Simulation of soot formation and analysis of the "Advanced soot model" parameters in an internal combustion engine

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ABSTRACT

Environment issues have been in the public focus for decades, resulting in various steps to prevent or minimize dangerous combustion emissions. With the general traffic (transformation of the chemical energy into mechanical) being the main source of the emissions discussed here, main issue in this paper will consider a possible way to minimize emissions in this region.

Lately, development of computer based simulations led to new mathematical models and approaches to combustion modelling. Along the usual conventional combustion models which assume certain premises to simplify the problem, new and advanced models that include complex chemical kinetics are being developed.

This paper focuses on the soot formation process and the possibilities of its prediction and minimization, if possible. Based on a heavy-duty diesel engine cylinder geometry, a series of calculations were performed using a CFD software package "CFD Workflow Manager" and compared to measurements at five different load points. Variations of the mathematical soot model parameters showed certain patterns which are also described. Also, a description of the rezone meshing strategy that was used for numerical stability is given.

Keywords: Soot, CFD, diesel engine, combustion

1. INTRODUCTION

Lately, development of computer based simulations led to new mathematical models and approaches to combustion modelling. Along the usual conventional combustion models which assume certain premises to simplify the problem, new and advanced models that include complex chemical kinetics are being developed. These are still very much limited with current computer resources, and as such enable inclusion of relatively small number of chemical reactions.

Soot, although welcome in furnace combustion processes contributing greatly to radiation heat transfer, is a dangerous product of combustion processes found in internal combustion engines.

Soot creation mechanism still isn't chemically, and especially mathematically, described, but it is known that it includes hundreds of chemical reactions and species. Therefore, in simulations of soot creation statistical and other empirical based models are used.
Since the heavy-duty engine was used for simulations, a 3d cylinder model, representing 1/8 of a real cylinder, was made in "Imagine" module of the "CFD Workflow Manager" package. Dozens of calculations were performed varying several engine parameters as well as soot model parameters.

2. ENGINE PARAMETERS AND 3D MODELLING

Engine used for simulations was a HD (heavy-duty) diesel engine usually found in trucks and buses. Geometrical parameters of the engine are:

- bore – 130 mm
- stroke – 150 mm
- swept volume 1.99 l
- connecting rod length – 263.8 mm

The following temperatures were used for setting the boundary conditions:

- head temperature – 500 K
- liner temperature – 410 K
- piston temperature – 510 K

The calculations were performed for five different load points varying load (the amount of injected fuel), speed (in rpm), and the moment of fuel injection. The different loads were at 25%, 50% and 75%, speeds were at 1130 rpm, 1420 and 1710 rpm. The injection times were at top dead centre (TDC) or 0 °CA (crank angle degrees), and -4 °CA (four degrees before reaching TDC). Variations are denominated according to ESC (European stationary cycle) standard [1], and are:

- A_25_A_0 (low speed, low load, injection at 0 °CA)
- A_75_A_0 (low speed, high load, injection at 0 °CA)
- A_75_A_-4 (low speed, high load, injection at -4 °CA)
- B_50_A_0 (medium speed, medium load, injection at 0 °CA)
- C_25_A_0 (high speed, low load, injection at 0 °CA)

Discrete volume mesh was created representing 1/8 of the cylinder, gradually deforming from 247 °CA to 360 °CA (compression stroke) and then back to 470 °CA (expansion stroke). When this cell deformation takes place the cell layers are being squished to near zero height. Therefore, to avoid any numerical disturbances, a rezone strategy is being used to change the layer distribution along the deforming part of the mesh. Also, rezone is performed in expansion stroke to increase the number of cell to get the best results. In this case rezone action is performed at following time steps: 300 °CA, 340 °CA, 370 °CA, 380 °CA and 420 °CA. Figures 1 and 2 show the results of a rezone procedure at 300 °CA or 420 °CA (symmetrical in respect to TDC). In the case of 420 °CA figure 2 shows the mesh before rezone.

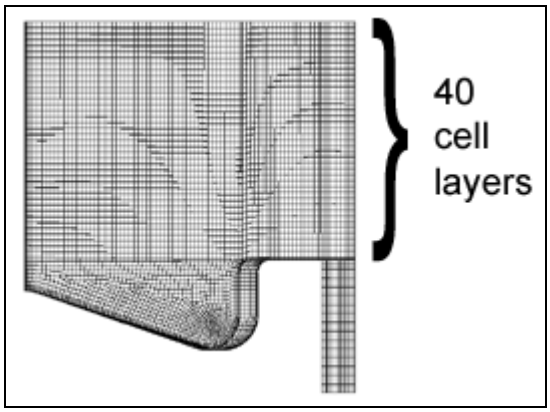

Figure 1. Mesh before rezone

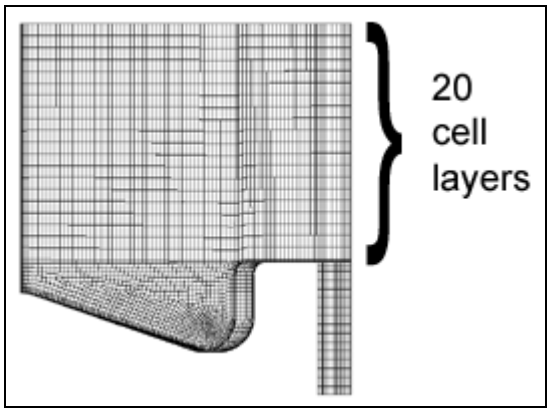

Figure 2. Mesh after rezone

3. THEORETICAL BACKGROUND (MATHEMATICAL MODELS USED IN CALCULATIONS)

3.1. Turbulent flow

Turbulent flow inside a cylinder was in this case simulated using k-ε turbulence model. This model is one of the most used turbulence models in industrial computations because of its proven robustness and accuracy in acceptable boundaries and is implemented in most of the CFD software. Turbulent kinetic energy is represented with a symbol k, and ε is a turbulent dissipation of the kinetic energy (Eq. 1) [2].

$$\tilde{\varepsilon} \sim \frac{\tilde{k}^2}{l_t} \tag{1}$$

Turbulent viscosity coefficient is calculated according to Eq. 2 (C_μ is an empirical constant) [2].

$$\mu_t = \bar{\rho} C_\mu \frac{\tilde{k}^2}{\tilde{\varepsilon}} \tag{2}$$

Transport equations for k and ε are then derived from Navier-Stokes equations.

3.2. Combustion

Considering the extremely wide scope of the whole field of combustion theory, only the specific models that are used according to the problem will be regarded here – combustion of fuel spray and droplet combustion.

Liquid fuel combustion is usually achieved by injecting the liquid through a certain opening into the gaseous combustion chamber domain. This jet is then dispersed into the dens cloud of fuel droplets that penetrate the combustion region. Heat transfer onto each of the droplets raises the vapour pressure to the final combustion of the gas phase

Spray was simulated in "CFD Workflow manager" using mathematical models called WAVE (for dispersion), and WALLJET (for spray-wall interaction).

Type of flame that we meet while discussing combustion in an IC engine cylinder is referred to as turbulent nonpremixed flame. The main characteristic of these flames, as their name suggest, is the separate introduction of fuel and oxidizer to the combustion chamber. Since the modelling of turbulent nonpremixed flames is based on many statistical assumptions, using probability density functions and flamelet models is more than welcome. First approach defines a probability function representing a probability of a certain physical property appearing in specific intervals [3].

Flamelet model of nonpremixed flames describes turbulent flame as a laminar premixed flame imbedded in a turbulent flow field. One of basic empirical model called Eddy-breakup model was used in these simulations. This model assumes the time scale of chemistry being much smaller than the turbulent time scale and the reactants being contained in different eddies. Breakup and mixing of these eddies determines the reaction rate [4].

3.3. Soot

Soot is usually formed during combustion when the equivalence ratio is greater than 1. Investigation of premixed flames showed that the fuel molecules are broken down to radicals, mostly acetylene. In time, these radicals grow in two dimensions by chemical reactions, H abstraction and acetylene addition. These processes form large aromatic rings out of aliphatic species. In further stages molecules become three-dimensional and form carbonaceous particles by coagulation. The most important influences during the soot formation process come from local fuel-air ratio (C/H and C/O ratios), temperature, pressure, and residence time [4].

The "Advanced soot model" developed by Lund LTH University, calculates the volume fractions of the soot source, integrated over the mixture fraction (Eq. 3) probability density function.

$$Z = \frac{m_u + m_b}{m_{tot}} \tag{3}$$

Soot source consists out of four parts: particle inception, surface growth, fragmentation and oxidation. Different sources can be adjusted to each problem. Four scaling parameters are, therefore, introduced. For each of the soot source part there is one scaling parameter which is then multiplied with the integral surface of the different elements to qualitatively define the influence of each source on the final volume soot source [4].

4. CALCULATION RESULTS

4.1. Pressure and temperature

Figure 3 shows good agreement comparing calculated and measured pressure during compression and combustion. Only discrepancy is seen at the beginning of the combustion due to the fast chemistry assumed when using Eddy-breakup combustion model.

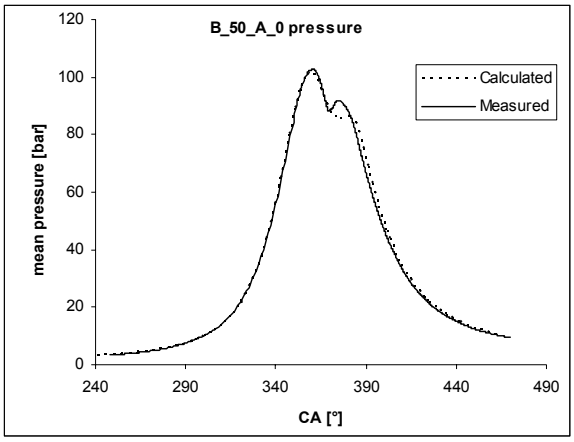

Figure 3. Mean pressure in B_50_A_0 case

Since no experimental data was available for temperature comparison, Figure 4 shows temperature comparison for each calculated case. This chart can be used to discuss the temperature influence on soot formation.

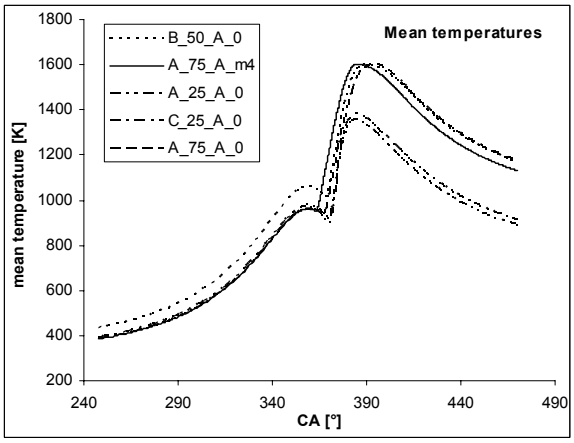

Figure 4. Mean temperature in all cases

4.2. Particle inception parameter variations

As seen in following figures (Fig. 5 and 6) variations of this parameter produced strictly linear dependence of soot mass at the end of combustion on this parameter. This kind of dependence carries low physical value, but can be used to adjust the tendencies acquired by setting other parameters.

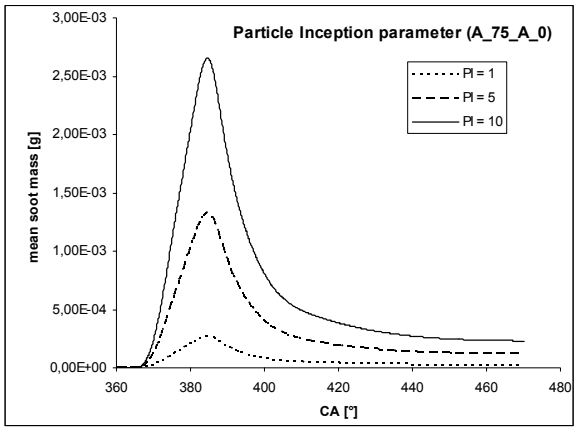

Figure 5. Particle inception parameter variations

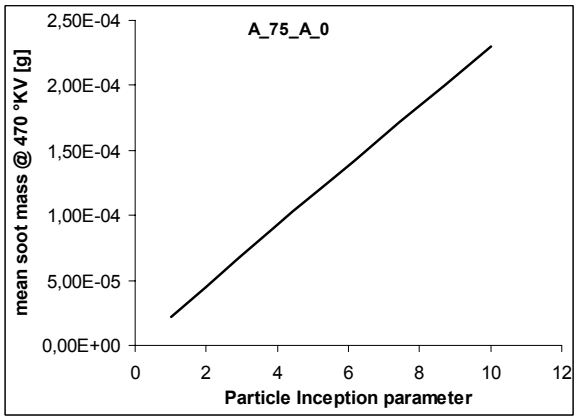

Figure 6. Soot mass dependence on particle inception parameter

4.3. Oxidation parameter variations

Since the oxidation part of the soot source has a negative sign (thus representing the sink), the increase of the resulting soot mass occurs when lowering the oxidation scaling parameter. When its value comes close to zero, which could represent the total lack of the oxidation in the soot formation process, the final soot mass values are stabilized at a certain level dependant on the fuel amount (or load) and other parameters (pressure, temperature, other soot model parameter values). Increasing the parameter values over 1, the soot values would be decreased close to zero, since the oxidation is in that case a dominant process.

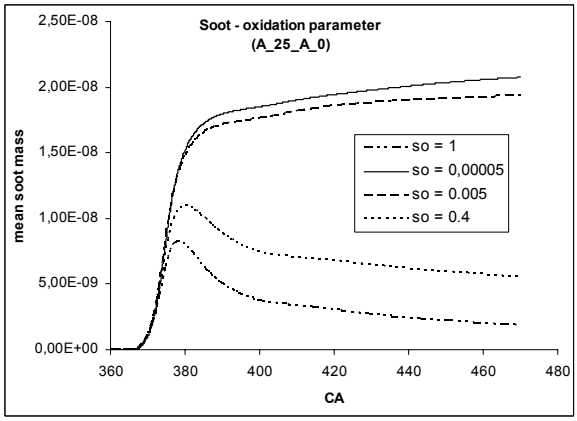

Figure 7. Oxidation parameter variations

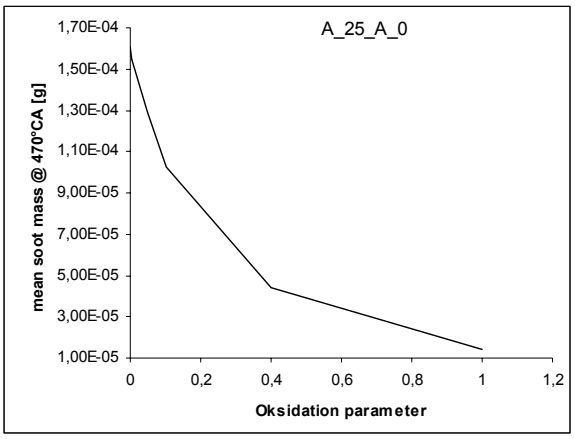

Figure 8. Soot mass dependence on oxidation parameter

4.4. Surface growth parameter variations

In Figure 10 which is showing the final soot mass dependence on the surface growth parameter, one can see that it is almost exponential. Setting the greater values of this parameter the soot concentration (or the soot mass) increases, which cannot be effectively eliminated with the oxidation in the latter part of the combustion process (this could, of course, be regulated by the adequate oxidation parameter).

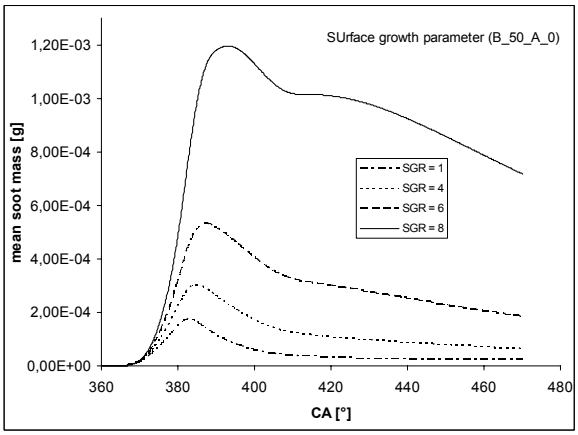

Figure 9. Surface growth parameter variations

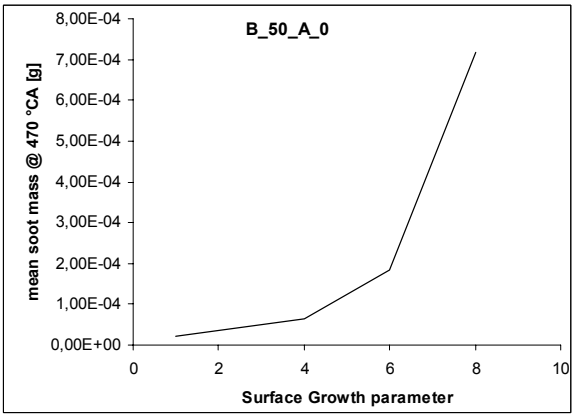

Figure 10. Soot mass dependence on surface growth parameter

4.5. Fragmentation parameter variations

As shown in figures 11 and 12, varying this parameter show vary small deviations from the initial ones acquired using the default parameter value (1).

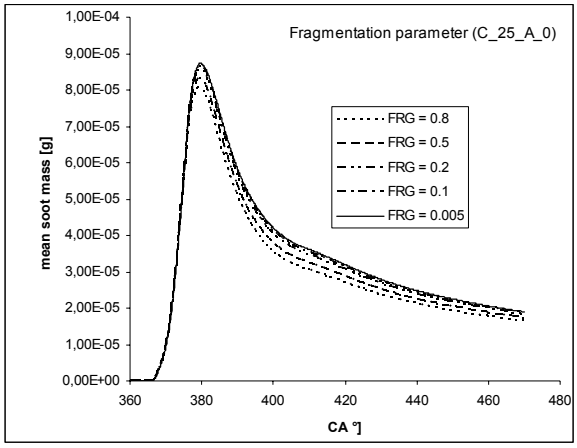

Figure 11. Fragmentation parameter variations

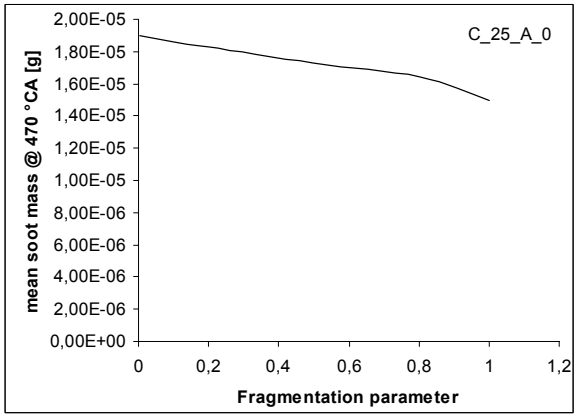

Figure 12. Soot mass dependence on fragmentation parameter

4.6. Optimized parameter set?

Since the really significant results were obtained varying the oxidation and surface growth parameters, their values were set to 2 (surface growth) and 0.9 (oxidation), while leaving the other two parameters (fragmentation and particle inception) at their default values of 1. Calculation results (shown in figure 5.17) show relatively good agreement (and tendencies) at the last time-step in the high-load cases (A_75_A_0, A_75_A_-4 and B_50_A_0), while the calculation results for the low-load cases are much underestimated according to the measured values. This is especially evident in the A_25_A_0 case (low load and low rotational speed), in which the calculated values are about ten times lower than the measured ones. Looking at these results, one can conclude that the final soot mass calculated by this mathematical model is heavily dependant on the amount of the injected fuel, thus giving the higher values at high-load, and lower values at low-load cases, which isn't realistic.

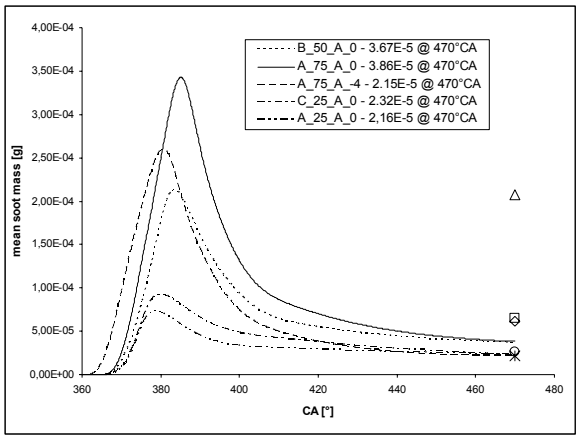

Figure 13. Mean soot mass comparison for a single parameter set on all cases

5. Conclusion

These results have shown that using the advanced soot model, one gets the soot production mostly dependant on the mass of the injected fuel (or the load), what makes it hard to define a single set of optimized parameters for all the load cases. Also, two of the four soot model parameters have show little physical significance, one (particle inception) not giving realistic results, and the other (fragmentation) making practically no influence on the resulting values. This has shown the dominant influence of the other two parameters, oxidation and surface growth. Since only the measured values at the exhaust (last time-step) were available, it wasn't possible to assess the quality of the model during the entire soot formation process, but, as seen in the high load cases, has shown pretty good tendencies when changing the start time of the injection.

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