A Coupled Diesel Combustion and Soot Formation Model for KIVA II Code: Characteristics and Experimental Validation

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ABSTRACT

A modified version of the Kiva2 code was used to study the combustion and the soot formation processes in a direct injection, naturally aspirated Diesel engine. The modified submodels concern the following topics:
- the drop break up,
- the spray-wall interaction,
- the autoignition phenomenon and the high temperature combustion.

Using the improved version of the code, the main combustion features of the tested engine were investigated: numerical results were compared with those deriving from the experiments.
Once tuned the combustion model constants and obtained predictions of in cylinder pressure cycles well related with the experimental data for different test cases, a multistep soot formation model was implemented and tested.
The model performances are discussed in comparison with detailed in cylinder experiments carried out with the two colours technique.

INTRODUCTION

The increasing impact of the internal combustion engines on the environment has led to the introduction of more restrictive legislation to control pollution by engine exhaust emissions.

EEC [g/Km]	CO	HC+NOx	PM
91/441 (current)	2.72	0.97	0.14 IDI 0.18 DI
Phase II 1996: gasoline	2.2	0.5	
IDI Diesel	1.0	0.7	0.06
DI Diesel	1.0	0.9	0.1
Phase III 1999:			
(MVEG) gasoline	1.5	0.2	
Diesel	0.5	0.45	0.04

Table 1: The forecast evolution of EEC limits for passenger cars (<2500 Kg)

In particular the European legislation, reported in tables 1 and 2 both for light duty and heavy duty applications, will closely match, by the end of the century, the California ULEV standards.

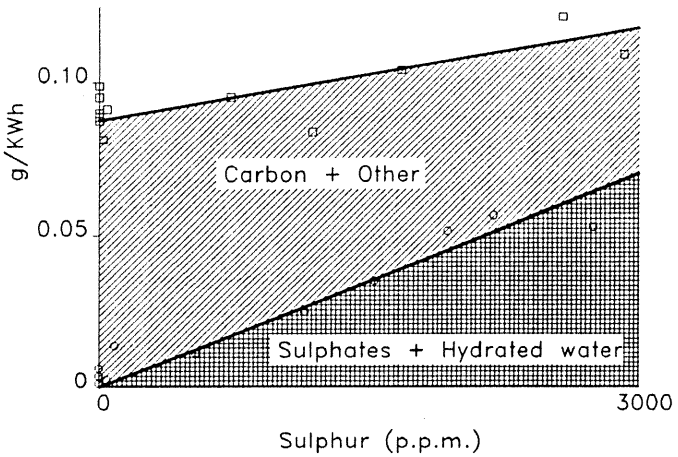
Date	from Jul 92 Euro 1		95/96 Euro 2	1999 * Euro 3
Applicability	T.A.	C.O.P.	T.A. C.O.P.	T.A. C.O.P.
CO [g/kWh]	4.5	4.9	4.0	2.5
HC [g/kWh]	1.1	1.23	1.1	0.7
NOx [g/kWh]	8	9	7	< 5
PM [g/kWh]				
< 85kW	0.61	0.15	0.15	< 0.12
> 85kW	0.36			

T.A.: Type Approval C.O.P.: Conformity of production
* In discussion

The forecast evolution of EEC limits for heavy duty engines
Table 2

It is interesting to notice that, for light duty applications, in the next future the emission limit for diesel powered vehicles will be different from the spark ignition engine powered ones'.
The European emission test procedure for heavy duty engines applications is based on the 13 modes steady state cycle (ECE R49); it's a common experience of engine manufacturers and research laboratories that the Euro 3 limits are probably more severe than the USA '98 limits for heavy duty trucks on transient procedure (HC=1.2, NOx=4, PM=0.1 [g/BHP/h]) [1].
Therefore the diesel engines for both heavy duty and light duty applications have to be improved to match the emission limits provided for the end of the century. Because of the well known trade off between NOx and particulate emissions, any attempt to reduce NOx leads to further problems in particulate emissions control.
In the emission test procedures, the particulate is measured by filtering part of the diluted engine exhausts under controlled test conditions. The particulate sample is composed by the insoluble and the soluble fractions, whose amounts vary in dependence of the combustion system and the ring pack design, as well as of the engine operating conditions.

However it can be noted that, with a careful optimisation of the engine's structural design (piston, ring pack, cylinder liner, heads and seals) and of the injection apparatus, the modern diesel engines have achieved a significant reduction of the global HC emission levels and of the lube oil consumption. Therefore also the soluble organic fraction in the particulate is strongly reduced [2].
The insoluble fraction is mainly composed by carbonaceous materials (usually named soot), sulphates and bonded water. In Europe as well in USA the tendency to use fuels with low sulphur content is well assessed [3]. Therefore the soot contribution to the insoluble organic fraction will be predominant, as shown in fig. 1 [2].



Insoluble particulate emissions versus fuel sulphur contents
Fig. 1

Any strategy aimed to further reduction of the total particulate matter must be turned to improve the in cylinder diffusion combustion and to deep the knowledge of the fundamental processes leading to soot formation and oxidation.
The multidimensional modelling of the combustion phenomenon and of the pollutants formation processes may be considered an useful tool for the combustion system design in the next future.
Therefore in the present paper the status of development of a new coupled diesel combustion and soot formation submodel for the Kiva2 code is pointed out. The main features and performances of the model are discussed, comparing the numerical results with some experimental data.

THE NUMERICAL CODE

In this work, to simulate the diesel engine combustion, the Kiva2 code, with some improvements, was used [4].
In fact, any pollutant emission model needs to start from a proper set of pressure, temperature and fluid dynamic conditions. The original version of the code is not able to reproduce correctly the diesel combustion characteristics, as pointed out by Gonzales et al. [5] for direct injection systems, or by Patterson et al. [6] for D.I. quiescent combustion systems, or by Belardini et al. [7], [8] for D.I. swirl supported combustion systems.
Therefore some modifications have been introduced in the code, as it will be briefly described in the following.

The spray model

The atomisation process is treated in the KIVA code by the TAB model [10]. Liu et al. [9] found that in comparison with experiments this model gives worse results than the Wave Model, developed by Reitz [11].
Both models start with the injection of a blob with the same diameter of the nozzle hole and study the blob atomisation process.
It can be noted that the TAB model as well as the Wave model include a set of characteristic constants, whose values influence both the Sauter mean diameter of the drops and the tip penetration. In the case of the TAB model, the constants are those involved in the equation of the equivalent mass-spring damped system:

$$m\ddot{x} = F - kx - d\dot{x}$$

where x equals the displacement of the equator of the drop from its equilibrium position. The relationships between the mechanical and the fluidynamical parameters are:

$$\frac{F}{m} = C_F \rho_g \frac{u^2}{\rho_l r}; \quad \frac{k}{m} = C_k \frac{\sigma}{\rho_l r^3}; \quad \frac{d}{m} = C_d \frac{\mu_l}{\rho_l r^2},$$

where ρ_l and ρ_g are the liquid and gas density, r is the radius and σ the fuel surface tension.
The values assigned of the constants C_F, C_K and C_D in the original model are $C_F = 1/3$, $C_K = 8$, $C_D = 5$.
Finally, an other parameter of the model is the initial amplitude of oscillation, settled by Amsden et al. [10] at 0.2.
The Wave model results from a linear stability analysis of liquid jets leading to a dispersion equation relating the growth of an initial perturbation on a liquid surface of infinitesimal parameters of both injected liquid and ambient gas. In the atomisation regime the new drop radius r is:

$$r = B_0 \Lambda$$

The law of variation of the blob radius a, due to break-up is:

$$\frac{da}{dt} = -(a - r) / \tau$$

The break-up time is expressed by:

$$\tau = 3.726 B_1 a / \lambda \Omega$$

with Λ = wavelength of the most instable wave disturbance and

$$\Omega = \rho_l a^3 / \sigma.$$

The two model constants B_0 and B_1 must be adjusted to tune the numerical results to the experimental ones.
In particular B_0 is settled at the same value B_0 =0.61 by Reitz et al. [11], Liu et al. [9] and Patterson et al. [6], while in these works different values of B_1 were chosen in the range from 1.7 to 30.
Belardini et al. [12] carried out a sensitivity analysis of both TAB and Wave models varying the model constants.
The numerical results were compared with the experimental findings obtained both in bomb experiments as well as by high speed cinematography in the same experimental D.I. Diesel engine used in this work.
The TAB model was found strongly sensitive to the value of the constant C_k, while C_D and Amp0 values slightly affect the numerical results.
Increasing the Ck value from 8 to 144 a better fit with the experimental data can be obtained. As concerns the Wave model, the best fit with the experimental data was obtained setting B_0 = 0.61, as the standard value, and B_1 =5.
Moreover Belardini et al. [12] demonstrated that adopting a different model based on both the Wave and TAB models a very good fit with experimental results can be obtained. In fact, the TAB model underestimates the tip penetration, because of its tendency to break-up the jet in very small droplets too quickly. On the contrary the Wave model has a better behaviour in the first phase of the atomisation process.
The new model works as follows. At the beginning the Wave model is used, considering the high diameter of the injected drops. After that the TAB model is called when the diameter is less than 95% of the maximum diameter of the injected drops. The setting for the optimum values of model constants is B_0=0.61, Ck=144 and C_D=200.

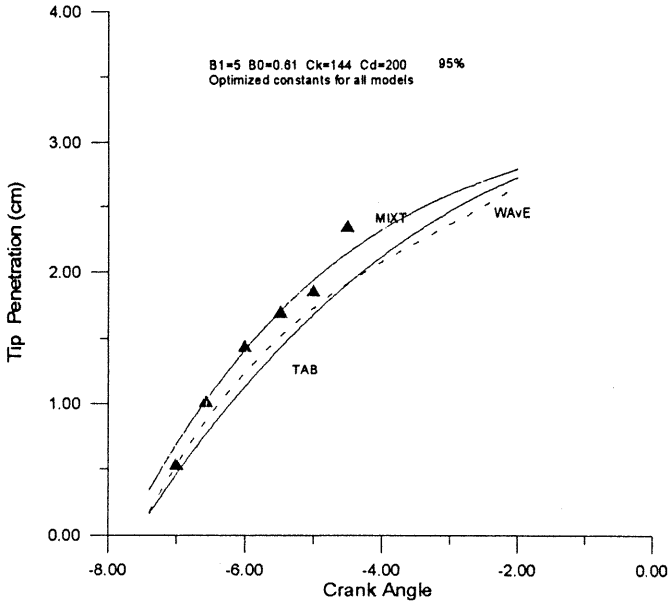


Fig. 2: Experimental and computed tip penetrations

In fig. 2 the computed tip penetration with TAB, Wave and the new model, all settled with the optimum values of the constants, is compared with the experimental one. It's quite evident that the new "mixed" model shows the best performances.

Finally the fuel injected model was further refined adding a spray - wall interaction model in the form described by Naber et al. [13] and Amato et al. [14].

The ignition delay model

In diesel combustion computations the low temperature chemistry must be described with a sufficient degree of accuracy to predict the ignition delay time.
To simulate the diesel combustion low temperature chemistry different schemes have been adopted in literature. The most diffused one is based on the so called Shell model, adopted by Gorokhovski and Borghi [15] and Patterson et al. [6]. However it can be noted that the tuning of the constants for this kind of model is dependent on the fuel characteristics.
Abraham and Bracco [16] proposed to model autoignition in diesel engines in a very simple way, using a single Arrhenius type equation, following the evolution of a specie representative of the radicals that lead to self- ignition. Also this kind of approach requires that the model constants be tuned with the fuel tendency to ignite.
An approach, as simple as the previous mentioned one, has been followed by Nishida et Hiroyasu in their work [17].
In this approach in each computational cell the autoignition starts when it is reached the condition:

$$\int_0^{t_{ig}} \frac{1}{\tau_d} d\tau_d = 1$$

In the present work, for τ_d the Hardenberg and Hase [19] formula was used:

$$\tau_d = \frac{n}{6} * \left(0.36+0.22S_p\right) * \exp\left(E_A * \left(\frac{1}{RT} - \frac{1}{17190}\right) + \left(\frac{21.2}{p-12.4}\right)^{0.63} \right)$$

where 0 is the time at which injection starts, n is the engine speed [rpm], T is the cell temperature [K], p is the cell pressure [bar], S_p is the mean piston speed [cm/sec]. This formula is sensitive to the fuel cetane number via the term:

$$E_A = \frac{618840}{CN + 8} [J / mol]$$

With respect to the original formulation, this term has been slightly modified by Belardini et al. [8], in order to obtain a better fitting of the experimental data in a number of test cases.

The combustion model

As in the standard version of the Kiva2 code, the high temperature fuel oxidation mechanism is modelled by a single step oxidation reaction:

$$C_n H_m + (n + \frac{m}{4}) O_2 \Leftrightarrow nCO_2 + \frac{m}{2} H_2O$$

The corresponding reaction rate ω has been expressed [8] as: $\omega=\min(\omega_{premix},\omega_{diff})$, where:

$$\varpi_{premix} = A\rho^2 (y_{fuel})^m (y_{ox})^n e^{-\frac{E}{T}}$$

$$\varpi_{diff} = B\rho\frac{\varepsilon}{\kappa} * \min\left(y_{fuel}, \frac{Y_{ox}}{s}\right).$$

In these formula y_{fuel} and y_{ox} are the fuel and oxygen mass fractions, ρ, κ and ε are respectively the gases density, the turbulent kinetic energy and its dissipation rate; s is the stechiometric ratio. A and E are respectively the preesponential factor and the activation temperature for the premixed combustion; B is the proportional factor for the diffusive combustion.
This model, derived from Magnussen, is the most diffused in multidimensional diesel combustion computations: it is used by Nishida and Hiroyasu [17], by Zellat et al. [18], by Belardini et al. [7], [8].

The soot formation and oxidation model

Many of the physical and chemical details of the soot formation process remain unknown up today. Despite of this, the attempts to model this complex phenomenon in practical combustion environments are increasing.
Limiting our attention to diesel combustion systems, many authors adopted for the soot formation mechanism a simplified formulation based on a single step Arrhenius type equation.
Hiroyasu [20] in the 1-st Comodia Congress (1985) gave a best revue of this kind of simple model, showing that there is a large scatter in the frequency factor as well as in the activation energy of the rate of the soot formation equation.
The need to introduce in multidimensional combustion calculations a soot formation and oxidation model at the lowest level of computational cost induced many researchers to use these simple formulations to obtain soot predictions.
In particular Hiroyasu et al., in a number of paper like [17], set up and tested a model based on a two steps formulation, one for the soot formation and one for the soot oxidation, in a simple Arrhenius form. The computed results were compared with the experimental findings at the engine exhausts.
The Hiroyasu model was also used by Belardini et al. [7], comparing the numerical results with the measured data of in cylinder combustion products, obtained with the high speed sampling technique.
Patterson et al. [6] performed extensive calculations, modelling combustion in a quiescent chamber engine, in order to evaluate the NOx-particulate trade off, varying the injection timing, the injection pressure and the split injection dwell angle. They used an improved Kiva2 version, adopting the Hiroyasu expression for soot formation and the Nagle et al. [21] mechanism for soot oxidation. The comparisons between the prediction in the late expansion stroke and the measurements of the insoluble fraction, performed with the dilution tunnel and the filter extraction, was quite good.
Zellat et al. [18], modelling a swirl chamber engine, adopted a different approach: they introduced in Kiva2 code a soot formation model derived from Tessner et al [22], and a soot oxidation model based on the Magnussen et al. hypothesis [23], considering the soot combustion process controlled by mixing rather then by kinetics. The predictions obtained by Zellat in four different engine operating conditions show a qualitative agreement with the experimental results.
Also Nagakita et al. [24] applied the Tessner model [22] jointly with the Farmer model as concerns the soot formation process, while the soot oxidation phenomenon was described using the Nagle [21] and Magnussen [23] theories. As switch criterion between the different models, during the formation as well as the oxidation phases, Nagakita et al. adopted the choice of the smaller rate. Their computational results, compared with in cylinder measurements obtained by back illuminated photography, show a good qualitative agreement.
Gorokhovski and Borghi [15] followed a different approach, using a linked ignition - combustion - soot formation kinetic model. A set of two equations is assumed to predict the soot volumic fraction and the global intermediate specie for soot formation. The soot formation rate is expressed as a first order equation of the intermediate specie concentration: the proportional constant is deduced from literature data in dependence of the cell values of temperature and carbon to oxygen ratio. The soot oxidation rate was computed as Lee et al. [25]. The computational results seem to be reasonable, but they were not compared with experimental data.
From the previous picture it is evident that there is a lack of detailed experimental data as well as of detailed knowledge about the soot formation process.
More recently some attempts were made to use multistep models. In particular Yoshihara et al. [26] used a simplified approach to calculate mixing of a natural gas fuelled diesel combustion. On the contrary the chemistry was extensively treated, having respectively 70, 6 and 12 reactions for methane combustion, for benzene and for the PAH growth. The nucleation is described as coalescence from pyrene, while the surface growth is described by "HACA" reaction sequence as reported by Frenklach and Wang [27]. The soot particle oxidation by the OH radicals was considered as probability of the reaction upon collision of the OH radical with the particle surface. The model is able to compute the right amount of soot at the engine exhausts, for the test case under examination. Anyway the proposed model, even if attractive, remains prohibitive in terms of computational time in 3D CFD calculations.
A right compromise between a comprehensive description of the process and the computational time may be the model firstly proposed by Leung et al. [28] and by Fairweather et al. [29]. In this model the acetylene was assumed as crucial pyrolitic specie for the nucleation and the surface growth processes, as affirmed by Smith [30], Glassman [31], Wagner [32], and Ciajolo et al. [33].
The three steps are the following:

r1:	$C_2H_2 \Rightarrow 2C + H_2$	nucleation
r2:	$C_2H_2 + nC \Rightarrow (n+2)C + H_2$	surface growth
r3:	$C + 0.5O_2 \Rightarrow CO$	oxidation

Belardini et al. [8] implemented this model in the standard kinetic routine of the Kiva2 code, running the soot model simultaneously with the ignition delay and the combustion models. They assumed that the fuel vapour undergoes to acetylene by a single step mechanism:

r0: $$C_mH_n \Rightarrow \frac{m}{2}C_2H_2$$

Preliminary results of the model, in comparison with experimental data of tetradecane combustion, were presented: but further refinements were clearly necessary. Therefore in the present paper further computations are presented: the problem of the model constants setting is discussed, comparing the numerical predictions with experimental measurements obtained in a number of test cases.

THE EXPERIMENTS

For the experiments a single cylinder diesel engine was used, whose characteristics are reported in table 3.
In the head of the engine two small quartz windows have been mounted, in order to obtain pictures of the injection and combustion processes by high speed cinematography, and to apply the two colours technique for soot temperature and soot loading measurements. In addition the engine may be also equipped with a second head, in which a fast acting valve allows the direct sampling of the combustion products. In present paper, the soot loading was measured only by the two colours technique, implemented as outlined in [8].
The same engine was also characterised from the fluid dynamic point of view [34]. For the purposes of the present paper the test cases reported in table 4 were chosen. For each test condition measurements of indicated pressure line pressure and needle lift low were taken.
Massoli and Di Stasio [35] performed a careful analysis of this kind of measurement. They deduced that, starting from the algorithm chosen for the two colours method and supposing a soot diameter distribution between 5 and 35 nm (Tree and Forster [36]), for the soot volumic fraction f_v the error lies in the range of the 20-30% at the peak concentration in the combustion chamber.
At lower soot concentrations this value rises up to 60%.

Compression ratio	18
Bore	10.0 cm
Stroke	9.5 cm
Conn. rod length	17.8 cm
Comb. chamber	Toroidal
E.A.R.	4.6
Injection	4 holes ϕ=0.28
Spray cone angle	160/140

Table 3: The engines characteristics

This analysis must be kept in mind when performing comparisons between predicted and measured values.

RESULTS AND DISCUSSION

To test the model sensitivity to the fuel cetane number, tests were performed according to the table 4, using tetradecane (C.N.=93), n-eptane (C.N.=56), and two different diesel fuels, actually DNC20 and HDT70, whose characteristics are reported in table 5.
These special diesel fuels [2] are practically sulphur and polyaromatics free. In numerical runs they were simulated as n-dodecane, but using in the ignition delay model the proper value of cetane number.
In [8] it was shown that, expressed the reaction rates in [moles/cm3 sec], as used in Kiva2, and settled the A, E and B constants in the combustion model respectively to 0.65E+11 [cm^3/moles sec], 15780 [K] and to 5, it is possible to obtain very close values of computed and measured heat release patterns, burning tetradecane as well as diesel fuel. In the case of n-eptane it is necessary a different tuning of the activation temperature in the premixed combustion: it was used E=14000 [K].
In fig. 3 there are reported the experimental heat release patterns obtained with different fuels, but setting the injection timing to obtain that combustion starts at about the same crank angle. The effect due to increasing values of cetane number is quite evident: in fact the increase of cetane number leads to reduction of the premixed burnt fraction and to increase of the diffusive phase.
The two colours measurements of soot volumic fraction and soot temperature, in the same operating conditions, are reported in figs. 4 and 5. Within the measurement accuracy,

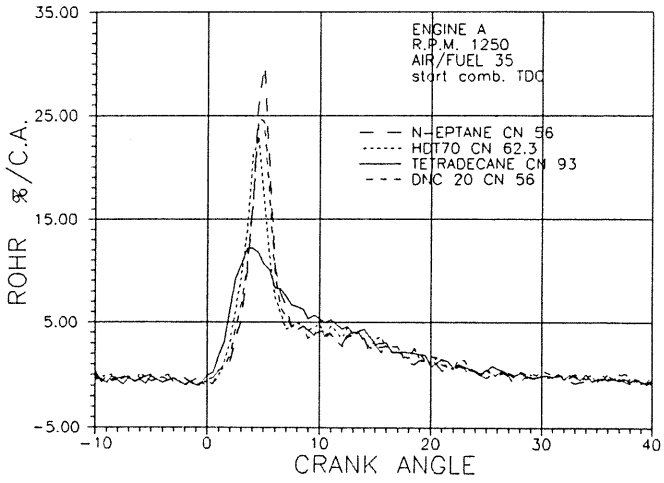
Fuel	A/F	Injection	M/cycle	inj.start	inj.dur.
Tetradecane	35:1	4-0.28-160	0.02 g	-7.5 CA	6.5 CA
Tetradecane	35:1	4-0.28-160	0.02 g	-4.5 CA	6.5 CA
N-eptane	35:1	4-0.28-160	0.02 g	-7.5 CA	7.0 CA
N-eptane	35:1	4-0.28-160	0.02 g	-4.5 CA	7.0 CA
N-eptane	35:1	4-0.28-140	0.02 g	-8.5 CA	7.5 CA
N-eptane	35:1	4-0.28-140	0.02 g	-5.5 CA	7.5 CA
Diesel:DNC20	35:1	4-0.28-160	0.02 g	-7.5 CA	7.0 CA
Diesel:DNC20	35:1	4-0.28-160	0.02 g	-5.0 CA	7.5 CA
Diesel:HDT70	35:1	4-0.28-160	0.02 g	-7.5 CA	6.5 CA
Diesel:HDT70	35:1	4-0.28-160	0.02 g	-4.5 CA	6.5 CA

Table 4: engine test cases

the scaling of the soot loading peaks among different fuels is well linked to the heat release analysis. Vice versa the soot temperature values don't seem to be affected by differences in cetane number.
The figures 6, 7, 8, 9 show the comparisons between measured and predicted values of soot volumic fraction.
Tests are referred to the engine, operating at two different injection timings. The combustion volume was discretised with a 21x21x28. The soot data are referred to the sample volume of the optical probe, that is a relatively small fraction of the whole combustion chamber: in the present set of experiments, this volume is approximately a frustum of solid

FUEL	HDT70	DNC20
Density [Kg/dm^3]	0.81	0.818
Sulphur [ppm]	1	1
Dist. T [°C] 10 %	211	206
50 %	268	245
95 %	380	347
Cetane number	62.3	56
Aromatics W% Mono	6.1	3.9
Di	0.5	0.2
Tri	/	/
Total	6.6	4.1

Table 5: Diesel fuel characteristics



Experimental heat release patterns for different fuels.
Fig.3

cone, of about 32° degree angle, located downstream the first fuel jet, with an angle of 5° with respect to jet axis.
Therefore it must be noted that, in the experimental as well as in the numerical analysis, these results are the picture of a small volume inside the combustion chamber. This is an important remark, because in our opinion a three dimensional code should be able to keep the details of the combustion process.
The model seems to be able to reproduce the main features of the diesel combustion process, confirming the experimental trends.
Therefore, accordingly with the experimental trends, retarding the injection timing and increasing the cetane number, higher values of computed soot volumic fraction are obtained.
The agreement between computed and measured soot volumic fractions may be considered satisfactory, taking into account the previously outlined measurement limits of accuracy.

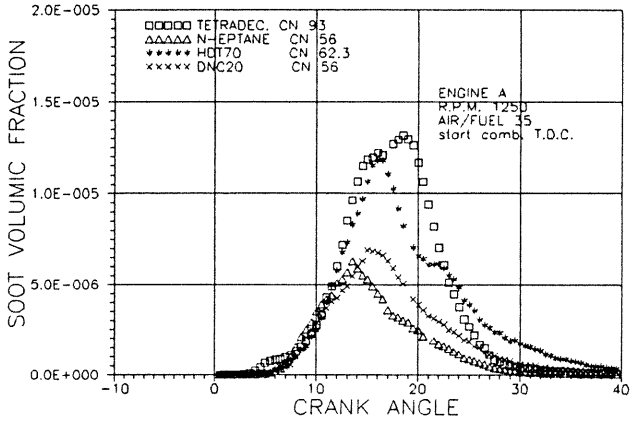


Fig.4: Experimental values of soot volumic fraction for different fuels.

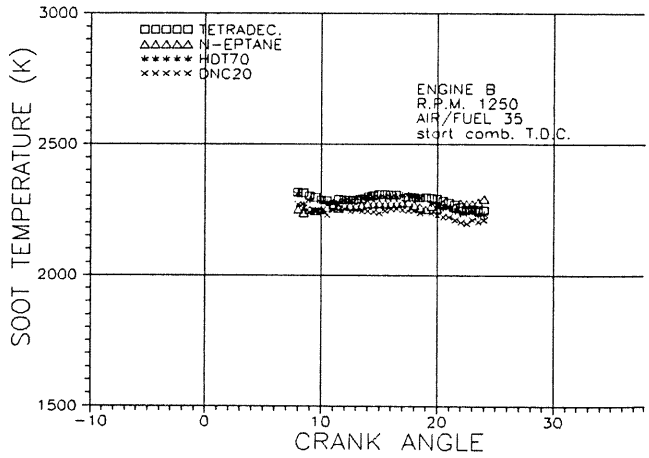


Fig 5: Experimental soot temperatures with different fuels.

However, to tune numerical and experimental data the tuning of the model constants is an essential step. Table 6 shows the values adopted for the preesponential factor and for the activation temperature in the kinetic reaction rates of the model: for the acetylene formation equation the proportional constant reported in the table corresponds to the full term $m/2 * A_0$ [8]. It is also outlined that it was necessary to use different values of the constants in the equation of the acetylene formation, when using different fuels. Surely this is due to the strong simplification to treat the acetylene formation process by a single step. Therefore more experimental data and further refinements are needed to improve the reliability of the model.
Another lack of the model can be attributed to the soot oxidation mechanism, treated as Leung with the Lee formula [25], but probably improper in the high temperature range

typical of the Diesel combustion. Numerical tests assessed the strong sensitivity of the results to the soot oxidation model constants: many efforts have to be directed in this direction.

	eq. ro	eq. r1	eq. r2	eq. r3
n-eptane				
pre EXP	1.2 E+14	1.0 E+06	2.4 E+05	1.6 E+04
act.TEMP	60418	21000	12100	19680
tetradecane				
pre EXP	2.4 E+15	1.0 E+06	2.4 E+05	1.6 E+04
act.TEMP	60418	21000	12100	19680
df2:hdt70p				
pre EXP	1.4 E+15	1.0 E+06	2.4 E+05	1.6 E+04
act.TEMP	60418	21000	12100	19680
df2:dnc20p				
pre EXP	7.2 E+14	1.0 E+06	2.4 E+05	1.6 E+04
act.TEMP	60418	21000	12100	19680

Table 6: Soot model constants used for different fuels.

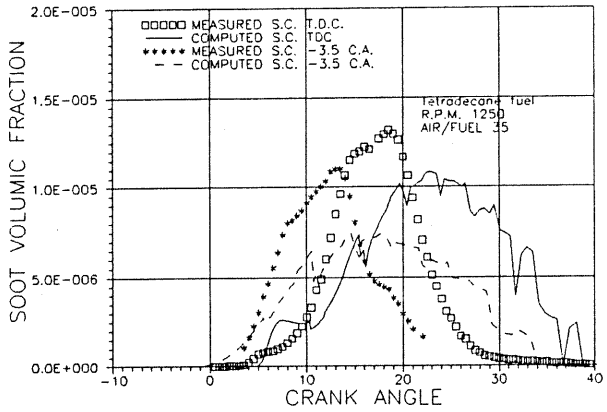


Fig 6: Computed and measured values of soot volumic fraction for tetradecane fuel

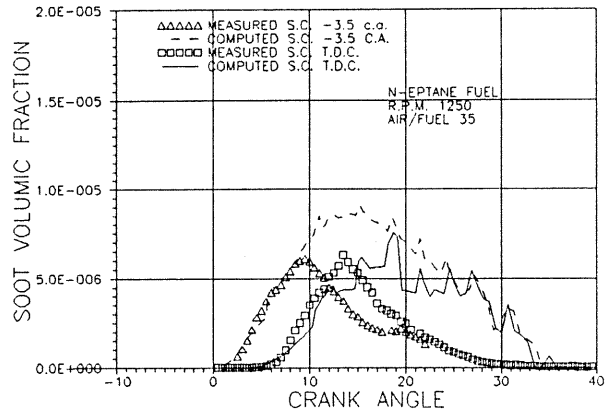


Fig 7: Computed and measured values of soot volumic fraction for n-eptane fuel.

However in this work this aspect was not treated, limiting to perform a set of numerical runs aimed to define compromise values of the constants, to be adopted in all test cases.

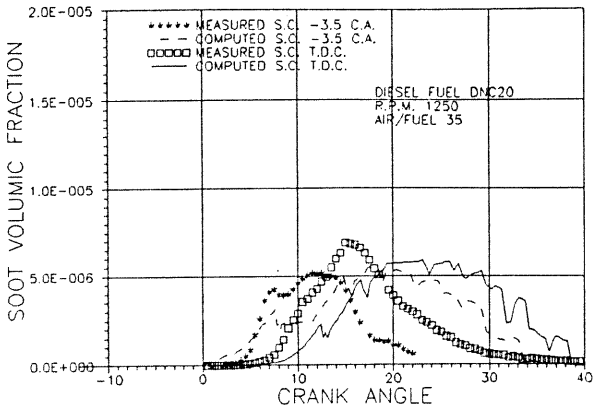


Fig.8: Computed and measured values of soot volumic fraction for Diesel fuel DNC20

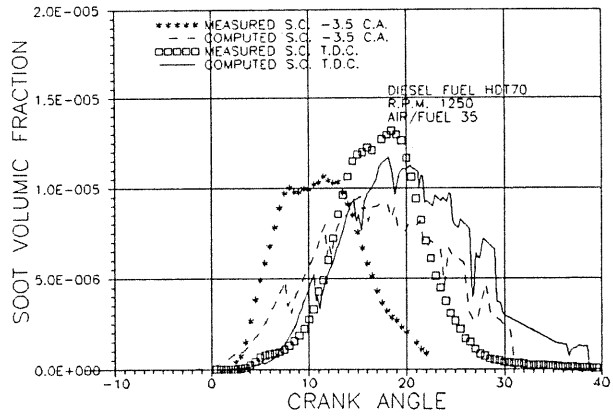


Fig 9: Computed and measured values of soot volumic fraction for Diesel fuel HDT70.

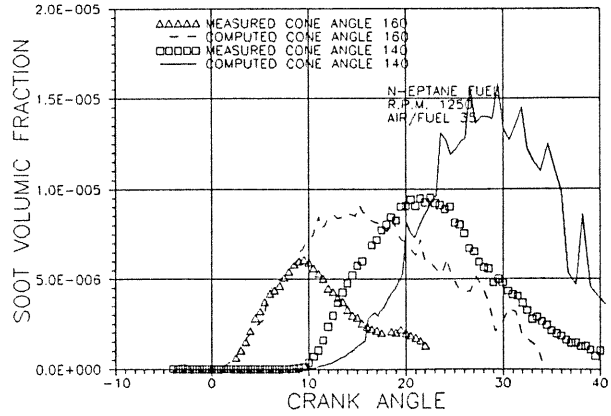


Fig 10: Soot volumic fraction computed and measured for different spray cone angle.

Finally the sensitivity of the model to changes in the combustion system design was evaluated, running the n-eptane test cases with an injector spray cone angle equal to 140° as well as to 160°, as reported in table 4.
The model seems to be sensitive to changes in the details of the combustion system design.

Anyway, comparing numerical and experimental data, much attention may be spent to properly evaluate the measurement volume: different positionings of the control volume give consistently different results. This is a one more problem in a study that should be as more accurate, but is very difficult to be treated from the experimental as well as from the numerical point of view.

CONCLUSIONS

A new multistep soot formation and oxidation mechanism was introduced in an improved version of the Kiva2 code.
The main modifications to the original version of the code concern the fuel break up routine, the combustion routine and a simple mechanism to compute ignition delay time.
The improved code is able to predict correctly the combustion pressure and heat release patterns in a number of test cases obtained varying injection timing and fuel quality, without changing the values of the model constants, with the exception of the n-eptane fuel.
As concerns the soot volumic fraction predictions, the preesponential factor of the acetylene formation reaction rate must be changed in dependence of the used fuel, while the other model constants may remain unmodified. Therefore the main limitation of the proposed model is the availability of more accurate experimental details concerning the acetylene formation mechanism starting from different fuels. Moreover, considering the sensitivity of the model to the soot oxidation constants, the problem of the oxidation must be deepen.
Despite this limitation, the proposed model works quite acceptably, keeping the main features of the diesel combustion locally in the combustion chamber and reproducing the main changes due to the different fuel cetane number.
Anyway further work is required both numerically and experimentally.

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