of both NO and soot emissions (up to almost 50% concerning soot), while retarding it causes a decrease in soot emission and an increase to NO emission, compared to the nominal case. Different mechanisms for each behavior lie behind these trends. On one hand, soot obtains higher values with advanced EVO timing due to the lesser available time for its oxidation during expansion; this can be also documented in the middle sub-diagram of Fig. 7, showing the development of NO and soot during the closed part of the engine cycle. On the other hand, NO emission is mainly influenced by the maximum cycle temperature, which is directly affected by the fuel-air equivalence ratio value. Advanced EVO timing causes a reduction in piston work (shorter effective expansion stroke), forcing the governor to increase engine fuelling even more, in order to respond to the load increase. At the same time, the energy delivered to the turbine is higher, leading to higher boost pressures. The combination of increased fuelling and boost pressure ultimately leads to higher values of fuel-air equivalence ratio. In the case of retarded EVO, the decrease in boost pressure is dominant (due to the lower energy delivered to the turbine), resulting again in higher values of equivalence ratio.

SUMMARY AND CONCLUSIONS

A comprehensive two-zone transient diesel combustion model has been applied for an extensive parametric study of NO and soot exhaust emissions prediction during transient operation of turbocharged diesel engine. The main findings of the analysis, for the current engine-load configuration, are the following:

- NO and soot emissions development during transient operation after a load increase follow closely the temperature and fuel-air equivalence ratio profiles. Turbocharger lag, mainly during the early cycles, worsens emissions and is the main reason for the black smoke coming out of the exhaust pipe.
- The magnitude of the applied load directly affects emissions; increased values of NO and soot emissions are noticed for higher load changes.
- The load-time schedule has a strong impact on the profile and peak values of exhaust emissions, while the final steady-state values are practically unaffected.
- A larger exhaust manifold volume worsens engine response and increases exhaust emissions, mainly NO.
- A smaller turbine inlet area improves slightly exhaust emissions.
- The higher the degree of cylinder wall insulation, the higher the NO emissions. Soot emission is influenced moderately.
- Advancing EVO timing increases dramatically soot emission (up to almost 50% for the cases examined), while a retarded EVO timing improves it. NO emission is increased in both cases.

Table 1 summarizes the results concerning the change in peak and cumulative (for all cycles up to equilibrium) values of NO and soot emissions for the cases examined compared to the nominal case (load change 10-80%, load change duration 1.3 sec, cast iron wall). It is suspected that even greater differences between the cases examined exist, which could not be revealed due to the high mass moment of inertia of the engine under study. A comprehensive experimental validation of the model's exhaust emissions results is under way.

Table I: Percentage change of peak and cumulative exhaust emissions values for the cases examined compared to the nominal case.

Parameter		Peak values		Cumulative values	
		NO	Soot	NO	Soot
Final Load	65%	-8.0%	-15.4%	-17.1%	-12.5%
	90%	1.8%	7.5%	47.9%	43.8%
Load Change Duration	0 sec	11.7%	8.2%	66.4%	59.4%
	3.0 sec	-6.1%	-8.5%	-17.4%	-5.0%
Exhaust Manifold Volume	1/5th	-1.4%	-0.2%	-1.1%	–
	x 10	25.1%	5.2%	9.9%	3.0%
Turbine Inlet Area	-10%	-3.8%	-0.2%	-0.3%	–
	+10%	6.7%	1.1%	-0.9%	0.1%
Insulation	4.0 mm SN	7.3%	1.3%	2.6%	0.4%
	1.0 mm PSZ	17.5%	1.8%	10.4%	1.4%
	1.5 mm PSZ	23.4%	3.7%	16.2%	2.6%
EVO timing	20 ^{o}CA adv.	3.9%	26.3%	-0.5%	–
	30 ^{o}CA adv.	11.4%	49.0%	44.9%	37.4%
	20 ^{o}CA ret.	15.9%	-9.6%	7.0%	1.9%

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