An Evaluation of a Discrete Particle Model for Soot Formation, Growth, Transport and Oxidation in Diesel Engines

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ABSTRACT

A multidimensional model for flows, sprays and combustion including pollutants in Diesel engines is employed to evaluate a discrete particle model for soot formation, growth, transport and oxidation in Diesel engine. Results of computations in a constant volume chamber, where the ambient state conditions and the spray conditions relate closely to that in a Diesel engine, and in an optical-access Diesel engine are presented. The soot is represented as particles whose initial size is selected stochastically from an initial size distribution that may represent sizes during soot formation in a Diesel engine. The particles then grow in size by surface growth and change in size due to collisions, coalescence and oxidation. In evaluating oxidation rates, the effect of mixing on oxidation is evaluated relative to kinetics. It is shown that mixing rates have a controlling effect on the oxidation of soot during the later stages of oxidation. Transport effects including mean and turbulent convection and thermophoretic effects are also modeled.

INTRODUCTION

Diesel engines are a major source of small particulate matter emissions in the environment. Recent concerns about the harmful effects of small particulate matter in the environment have led to stringent regulations on the emissions of particulates from Diesel engines. It has been shown that fine particulate matter which are below 2.5 μm in aerodynamic diameter and ultrafine particles and nanoparticles pose serious health hazards [1,2]. In addition to the size of particles, the number in the exhaust is an important parameter as well. The Environmental Protection Agency has imposed stringent standards on ambient fine particles which are smaller than 2.5 μm in aerodynamic diameter [3].

Optimizing engine designs and operating conditions to achieve lower particulate matter emissions in terms of mass and number is a challenging task involving many interacting variables. Multidimensional models for Diesel engine processes including flows, sprays, combustion and toxic pollutants are being evaluated to aid in understanding and optimizing engine designs [4-6]. In the case of modeling of soot, the common approach is to consider the soot as a trace species, modeled like the other species, and whose mass is a balance between formation and oxidation. Such approaches do not provide information about the number density or sizes of the particles nor do they naturally adapt to surface dependent oxidation rates.

Recently, an approach has been proposed whereby the soot is modeled as particles with a size distribution and number density [7]. This approach includes the effects of collisions, coalescence and thermophoretic effects. In this paper, this approach is extended to include surface growth and surface area dependent oxidation rates. The approach is then employed to compute soot distribution in a combusting spray under Diesel conditions and also in a Diesel engine. The results are qualitatively compared with published measured results in an optical engine. The next section briefly discusses the experimental results employed for the comparisons. The three-dimensional model is then discussed. Results from computations in the constant volume chamber and in the engine are then presented. We close the paper with summary and conclusions.

THE EXPERIMENTAL RESULTS

The experimental results that we have employed for our comparisons with our computed results are those that
have been obtained in an optical-access Diesel engine at the Combustion Research Facility at Sandia National Laboratories [8-9]. This engine is a modified single cylinder version of a Cummins N-14 engine. Figure 1 shows a cross section of the engine. The ambient and injection conditions for the cases considered are given in Table 1. Measurements were made of distributions of liquid-phase and vapor-phase fuel, chemiluminescence, PAH, soot and of OH radicals which are indicative of heat release in the flame. Vapor fuel distribution was derived using quantitative planar laser Rayleigh scatter imaging. Soot distribution was obtained using laser induced incandescence (LII) and elastic-scatter imaging. The elastic scatter images are biased towards larger soot particles compared to the LII. The relative soot size distribution may thus be deduced from the images.

Based on these measurements, a conceptual model of Diesel combustion has been proposed by Dec [9]. Figure 2 shows a schematic of the conceptual model. The figure shows a temporal sequence of the liquid fuel, vapor fuel and soot distribution and the development of the diffusion flame. The sequence starts at 4.5° CA after start of injection (ASI) to 10° CA ASI. The liquid fuel reaches a steady penetration of about 20 mm at 4.5° CA. The vapor fuel continues to penetrate. Soot is first noticed at 6.0° CA. The soot concentration increases with time. A key observation is that soot is observed at the center of the jet from the time it begins to form. Maximum concentration and the largest size particles are observed in the head of the jet.

THE COMPUTATIONAL MODEL

The three-dimensional model for flows, sprays and combustion that is employed in this work has two distinct components: the physics and the numerics [10]. For the physics, the unsteady general conservation equations for two-phase flows with submodels for turbulence, heat and momentum fluxes at the walls, sprays and combustion are solved [4,11-13]. Turbulence is represented using a two-equation k-ε model with terms that account for spray/turbulence interactions and the effects of compressibility. Wall functions are used to compute heat and momentum fluxes at the walls. The spray model incorporates a line source for drops [14]. It solves equations for the exchange of heat, mass and momentum between the gas and liquid phases, turbulent dispersion of drops and collisions and coalescence. All constants of the model are those used in reference [4,10-14]. The combustion submodel, that is employed here, includes a model for predicting autoignition and one for computing the subsequent combustion of the ignited gas [4].

In the present work, the soot is modeled using a stochastic discrete particle approach. This has been described before [7]. Briefly, in the approach, in principle, we solve an equation for the distribution function of soot particles. The distribution function f is defined in such a way that \( f(r,x,v,t)drdt \) is the probable number of soot particles per unit volume at position x and time t with velocities in the interval \( (v, v+dv) \), radii in the interval \( (r, r+dr) \). The solid volume fraction \( \theta \) is given by

\[
\theta = \int \int \frac{4}{3} \pi r^3 dv dr
\]

(1)

This calculation is valid for \( \theta < 1 \). The evolution equation for f is given by

\[
\frac{\partial f}{\partial t} + \nabla_x \cdot (fv) + \nabla_v \cdot (fF) + \frac{\partial (fR)}{\partial r} = f_{\text{coll}} + f_n + f_{\text{ox}}.
\]

(2)

In this equation, the term \( \frac{\partial f}{\partial t} \) is the time rate of change of the distribution function f at a fixed value of x. The term \( \nabla_x \cdot (fv) \) is the time rate of change of f due to convection of particles. \( \nabla_v \cdot (fF) \) accounts for the transport of particles in velocity space and \( \partial (fR)/\partial r \) accounts for a change in radius of the particle. F and R are the time rate of change following an individual particle, of its velocity and radius. \( f_{\text{coll}} \) is the source term due to soot collisions and \( f_n \) is the source term due to soot nucleation. \( f_{\text{ox}} \) represents the sink term due to soot oxidation. In practice, we solve this equation using a discrete particle, Monte-Carlo approach, like the one used to solve the spray equation in reference [15]. We have discussed the models for collisions and coalescence before [7]. Below, we discuss only the models for formation and oxidation.

The nucleation term, \( f_n \), is modeled using two approaches. The soot formed is modeled as discrete particles. We assume that these particles are spherical. Since the total number of particles would be prohibitively large from a computational point of view, the particles are grouped into parcels with each parcel containing a large number of identical soot particles. The size of each particle is randomly selected from a log-normal distribution. The number of particles in each parcel may then be determined. The two models for formation of soot that are employed are one due to Hiroyasu et al. [16] and the other due to Moss et al. [17]. While both models consider the soot formed in terms of the mass of soot, in our work this mass of soot is transferred into particles when its value in a computational volume reaches a value that is set a priori.

In employing the model of Hiroyasu et al. [16], the formation of soot is modeled as:

\[
\frac{dM_s}{dt} = k_f M_{fv}
\]

(3)

where \( M_s \) and \( M_{fv} \) are the mass of soot and fuel vapor respectively, and

\[
k_f = 300 p^{0.3} e^{-E_f/RT} \quad [s^{-1}]
\]

(4)

In this expression, \( p \) and \( T \) are pressure in bar and temperature respectively, \( \mathcal{R} \) is the universal gas constant and \( E_f = 12500 \text{ cal/mol} \).

In the approach proposed by Moss et al. [17], simplified representations for the processes of nucleation, heterogeneous surface growth and coagulation are employed in ordinary differential equations for the soot volume fraction, \( f_v \) and the particle number density, \( n \). However, in
our approach here, we employ only the nucleation model of Moss et al. since other elements of the model are included in the stochastic discrete particle approach employed here. The nucleation model is:

$$\frac{d}{dt}(\rho_s f_v) = \delta$$  \hspace{1cm} (5)

where $\rho_s$ is the density of the soot and $f_v$ is the local volume fraction of soot.

For each particle of mass $m_p$, the growth in soot mass due to surface growth is modeled as:

$$\frac{dm_p}{dt} = \gamma$$  \hspace{1cm} (6)

where $\delta$ and $\gamma$ are related to the local density, temperature, and fuel concentrations by the following equations:

$$\delta = C_\delta \alpha$$  \hspace{1cm} (7)

$$\alpha = C_\alpha \rho^{3/2} T^{1/2} X_c \exp(-T_s/T)$$  \hspace{1cm} (8)

$$\gamma = C_\gamma \rho^{1/2} T^{1/2} X_c \exp(-T_s/T)$$  \hspace{1cm} (9)

where $C_\delta$, $C_\alpha$, and $C_\gamma$ have the following forms:

$$C_\delta = 144.$$  \hspace{1cm} (10)

$$C_\alpha = 6 \times 10^6 \,[m^3kg^{-2}K^{-1/2}s^{-1}]$$  \hspace{1cm} (11)

$$C_\gamma = 4.8 \times 10^{-18} \,[m^3K^{-1/2}s^{-1}]$$  \hspace{1cm} (12)

The term $R$, which is the time rate of change in the particle radius following individual particles includes the contribution from soot oxidation. For soot oxidation, we employ the Nagle and Strickland-Constable (NSC) model [18] and a mixing controlled (MIX) model [4,19]. The NSC model is formulated as:

$$\omega_{NSC} = 120[(k_A P_O_3 \chi)/(1 + k_B P_O_3) + k_B P_O_3(1 - \chi)]$$  \hspace{1cm} (13)

The expressions for $k_A$, $k_B$, $k_T$, $k_Z$ and $\chi$ are given below:

$$k_A = 20 \exp(-15098/T)$$  \hspace{1cm} (14)

$$k_B = 4.46 \times 10^{-3} \exp(-7650/T)$$  \hspace{1cm} (15)

$$k_T = 1.51 \times 10^5 \exp(-48817/T)$$  \hspace{1cm} (16)

$$k_Z = 21.3 \exp(2063/T)$$  \hspace{1cm} (17)

$$\chi = [1 + (k_T/(k_B P_O_3))]$$  \hspace{1cm} (18)

The mixing controlled rate is based on characteristic mixing times $\tau_1$ and $\tau_2$ derived from the local and instantaneous values of $k$ and $\epsilon$ as follows [4,19]:

$$\tau_1 = C_{m1}(k/\epsilon)$$  \hspace{1cm} (19)

and

$$\tau_2 = C_{m2}(k/\epsilon)(\rho_s \alpha_s + \rho_f \alpha_f)/\rho_O_2$$  \hspace{1cm} (20)

$C_{m1}$ and $C_{m2}$ are two constants. $\alpha$ refers to the stoichiometric oxygen requirement to burn the soot or fuel, and the subscripts $s$, $f$, $O_2$ denote soot, fuel and oxygen respectively. The factor $(\rho_s \alpha_s + \rho_f \alpha_f)/\rho_O_2$ is the ratio of oxygen required to burn the soot and fuel to the actual amount of oxygen available. If this factor is greater than 1, i.e. oxygen is not readily available as in fuel rich regions, then $\tau_2$ will be the longer of the two characteristic times $\tau_1$ and $\tau_2$. On the other hand, in regions where the local concentration of soot is low compared to the concentration of oxygen, $\tau_1$ will be the longer of the two times. In the approach considered below, this characteristic mixing time is compared with a kinetic time, $\tau_k$ derived from the NSC model. $\tau_k$ is derived from $\omega_{NSC}$ as follows:

$$\tau_k = (\rho_s \tau)/(3\omega_{NSC})$$  \hspace{1cm} (21)

During expansion, as the combustion products cool, this kinetic characteristic time will become more dominant. The controlling characteristic time, $\tau_c$ of oxidation of soot is then estimated as:

$$\tau_c = \max(\tau_1, \tau_2, \tau_k)$$  \hspace{1cm} (22)

The rate $\omega$ of soot oxidation for each particle is then

$$\omega = (\rho_s \tau)/(3\tau_c)$$  \hspace{1cm} (23)

where

$$\frac{dm_p}{dt} = -\omega$$  \hspace{1cm} (24)

The radius of the soot particle associated with the parcels in the cell is then reduced to account for the oxidized mass. R may then be calculated as the time rate of change in radius.

RESULTS AND DISCUSSION

Results are presented below for computations in an axi-symmetric constant volume chamber and in an engine. The objective of the constant volume chamber computations are to assess the implementation of the model. Our previous work has shown that when injection mass and momentum flow rates are kept the same, the penetration and dispersion of gas jets are similar to those of sprays [11,20]. Computations with gas jets also enable the jet to be resolved in the region of the injector orifice unlike in the case of sprays where such high resolution cannot be employed and hence the results are grid sensitive. For this reason, the computations in the constant volume chamber are reported for transient gas jets where the injection conditions correspond to those of the spray in the optical-access engine as given in Table 1. The ambient conditions
in the chamber correspond to that in the optical engine at the start of injection. The injector used in the engine has an 8-hole tip. The holes were spaced equally around the tip and this arrangement lends itself to a periodic treatment of the chamber. Therefore, the computations are made for a 45° sector with periodic boundary conditions in the azimuthal direction. The engine had a cylindrical bowl. Figure 3 shows the grid arrangement in a transverse and a radial plane. The grid is generated such that there is higher resolution near the injector orifice. In the case of the engine, computations are made with the actual experimental conditions including those for sprays.

Figures 4-7 show the computed structure of the gas jet. The figures show the computed fuel mass fraction contours, the temperature contours, soot concentration contours and soot parcels respectively at 1 ms and 2 ms after start of injection. It may be seen that the soot parcels increase in number from 1 ms to 2 ms. Also indicated on the figures are the outlines of the jet as measured by Dec et al. [9] showing that there are discrepancies in penetration and spread. Consistent with the experimental findings, the maximum soot concentration is found towards the head of the jet. However, unlike the experimental results, soot does not appear to form along the centerline of the jet. The soot appears to form in the high temperature region of the jet on the fuel rich side. The soot parcels then diffuse and are convected towards the centerline. Figure 8 shows the computed mass of soot in the chamber as a function of time when the Hiroyasu formation model and the NSC oxidation model and a combination of the NSC and MIX oxidation models are used. Also shown on the figure are results when the Moss formation and NSC oxidation models are employed. It may be seen that the mass increases at early times when the formation and growth processes are dominant and then decreases as oxidation becomes more dominant relative to formation. It may be seen that the oxidation in the later stages appears to be mixing limited. Figure 9 shows the sootier mean diameter (SMD) of the soot particles as a function of time for the soot models that we have considered here. Figure 9 also shows the SMD when the Moss model is employed. In this case, growth on the particle surface appears to lead to a significant increase in particle size. However, when no growth model is employed as is the case with the Hiroyasu model, it would appear that collisions and coalescence do not result in significant increase in particle size.

Figure 10 shows the computed flowfield in the engine. The figure shows the temperature contours and the soot parcels at 0° CA which is about 1 ms after start of injection. Also indicated on the figure showing the soot parcels are outlines of the measured jet profile. From these results, the following composite picture emerges: As observed in the case of the transient jets in the constant volume computations, the soot concentration is highest towards the head of the spray and soot is not found close to the injector orifice. This is consistent with the experimental findings [9]. However, there is a discrepancy between the computed and measured jet penetrations [11].

**SUMMARY AND CONCLUSIONS**

A three-dimensional model for fluid flows, sprays and combustion including pollutants in Diesel engines is employed to compute a combusting Diesel spray in a constant volume chamber under Diesel conditions and in an optical-access Diesel engine. A stochastic discrete particle approach is employed to model soot dynamics and transport. Two models for soot formation and two models for soot oxidation are evaluated. The computed results reproduce some aspects of the experimental findings. The maximum soot concentration is found in the head of the jet. The model reproduces the measured trend of increasing particle size along the axis towards the head of the jet. The model appears to suggest that collisions of soot particles from relatively widely separated regions are not important in contributing to the growth of soot particles but that growth on the soot particles could result in such increase in size. The model does not reproduce the measured trend of the formation of soot along the axis of the jet. Additional detailed measurements of size distribution in such transient combusting jets are necessary to further assess the accuracy of the models and the approach.

**ACKNOWLEDGMENTS**

Partial support for this work has been provided by Cummins Engine Company and Detroit Diesel Corporation. V.M. would also like to thank the support of MURST and CNR, Italy.

**REFERENCES**


Table 1: Engine, ambient and injection parameters

<table>
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<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Bore</td>
<td>140 mm</td>
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<tr>
<td>Stroke</td>
<td>152 mm</td>
</tr>
<tr>
<td>Displacement</td>
<td>2.34 liters</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>11:1</td>
</tr>
<tr>
<td>Number of Holes in Injector</td>
<td>8</td>
</tr>
<tr>
<td>Hole Diameter</td>
<td>0.203 mm</td>
</tr>
<tr>
<td>Angle of Fuel jet Axis (from horizontal)</td>
<td>14 degrees</td>
</tr>
<tr>
<td>Engine Speed</td>
<td>1200 RPM</td>
</tr>
<tr>
<td>Intake Air Temperature</td>
<td>433 K</td>
</tr>
<tr>
<td>Intake Air Pressure (absolute)</td>
<td>206 kPa</td>
</tr>
<tr>
<td>Average Equivalence Ratio Load</td>
<td>0.21 (Low)</td>
</tr>
<tr>
<td>Injected Fuel</td>
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<tr>
<td>Peak injection pressure</td>
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<tr>
<td>Specific gravity of injected fuel</td>
<td>0.7865</td>
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<td>Injection duration</td>
<td>1.4 ms</td>
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<td>Estimated motored ambient density at TDC</td>
<td>16.67 kg/m³</td>
</tr>
<tr>
<td>Estimated motored ambient temperature at TDC</td>
<td>992 K</td>
</tr>
</tbody>
</table>

Figure 1: Cross section of the optical engine

(a) 1.0 ms
(b) 1.6 ms
(c) 2.0 ms

Figure 2: Heat release rate contours: Conditions of [9]: Min contour line = 1x10^7 W/cm³

Figure 3: Computational grid for engine
Figure 4: Fuel mass fraction contours

Figure 5: Temperature contours

Figure 6: Soot concentration contours

Figure 7: Soot particle distribution

Figure 8: Computed mass of soot using Hiroyasu and Moss formation models and two oxidation models

Figure 9: Plot of computed SMD vs time

Figure 10: Computed engine flowfield