

## Soot Modeling in Diesel Engine

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*Abstract:* - This paper presents an advanced version of the original software developed by the author in order to simulate the combustion in the Diesel engines, focusing on simulate soot formation. Complex kinetic mechanisms are need for realistic modeling of shoot formations, but this is applicable only for simple flame computations (e.g. one dimensional, laminar, etc.). For real turbulent flame calculations, their use is impractical, due to the complexity of the interacting processes (turbulence, radiation, heat transfer, etc.). A model derived by systematic reduction of multi-step chemistry is used. This reduction is based on the partial equilibrium assumption of the considered elementary reactions using the skeletal chemistry for n-decan for ignition, combustion and emissions. Subsequently, predictions of heat release rate, as well as NO and soot emissions are compared with experimental data. It is demonstrated that the model can predict the rate of heat release and engine performance with high fidelity. However, additional effort is required to enhance the fidelity of NO and soot predictions across a wide range

*Key-Words:* - soot formation, soot oxidation, NOx, fuel spray, kinetic reaction,

### 1 Introduction

Due to the growing importance of future emission restrictions, manufacturers of internal combustion engines are forced continuously to improve the mixture formation and combustion processes in order to reduce engine raw emissions. In this context, the numerical simulation and optimization of mixture formation and combustion processes is today becoming more and more important. One advantage of using simulation models is that in contrast to experiments, results can often be achieved faster and cheaper. Much more important is the fact that despite the higher uncertainty compared to experiments, the numerical simulation of mixture formation and combustion processes can give much more extensive information about complex in-cylinder processes than experiments could ever provide. Using numerical simulations, it is possible to calculate the temporal behavior of every variable of interest at any place inside the computational domain. This allows the obtainment of a detailed knowledge of the relevant processes and is a prerequisite for their improvement. Furthermore, numerical simulation can be used to investigate processes that take place at time and length scales or in places that are not accessible and thus cannot be investigated using experimental techniques.

The computer code makes by author and describe in details in [1] is quasi dimensional, designate to simulate combustion process and nitric oxide formation. The purpose of present work was to improve the capability

of the program and introduce a model for soot calculations. The final objective is to achieve a computing program that would enable us to model the combustion process and pollutant emissions (NOx and soot) accurately enough so that it may be used as a study tool.

### 2 Problem Formulation

The model is two-dimensional and it takes advantage of the symmetry, being it used only two of the three spatial coordinates. If axial symmetry approach of the combustion chamber is considered, which is common in most of the practical cases, it is appropriate to take into account the swirl movement. In this way the spatial resolution is enhanced and the third dimension is partially implemented. The governing equations are written in a two-dimensional form, the plane of calculation being the xy-plane. Vector notation is employed in order to have a compact set of relations.

#### 2.1 The fluid phase

For fluid phase, approximated as Newtonian fluid, we can use the known set of equations for fluid flow with additional terms which take into account the effect of chemical reactions and interaction between fluid mixture and spray droplets. The set of equations [2] is: continuity equation (1) for species  $k$  and fluid (2), momentum equation (3) for the mixture, angular

momentum (4), the internal energy equation (5), and the state relation assumed for ideal gas mixture:

$$\partial \rho / \partial t + \nabla \cdot (\rho_k u) = \nabla \cdot [\rho D \nabla (\rho_k / \rho)] + \dot{\rho}_k^c + \dot{\rho}_s^c \delta_{k1}, \quad (1)$$

$$\partial \rho / \partial t + \nabla \cdot (\rho u) = \dot{\rho}_s^c, \quad (2)$$

$$\frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot (\underline{\underline{\sigma}}) - \frac{(\sigma_0 - \rho w^2)}{x} \nabla_x + F + \rho G, \quad (3)$$

$$\frac{\partial}{\partial t} (R\rho w) + \frac{1}{x} \nabla \cdot (x^2 \rho w u) = \frac{1}{x} \nabla \cdot (x \tau) + N, \quad (4)$$

$$\frac{\partial}{\partial t} (\rho I) + \nabla \cdot (\rho I u) = -p \nabla \cdot (u) + \underline{\underline{\sigma}} : \nabla u + \tau \cdot \nabla \left( \frac{w}{x} \right) + \frac{(\sigma_0)}{x} u \nabla_x - \nabla \cdot J + \dot{Q}_c + \dot{Q}_s, \quad (5)$$

where:  $\rho_k$  is the partial density of the  $k$  species,  $\rho$  is the total density of the fluid mixture,  $\dot{\rho}_s^c$  is the rate of change of fuel ( $k=1$ ) density due to spray evaporation or condensation,  $\underline{\underline{\sigma}}$  is the viscous tensor,  $\sigma_0$  is the cylindrical viscous stress,  $F$  is the momentum transferred from spray droplets to the fluid,  $G$  is the external force,  $\tau$  is the swirl stress vector,  $N$  is the angular momentum transferred from spray,  $I$  is specific internal energy (exclusive chemical),  $J$  is the heat flux vector,  $\dot{Q}_c$  is the rate of chemical heat release,  $\dot{Q}_s$  is a source term associated with the interaction between the spray droplet and the fluid.

The mean values in the equations are mass weighted (Favre procedure). The fluctuation terms are ordinarily modeled by the gradient-flux approximation. In this approximation the averaged turbulent equations become identical in form to the laminar ones; the transport coefficients are simply replaced by the appropriate turbulent values (6), which are much larger:

$$\begin{aligned} \mu &= \rho v_0 + \mu_{air} + \mu_t, \\ K &= \mu c_v / Pr', \\ D &= \mu / \rho Sc', \end{aligned} \quad (6)$$

where:  $\mu$  is the viscosity,  $v_0$  is the constant uniform turbulent diffusivity,  $\mu_{air}$  is air viscosity,  $\mu_t$  is turbulent viscosity computed using SGS (SubGrid Scale turbulent viscosity) model [3].

## 2.2 Chemical reactions

The consequent chemical reactions used may be included in two categories:

- one kinetic equation, fuel stoichiometric in air combustion;
- six equilibrium equation, dissociation equations of combustion products;

- Three kinetic reversible equations expressing the extended Zeldovich mechanism for NO evaluation; The chemical source term (1) and the chemical heat release term (5) is given by equation 8 and 9,

$$\dot{\rho}_k^c = W_k \sum_r (b_{kr} - a_{kr}) \dot{\omega}_r, \quad (8)$$

$$\dot{Q}_c = \sum_r q_r \dot{\omega}_r, \quad (9)$$

where  $a_{kr}$  and  $b_{kr}$  are the dimensionless stoichiometric coefficients for the  $r$ -th reaction,  $W_k$  is the molecular weight of specie  $k$ ,  $\dot{\omega}_r$  is reaction speed of  $r$ -th reaction,  $q_r$  is the negative of the heat of reaction for  $r$ -th reaction at  $0^\circ K$ .

Reaction speed  $\dot{\omega}_r$  is computed for the kinetic reaction and is implicitly determined by the constrain condition imposed for the equilibrium reaction [4].

## 2.3 Soot model

Soot forms in the rich unburned-fuel-containing core of the fuel sprays, within the flame region, where the fuel vapor is heated by mixing with hot burned gases. Soot then oxidizes in the flame zone when it contacts unburned oxygen. Therefore, the concentration of soot in the exhaust is governed by the formation and oxidation of soot during the engine cycle, i.e.

$$\frac{dm_s}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{so}}{dt} \quad (9)$$

where  $m$  is mass; subscript  $s$ ,  $sf$ , and  $so$  denote soot emitted, soot formed, and soot oxidized, respectively. The general fact that the net soot formation rate is primarily affected by pressure, temperature and equivalence ratio has been fairly well established.

However, the details of the mechanism leading to soot formation are not known. Consequently, semi-empirical, two-rate equation models have been used to describe the soot dynamics. In particular, the soot formation model proposed by Hiroyasu et al. [5] is used in many models. The formation rate is calculated by assuming a first-order reaction of vaporized fuel,  $m_{fg}$ , as:

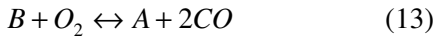
$$\frac{dm_{sf}}{dt} = A_f m_{fg} p^{0.5} \exp\left(\frac{-E_{sf}}{RT}\right). \quad (10)$$

The soot oxidation is predicted by assuming a second order reaction between soot,  $m_s$ , and oxygen.

$$\frac{dm_{so}}{dt} = A_o m_s \frac{p_{ox}}{p} p^{0.5} \exp\left(\frac{-E_{so}}{RT}\right) \quad (11)$$

where  $E_{sf}=1.25 \times 10^4$  kcal/kmol,  $E_{so}=1.40 \times 10^4$  kcal/kmol.  $A_f$  and  $A_o$  are constants that are determined by matching the calculated smoke with the measured soot in the exhaust gas.

Another soot oxidation model investigated in this study is the Nagle and Strickland-Constable [6] oxidation model. The NSC oxidation model is based on oxidation experiments of carbon graphite in an  $O_2$  environment over a range of partial pressure. In this model, carbon oxidation occurs by two mechanisms whose rates depend on the surface chemistry involving more reactive A sites and less reactive B sites. The chemical reactions are:



The NSC soot oxidation rate implemented in equation (9) is given by:

$$\frac{dm_{so}}{dt} = \frac{M_C}{\rho_s d_s} m_s w \quad (15)$$

where  $M_C$  is the carbon molecular weight (12 g/mole),  $\rho_s$  is the soot density (2.0 g/cm<sup>3</sup>), and  $d_s$  is the soot diameter ( $4.5 \times 10^{-9}$  m). The term  $w$  in equation (15) is the net reaction rate of reactions (12), (13), and (14) and is defined as:

$$w = \left( \frac{K_A p_{ox}}{1 + K_Z p_{ox}} \right) x + K_B p_{ox} (1 - x) \quad (16)$$

where  $p_{ox}$  is the oxygen partial pressure in atm. The proportion,  $x$ , of A sites is given by:

$$x = \frac{p_{ox}}{p_{ox} + \left( \frac{K_T}{K_B} \right)} \quad (17)$$

The rate constants used in the NSC oxidation model are given in Table 1.

**Table 1.** Rate constants for NSC soot oxidation model

Rate Constant	Units
$K_A=20 \exp(-15100/T)$	g-C/cm <sup>2</sup> ·s·atm
$K_B=4.46 \times 10^{-3} \exp(-7640/T)$	g-C/cm <sup>2</sup> ·s·atm
$K_T=1.51 \times 10^5 \exp(-48800/T)$	g-C/cm <sup>2</sup> ·s
$K_Z=20 \exp(-15100/T)$	atm <sup>-1</sup>

## 2.3 The spray

The equation of motion for the spray will be given in Lagrangian form for discrete computational particle [3]. The flow of liquid jet is computed using the general equation of jet simplified in stochastic approach and the evaporation using the equation deduced by O'Rourke.

The equations for fluid – particle interaction are:

$$\dot{\rho}_s = - \sum_k dm_k / dt \delta(r - r_k), \quad (18)$$

$$\underline{F} = \sum_k \left[ D_k (u_k - \underline{u}) - u_k dm_k / dt \right] \delta(r - r_k), \quad (19)$$

$$N = \sum_k [D_k (w_k - w) - w_k dm_k / dt] \delta(r - r_k), \quad (20)$$

$$\dot{Q}_s = \frac{1}{x} \sum_k \left[ - \frac{d}{dt} (m_k H_k) \right] \delta(r - r_k) + \sum_k \left[ D_k - \frac{1}{2} \frac{dm_k}{dt} \right] (u - u_k)^2 \delta(r - r_k). \quad (21)$$

where:  $dm_k$  is the mass of droplet  $k$ ,  $H_k$  is the specific enthalpy of liquid fuel,  $r$  position vector and  $\delta$  is the Dirac function.

## 3 Numerical Technique

The temporal differentiate is based on ICE (Implicit Continuous-fluid Eulerian) algorithm which is a partial implicit scheme. This iterative technique joins the continuity and moment equations and solves them simultaneously by using the state equation; the energy equation is solved in an explicit way. To move forward in time each cycle is achieved in three temporal sub-steps or phases. This approach is in direct connection to the spatial discretization based on ALE (Alternate Lagrangian Eulerian) method. Interaction of spray with the gas is treating based on the ideas of Monte Carlo method [1]. The spray is considered to be composed of discrete computational particles. Each of them represents a group of droplets of similar size, velocity, temperature [7].

The grid is adjustable and is consists of generalized quadrangle, whose corners are specified by co-ordinates dependent on time. This offers additional flexibility, the problem being solved in an Eulerian or Lagrangian way, as required.

The code is written in MATLAB language.

## 4 Numerical simulation

The model was used for the numerical simulation on T684 engine made by "Tractorul" Plant of Brasov, a four stroke automotive engine whit axial symmetric combustion chamber (Table 2). Experimental data are available for these engines [1].

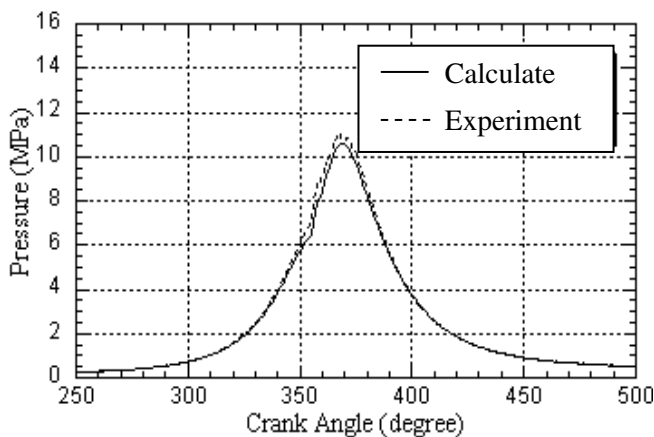
Model predictions of engine performance and emissions have been compared against corresponding measurements. Critical sub-models, such as for the heat release and emissions processes, contain empirical constants that need to be calibrated against experiments. The purpose of this effort is to explore the range of engine speed, load and injection timing conditions over which the multidimensional model predictions remain valid, following only an initial calibration.

**Table 2** Specification of T684 test engine

Bore (mm)	130	105 mm
Stroke (mm)	160	115 mm
Con. Rod length (mm)		182 mm
Compression ratio (-)		17.5
Rated speed/power (rpm/kW)		2400/45
Plunger diameter		10.5 mm
Plunger stroke		3.2 mm
Fuel pipe diameter		2 mm
Nozzle type		Hole type
Nozzle hole number		4
Nozzle hole diameter mm		0.24
Nozzle hole angle		90

Figure 1 shows predicted and measured cylinder pressure traces at the operating condition selected for model calibration  $n=1440$  rpm and load 100% and 7.5 timing injection. The predicted cylinder pressure trace falls in very good agreement with the experimental data. Therefore, both the magnitude and timing of occurrence of the peak pressure are precisely predicted by the model.

The observed cylinder pressure profiles reflect the effects of in-cylinder heat release, heat transfer to the cylinder surfaces and work transfers. Even though predictions of the gross heat release rate are directly available from the model, the apparent heat release rates have been calculated so as to compare them with experimental data. The equation for the apparent heat is:



**Figure 1** In-cylinder pressure

$$\frac{dQ_n}{dt} = \frac{\gamma}{\gamma-1} p \frac{dV}{dt} + \frac{1}{\gamma-1} V \frac{dp}{dt} \quad (22)$$

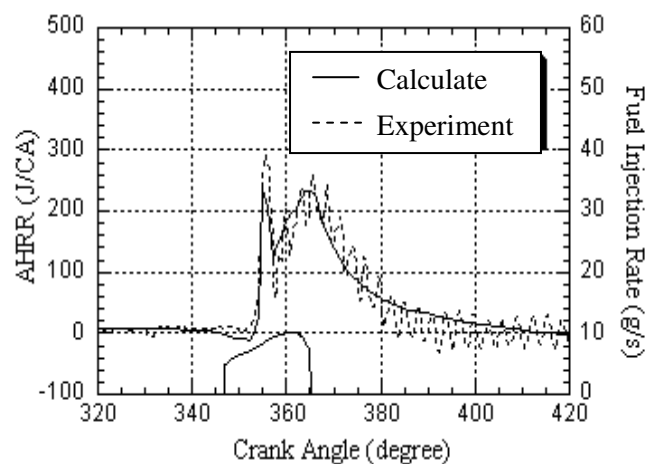
The ratio of specific heats is not necessarily constant through the compression, combustion, or expansion process. Here, the ratio is calculated by a relatively simple correlation for the purpose of comparing measured and predicted heat release rates, as follows:

$$\gamma = 1.338 - 6.0 \times 10^{-5} T + 1 \times 10^{-8} T^2 \quad (23)$$

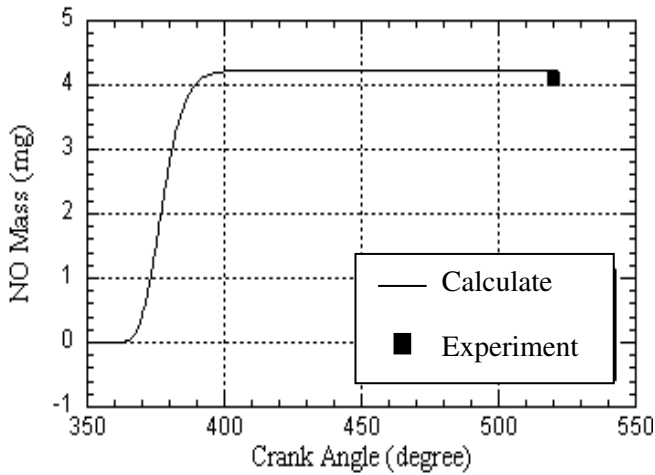
Figure 2 compares apparent heat release rates computed from predicted and measured pressure traces. Also shown is the fuel injection profile. Figure 2 exhibits the double-peak shape that characterizes the direct injection diesel combustion. The first peak due to premixed combustion strongly depends on the amount of fuel that is prepared for combustion during the ignition delay period. The second peak due to diffusion combustion is controlled by the fuel-air mixing rate. Diffusion combustion continues until combustion is completed. As can be seen in Figure 2, the shape, timing, and magnitude of both heat release peaks predicted by the model compare well with experimental data. This effectively validates that the spray dynamics, fuel droplet evaporation, fuel-air mixing, ignition delay, and combustion sub-models are properly working.

Figure 3 illustrates the in-cylinder NO formation history predicted by the model, and compares its cumulative value against the measured engine-out NO emissions. The predicted NO mass at the end of the expansion stroke is good accordance with measurements.

Model predictions of soot emissions are based on either the global rate equations for soot formation and oxidation proposed by Hiroyasu et al. [5] or the NSC



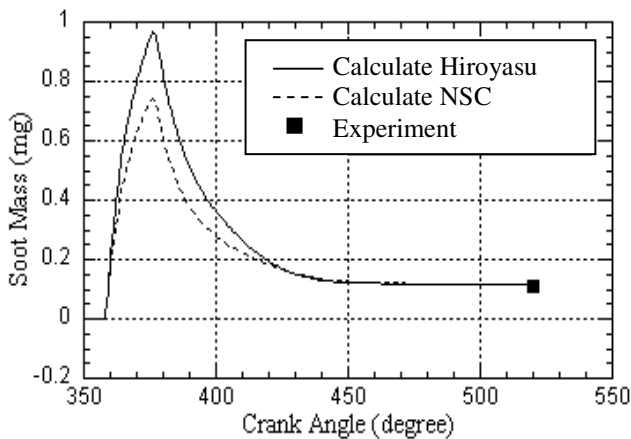
**Figure 2** Apparent heat release rates and rate of fuel injection.



**Figure 3** In-cylinder NO formation (Injection timing: 7.5 deg. CA BTDC)

soot oxidation model.

For the Hiroyasu et al model, the pre-exponential constant,  $A_f$ , in equation (10) is set here at 150  $\text{sec}^{-1}$ , which is, the same value used by Patterson et al. [8]. The other pre-exponential constant,  $A_o$ , in equation (11) is calibrated ( $A_o=24200$ ) to match the soot level with measurements under the baseline operating condition. On the other hand, the diameter of the soot particles for the NSC model is set to  $4.5 \times 10^{-9}$  m. In Figure 4, the in-cylinder mass of soot predicted by the global rate equation by Hiroyasu et al. [5] is compared with the mass predicted by the NSC soot oxidation model. Soot forms in the rich unburned-fuel-containing core of the fuel sprays, within the flame region, where the fuel vapor is heated by mixing with hot burned gases. Soot then oxidizes in the flame zone when it contacts unburned oxygen. Consequently, the concentration of soot starts building up earlier than NO during the early stages of combustion when rich unburned mixture is present.

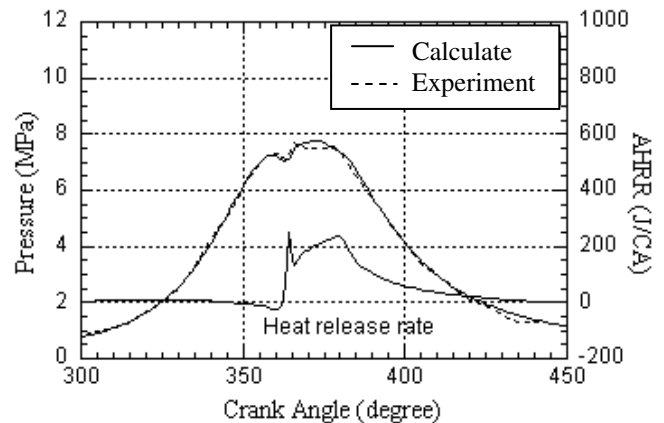


**Figure 4** In-cylinder soot formation by global rate equation vs. NSC model and measured exhaust soot mass (injection timing: 7.5 deg. CA BTDC)

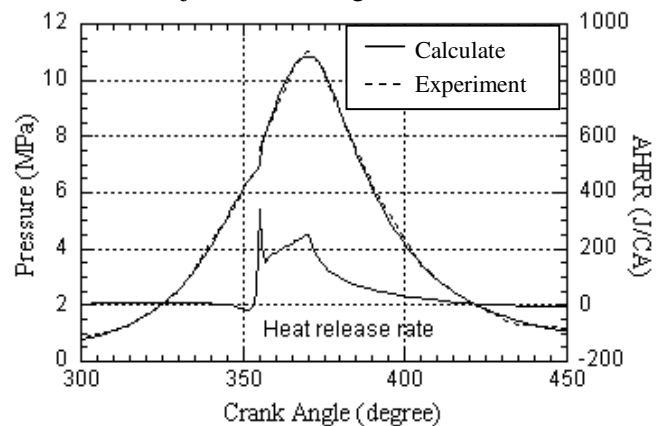
This can be observed by comparing the timings for the start of NO and soot formation from Figure 3 and 4. After reaching its peak, soot concentration decreases as oxygen is supplied by air entrainment. Soot destruction freezes later compared to NO dynamics since air entrainment promotes soot oxidation. In general, the soot formation and destruction trends predicted by the Hiroyasu et al. and NSC models are quite similar and in good agreement with experimental measurements.

Following model validation under the baseline operating condition, more extensive comparisons of predictions with measurements were carried out over a range of injection timings (from 5 to 15 degrees CA BTDC) at 1800 rpm and 80% load. The values of all model constants remain unchanged. As injection timing is advanced, cylinder pressure and temperature during the ignition delay period become lower. Therefore the ignition delay period becomes longer. These phenomena result in more fuel burned during the premixed combustion phase following the ignition delay period, as can be observed in Figures 5 and 6.

Higher cylinder temperatures with advancing injection timing generate more NO and less soot, resulting in the perennial NO-soot tradeoff. In Figure 7, NO-soot tradeoff curves are compared with the two alternative

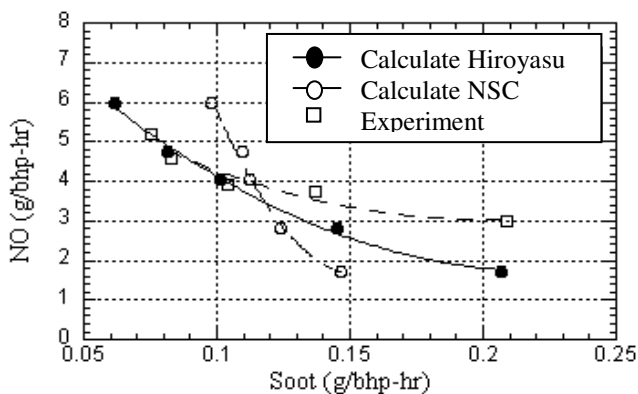


**Figure 5** Pressure and apparent heat release at timing injection of 5 deg. CA BTDC

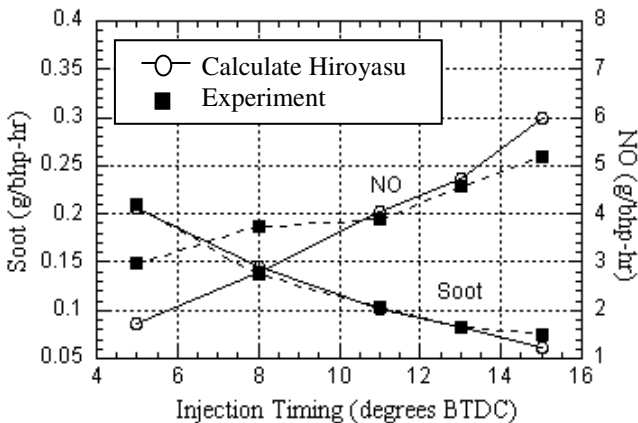


**Figure 6** Pressure and apparent heat release at timing injection of 15 CA BTDC

soot oxidation models and compared against measurements over a range of injection timings from 5 to 15 degrees CA BTDC. While the general experimental trend can be predicted by the multidimensional model using either soot models, it appears that the Hiroyasu et al. model predicts soot emissions better than the NSC model across the range. In Figure 8, the measured and calculated NO and soot emissions are plotted individually as a function of injection timing. The difficulty in predicting more accurately measured NO emissions for this engine appears to be responsible for the discrepancies in the NO-soot trend observed in Figure 7. In contrast, the global rate soot model emissions are in excellent agreement with measurements.



**Figure 7** NO-soot tradeoff curves for injection timings ranging from 5 to 15 deg. CA BTDC.



**Figure 8** NO and soot emissions for injection timings ranging from 5 to 15 deg. CA BTDC.

## 5 Conclusions

The software created meets the requirements (combustion modelling), i.e. to estimate the in-cylinder pressure with a 2-5 % error from the measured data.

Results are in good compliance with experiment for the full speed and load state of the engine.

Results closely depend on the constants of the

models and for this reason they have to be carefully analysed.

Accurate data is need for the calibration of model constants.

In general, the soot formation and destruction trends predicted by the Hiroyasu et al. and NSC models are quite similar and in agreement whit experimental measurements.

In particular Hiroyasu model tends to predicts soot emissions better than the NSC model across the range.

The performances of the program are limited by the models used, few of them requiring improvements, such as:

- the third dimension is need;
- a more accurate turbulence model is necessary ( $k-\varepsilon$  model);
- more chemical reactions are need for increase the performances of emissions model (soot and NO<sub>x</sub>);
- evaporation and boiling mechanisms for fuel droplets should be also improved;
- numerical algorithms should be redesigned in order to have an increased accuracy and lower run times.

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