

## **Numerical simulation of the turbulent combustion and soot of diffusion flame**

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### **Abstract**

*Modelling internal combustion engines (I.C.E.) can be made following different Approaches, depending on the type of problem to be simulated. A diesel combustion model has been developed and implemented in a full cycle simulation of a combustion model accounts for transient fuel spray evolution, fuel-air mixing, ignition, combustion and soot pollutant formation. The models of turbulent combustion of diffusion flame, apply to diffusion flames, which one meets in industry, typically in the diesel engines Particulate emission represents one of the most deleterious pollutants generated during diesel combustion engines oxidation in internal combustion engines. A phenomenological numerical Stringent standards on particulate emission along with specific emphasis on size of emitted particulates have resulted in increased interest in fundamental understanding of the mechanisms of soot particulate formation and oxidation in internal combustion model which can predict the particle size distribution of the soot emitted will be very useful in explaining the above observed results and will also be of use to develop better particulate control techniques. A diesel engine chosen for simulation is a version of the Caterpillar 3406. We are interested in employing a standard finite-volume CFD (computational fluid dynamics) code, KIVA3V-RELEASE2.*

**Key-words:** *Flame, turbulence, modelling, soot formation and oxidation.*

### **1. Introduction**

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. Soot is a solid black material that consists mostly of carbon and hydrogen in the core and with toxic components like metals, acids and organics absorbed on the surface area. Many studies have shown that human exposure to soot particles can lead to changes in heart. To avoid the formation of soot and soot precursors in combustion processes, complex pathways have to be examined. For this reason soot formation has been widely studied in the last decades but is nevertheless not fully understood, Laurie PESANT (2005). The mathematical and numerical description of soot formation and oxidation in technical combustion systems has been studied for decades. It can be regarded as a complex challenge, since the formation and destruction of soot involves many physical and chemical processes that are still under discussion. Modelling approaches range from rough empirical models that employ simple correlations based on experimental data to predict global soot formation characteristics. In this study a mathematical model based carbon black is formulated and implemented to a three dimensional KIVA3V-RELEASE2, a computer programme for chemically reactive flows with sprays used for simulating internal combustion engines. We wanted to create a relatively simple.

### **2. Soot Model**

The concentration of soot in the exhaust is governed by the formation and oxidation of soot during the engine cycle. The soot model is primarily based on that of V. F. Surovikin, while the oxidation of soot particles follows the procedure of Haynes and Wagner, with rate constants from Nagle and Strickland- Constable, Amsden, A.A. (1997). The eventual soot emission from a combustion device

is usually much less than the amount actually generated within. This difference arises because of the combustion of soot particles in oxygen-containing regions beyond the soot-formation zone, and is an important process. The concentration of soot in the exhaust is governed by the formation and oxidation of soot during the engine cycle.

### 2.1. Formation of soot

The soot model derived from Surovikin, the whole process from the moment when the hydrocarbon reaches the reaction temperature to the separation of particles of carbon black consists of three stages. First is the formation of radical nuclei. Second is the growth of the radical nuclei and their conversion to nuclei with a physical surface, on reaching a critical diameter. Third is the growth of the nuclei and their transformation into particles of carbon, Aerattukkara and Kumar (2002). First two stages of the process have a chemical nature and are due to the formation and growth of radical nuclei as a result of thermal decomposition of the molecules of the initial hydrocarbon with the splitting off of hydrogen and also the branching of nucleus formation through the reaction of the radical nuclei with molecules of the hydrocarbon. Third stage of the process consists of the interaction of the molecules of the hydrocarbon and of the radical nuclei with the extremely active surface of the growing nuclei of the carbon particles. This model is capable of predicting the total in-cylinder soot concentration and particle size distribution. (1) the formation of radical nuclei, (2) the growth of the radical nuclei and their conversion to nuclei with a physical surface, on reaching a critical diameter and (3) the growth of the nuclei and their transformation into particles of carbon. The first two stages of the process have a chemical nature and are due to (1) the formation and growth of radical nuclei as a result of thermal decomposition of the molecules of the initial hydrocarbon with the splitting off of hydrogen. And (2) the branching of nucleus formation through the reaction of the radical nuclei with molecules of the hydrocarbon. Both these stages take place from the beginning of the process to the complete consumption of the hydrocarbon. The third stage consists of the interaction of the molecules of the hydrocarbon and of the radical nuclei with the extremely active surface of the growing nuclei of the carbon particles. The three stages shown in Fig.1. The Surovikin model equations, Bosch (2001), presented by:

$\frac{dn}{dt} = F_0 + F_n - G_0 n^2 + K$	Rate of formation of radical nuclei (1)
$\frac{d(D_{r-n})}{dt} = \sqrt{\frac{6}{\pi}} \frac{1}{3} G_0^{\frac{1}{2}} \frac{dG}{dt}$	Rate of growth of radical nuclei (2)
$\frac{dV}{dt} = Z_{r-n} S_{r-n} + Z_m S_m$	Rate of consumption of hydrocarbon (3)
$\frac{dV_m}{dt} = \frac{\pi}{2} \left( \frac{D_{r-n} + D_m}{2} \right)^2 \frac{d \left( \frac{D_{r-n} + D_m}{2} \right)}{dt}$	Rate of growth of Particle nuclei (4)
$\frac{dn'}{dt} = F_0 + F_n' - G_0 (n')^2 - K$	Dependence of m (t) on n (t) (5)
$\frac{dn}{dt} = \frac{dn'}{dt} \frac{V}{V_m}$	Rate of formation of Particle nuclei (6)

Where: m: concentration of Particle nuclei, n': dependence of m (t) on n (t),  $D_{nuc}$ : diameter of particle nuclei

### 2.2. Oxidation of soot

The oxidation process for the soot particles is based on the formula of Nagle and Strickland-Constable, which uses empirical rate parameters, and is based on the concept that there are two types of sites on the carbon surface available for O<sub>2</sub> attack. For the more reactive sites, the rate is controlled by the fraction of sites not covered by surface oxides, whereas in the less reactive sites, the reaction rate has a first-order dependence on the oxygen concentration. 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, Dohoy and Dennis (2001). The chemical reactions are:



The NSC soot oxidation rate IS given by:

$$\frac{dm_s}{dt} = \frac{M_C}{\rho_s d_s} m_s w \quad (10)$$

Where  $M_C$  is the carbon molecular weight (12 g/mole),  $\rho$  is the soot density (2.0 g/cm<sup>3</sup>), and  $d_s$  is the soot diameter (2.248\*10<sup>-8</sup>m). The term  $w$  in equation (4) is the net reaction rate of reactions (7), (2), and (3) and is defined as:

$$w = \left( \frac{K_A P_{O_2}}{1 + K_A P_{O_2}} \right) x + K_B P_{O_2} (1 - x) \quad (11)$$

Where  $P_{O_2}$  is the oxygen partial pressure in atm. The proportion,  $x$ , of A sites is given by:

$$x = \frac{P_{O_2}}{P_{O_2} + (K_A / K_B)} \quad (12)$$

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

### 3. Specification of engine diesel used

Measurements and modelling taken on a representative, modern, controlled diesel engine commonly found in heavy-duty trucks. With four strokes, in-line, six cylinders, turbocharged, water-cooled, direct injection, Dohoy and Dennis (2001). version of the Caterpillar 3406 are listed in Tab. 2. And the combustion chamber employs a bowl shape, Amsden and Rourke (1989), shows in Fig. 2.

### 4. Results obtained and discussions

The accumulation of a number of radical nuclei (RN) and their growth takes place during the induction period in the 1<sup>st</sup> and 2<sup>nd</sup> stages of the process. After the 1<sup>st</sup> radical nucleus has reached the critical diameter due to the appearance of a physical surface, the surface, the process of the appearance and growth of the particle nuclei develops. At the end of induction period, the process of the appearance and growth of radical nuclei, destruction of radical nuclei and the appearance of new particle nuclei, all take place simultaneously. The competition of the process of the growth of radical nuclei and the growth of particle nuclei is due to difference in values of the activation energies of growth. The destruction of the radical nuclei is accelerated through the appearance of the rapidly growing surface of the particle nuclei. The kinetic characteristics of different stages of the process are shown in Fig. 5. Nucleation produces a large number of very small particles with insignificant soot loading. The bulk of solid phase is generated by surface growth, which involves the gas phase of hydrocarbon intermediates on the surfaces of the particles that develop from the nuclei. The two processes may not be separated in time and agglomeration may begin at the onset of soot nucleation. These stages of particle generation and growth constitute the soot formation process. The semi empirical formula of nagle and Strickland gives a surface mass oxidation rate  $\omega$  (g/cm<sup>2</sup>.s). according to this mechanism, the reaction is first order at low oxygen partial pressures. But approaches zero order at higher pressures. At a given oxygen pressure, the rate initially increases exponentially with temperature (equivalent activation energy is  $k_A / k_Z$ ). Beyond a certain temperature the rate decrease

as the thermal rearrangement favors formation of less reactive B sites. When, at sufficiently high temperature the surface is completely converted with temperature. Fig. 3 shows the oxidation rate predicted by NSC as a function of temperature and oxygen partial pressure. The rate  $\omega$  gives by equation (5) used to estimate the amount of soot can be oxidized in specified diesel engine. In the overall soot formation process, shown schematically in Figure1, oxidation of soot at the precursor, nuclei and particle stages can occur. The rate of consumption of the hydrocarbon consists of the loss of hydrocarbon molecules as the result of active collisions with the surface of the radical-nuclei. The hydrocarbon is converted into radical-nuclei and particle-nuclei. Fig.4 shows the rate of hydrocarbon ( $C_7H_{16}$ ) converted to soot species.

## 5. Conclusion

The model tested for physical behaviour of different growth species has been implemented to the full three dimensional KIVA code, version KIVA3V version KIVA3Vrelease2. The model is capable of predicting the total in-cylinder soot Concentration and particle size distribution. The phenomenological soot model developed in this work predicts temporal soot variation and the size distribution. The complete model also accounts for the creation and growth of soot particle nuclei, through the use of a fictitious soot-forming species, and particle destruction through particle-particle collisions. Finally, the cell-specific internal energies are reduced through radiative heat loss. In conclude for this study the soot phenomenon is treated globally, incorporate the details of sooting process such as particle inception, surface growth and particle oxidation. Rate expressions are developed for each processes, the rate coefficients for each process are adjusted to match experimental data. Economic in computation, the validity of the correlations is quite uncertain for situations that vary only slightly from the conditions where modelling parameters are calibrated, the Nagle and Strickland-Constable model is a model most accepted expression of the oxidation rate by  $O_2$ .

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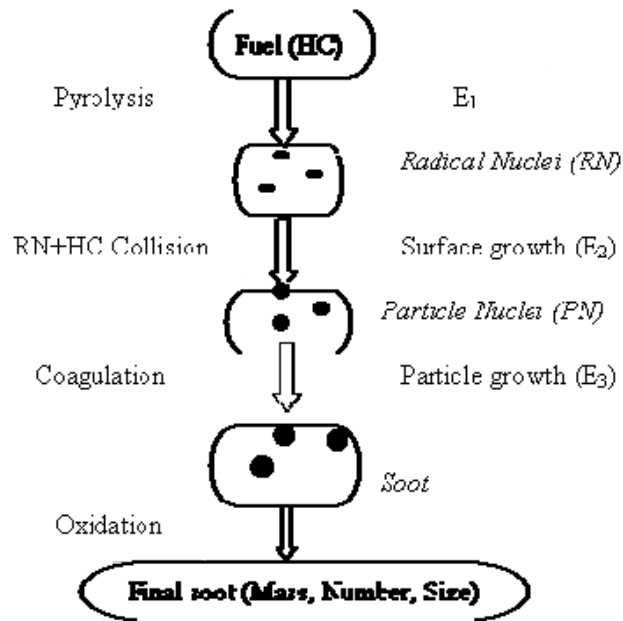


Figure 1: Phenomenological Surovikin soot model

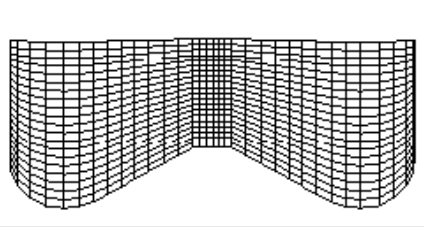


Figure 2. Bowl grid at crank = -30 BTDC

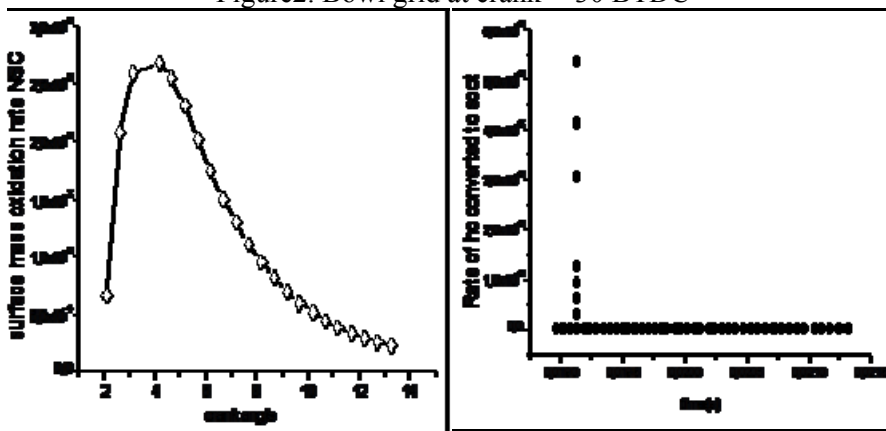


Figure 3: Soot oxidation rate

Figure 4: Hydrocarbon converted to soot

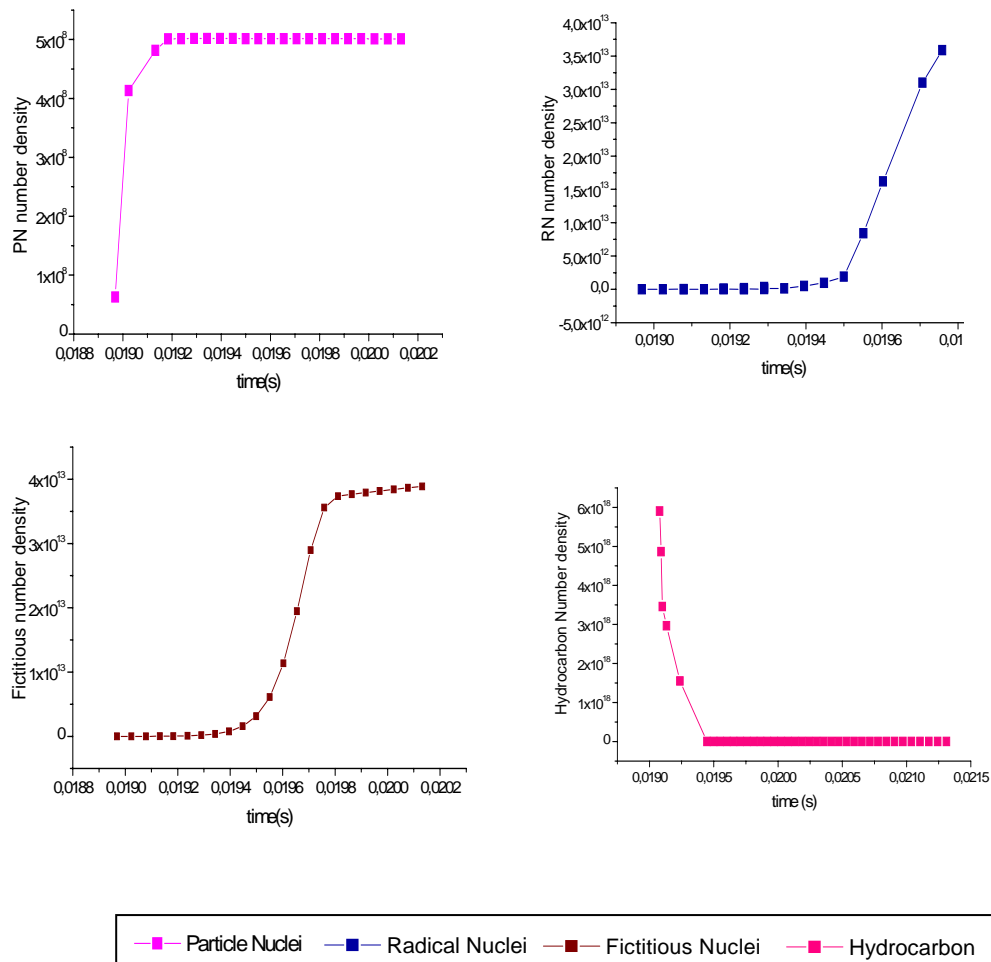


Figure 5: Surovikin soot Formation

Table 1: Rate constants for NSC soot oxidation model

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

Table 2. Heavy duty diesel engine Specification

Parameter	Value
Bore (mm)	100
Stroke (mm)	95.5
Conrod length (mm)	169.2
Compression ratio	15 : 1
Speed (rpm)	1600
Hole diameter (mm)	0.18
Hole length (mm)	1.1
Injection timing (deg. BTDC)	11
Inlet air temperature (deg. K)	400
Inlet air pressure (MPa)	1.5