Phenomenological Model of Particulate Matter Emission from Direct Injection Diesel Engines

A new phenomenological model is introduced by applying established conceptual models for direct injection combustion to develop a mathematical description of events. The model has the capability to predict particulate mass output, as well as a particulate mass history over a single combustion event. The model was developed in a Matlab-Simulink environment to promote modularity. Results of particulate mass output from single cylinder laboratory engine, and six-cylinder vehicular engine were used to determine the validity of the predictions made. Although predicted values do not perfectly match measured values, there is certainly reasonable agreement.

Keywords: Diesel engines, particulate emission, combustion chamber, fuel injection

Introduction

Particulate matter, or soot, is one of the major pollutants produced by diesel engines. The other major pollutant is nitrogen oxide (NOX). Soot, particularly small particles, has been shown to be a health hazard. The small particles can penetrate deeply into lung tissues. Because oxides of nitrogen and the particulates can not be easily reduced simultaneously without degrading the engine performance, they are the most critical pollutants. The overall objective of this research is to utilize current understandings presented from modern methods of experimentation to develop a new phenomenological model of particulate emissions that is flexible, computationally inexpensive, while maintaining reasonable fidelity. The model is developed based on a modular philosophy, in a Matlab-Simulink environment, and does not utilize a finite element or zonal approach. The conditions required by the model include: in cylinder pressure, mass rate of fuel injection, injection velocity, bulk mean temperature, energy release rate, and the characteristics of injector nozzles. With this information the model predicts: general geometry of developed spray plume, general characteristics of injector nozzles. With this information the model can operate either as a stand-alone device for predicting particulate matter output from a direct injection engine, or as a sub-model in a larger system model of a modern Diesel engine.

Nomenclature

- \( a \) = Empirical constant, 0.66 from SIEBERS (1999)
- \( A_0 \) = Section area of the injection orifice, m²
- \( aTDC \) = After top dead center
- \( b \) = Empirical constant, 0.41 from SIEBERS (1999)
- \( B \) = Thermodynamic balance
- \( C \) = Empirical constant dependent on ignition-delay characteristics of fuel
- \( C_A \) = Crankshaft angle, degrees
- \( C_{A0} \) = Coefficient of area-contraction of the injection orifice
- \( C_{SO} \) = Base soot formation constant
- \( D_T \) = Thermal diffusivity of the air-fuel mixture, m²/s
- \( d \) = Physical diameter of the orifice, m
- \( d_e \) = Effective diameter of the orifice, m
- \( E_R \) = Energy released in the cylinder, MJ/s
- \( E \) = Activation energy, cal/mol
- \( H \) = Total energy of products or reactants, kJ
- \( h \) = Enthalpy, kJ/kg
- \( h_f \) = Heat of formation of species, kJ/kg
- \( H \) = Total energy of products or reactants, kJ
- \( HF_{meas} \) = Measured volume of ISO 4113 oil in the standard discharge coefficient test, cm³
- \( l_h \) = Length of the injector orifice, m
- \( L^* \) = Dimensionless liquid length
- \( LHV \) = Lower heating value of the fuel, MJ/kg
- \( L \) = Liquid length, mm
- \( LO \) = Lift-Off length, mm
- \( M \) = Molar mass, kg/kmol
- \( m_A \) = Mass of fuel available in soot cloud, kg
- \( m_t \) = Mass of fuel injected, kg
- \( m_w \) = Mass of particulate, kg
- \( n_{orifices} \) = Number of injection orifices on injector
- \( P \) = Cylinder pressure, MPa
- \( R \) = Universal gas constant
- \( R_1 \) = Ratio of mass of oxygen to mass of fuel for stoichiometric mix
- \( R_2 \) = Ratio of mass of oxygen to mass of fuel for stoichiometric mix
- \( R_3 \) = Ratio of mass of oxygen in the oxidizer stream (0.232 is used for air; PETERS, 2000)
- \( R_e \) = Reynolds number of the liquid flow
- \( S_{f0} \) = Laminar flame speed of the stoichiometric mix, m/s
- \( T \) = Temperature, K
- \( U_0 \) = Injection velocity of the fuel, m/s
- \( W_{el} \) = Weber number of the liquid flow
- \( x^+ \) = Length scale, mm
- \( Y_{O2} \) = Molar fraction of oxygen present
- \( Z_0 \) = Stoichiometric-fuel-mixture fraction

Greek Symbols

- \( \Delta P \) = Pressure drop through the injector nozzle, Pa
- \( \nu \) = Compressibility factor
- \( \theta \) = Spray angle
The fuel is injected into the combustion chamber slightly before the desired time of combustion, as the piston reaches the end of the compression stroke. The liquid fuel atomizes into small droplets, evaporates and mixes with the hot and compressed air of the combustion chamber. Because the air temperature and pressure are above the fuel’s ignition point, spontaneous ignition occurs after a short delay. The time interval between the start of injection and the first heat release is called the ignition delay. After the ignition delay period, the subsequent Diesel combustion process is commonly divided into two stages. During the initial phase the fuel which has mixed with air to within the flammability limits combusts rapidly. This phase of the combustion process is commonly referred to as premixed phase and is associated with high rates of heat release over a few crank angle degrees. The combustion heat-release history during this interval depends strongly on the fuel-air mixture prepared during the ignition delay period.

DEC (1997), describes the formation and features of a quasi-steady diesel fuel jet, as shown in Fig. 1. It should be noted that this conceptual model applies to large bore, quiescent chamber combustion or a free fuel jet without wall interactions.

To characterize mass and momentum fluxes of fuel leaving the orifice, two of three coefficients for the injector tip are required (NABER & SIEBERS, 1996): the discharge coefficient ($C_D$), the velocity coefficient ($C_V$), and the area contraction coefficient ($C_a$). The discharge coefficient characterizes the mass flux from an orifice, while the area contraction or velocity coefficients allow the momentum flux to be characterized as well. The area contraction coefficient accounts for flow area loss as result of vapor bubbles generated by cavitation. The three coefficients are related by the Eq. (1). The more common situation in the literature however, is that only a discharge coefficient is available. At higher injection pressures, assuming a $C_V$ of one, would only result in a few percent over estimated of the momentum flux (SIEBERS, 1999).

\[
C_D = C_A \cdot C_V .
\]
The discharge coefficient of the orifices could be determined by a standard test, with the prescribed calibrating oil defined by ISO standard 4113, in the fixed temperature of 40 °C. In the test, with a nozzle holder without the pressure pin and under a pressure drop of 400 bar, the delivered oil volume in cm³ is measured in a glass gage for 60 seconds. It is possible to calculate the discharge coefficient from the measured volume by the Eq. (2), derived from Bernoulli’s equation (ARGACHOY, 2001), where ρISO 4113 is the density of the ISO 4113 oil in 40 °C (~ 807 kg/m³), HF meas is the measured volume (cm³), n orifices is the number of injection orifices on injector, A₀ is the section area of each orifice (m²), and ΔPf is the pressure drop through the injector.

\[
C_D = \frac{\rho_{ISO\ 4113} \frac{HF_{meas}}{n_{orifices}}}{6.10^7 (A_0 \sqrt{2 \rho_{ISO\ 4113} \Delta P_f})}.
\]  

(2)

### Spray Angle

When a liquid is injected, under pressure, into a volume of gas, the liquid breaks apart into a spray of droplets that eventually vaporize. Geometry of the injector orifice and the ratio of densities of the gas and liquid will determine the angle developed by the spray. A wider spray angle would result in a larger mass of gas being entrained as the liquid jet moves away from the nozzle. The model of REITZ & BRACCO (1979) for the spray angle (θ) in Eq. (3) and (4), uses the aspect ratio of the nozzle, where the aspect ratio refers to the length-to-diameter ratio of the orifice (lₙ/d), as well as the ratio of air and fuel densities (ρₐ/ρₕ) and the ratio of the Reynolds and Weber numbers of the fuel flow (Reₕ/Weₕ). The function f is a constant with the value of \(\sqrt{3/6}\).

\[
\tan\left(\frac{\theta}{2}\right) = \frac{1}{A} \cdot 4 \pi \left(\frac{\rho_a}{\rho_f}\right)^{1/2} \cdot f \left(\frac{\rho_f}{\rho_a} \cdot \frac{Re_f}{We_f}\right)^2.
\]

(3)

\[
A = 3.0 + (0.28) \left(\frac{l_n}{d}\right).
\]

(4)

Equation (3) simplifies into Eq. (5) for an injector which the spray atomizes at injector nozzle (HEYWOOD, 1988). Most modern Diesel injectors operate at sufficient pressures to cause atomization at the nozzle.

\[
\tan\left(\frac{\theta}{2}\right) = \frac{1}{A} \cdot 4 \pi \left(\frac{\rho_a}{\rho_f}\right)^{1/2} \cdot \frac{\sqrt{3}}{6}.
\]

(5)

### Liquid Length

The distance penetrated by the fuel before vaporization is known as the liquid length. SIEBERS (1999) developed a scaling law to predict the liquid length. The scaling law is based on the idealized spray model shown in Fig. 2.

\[
\frac{\rho_a}{\rho_f} = \frac{\rho_{iso\ 4113}}{\rho_{meas\ HF}} \cdot \frac{A_0}{\Delta P_f}.
\]

(6)

\[
x^+ = \sqrt{\frac{\rho_f}{\rho_a}} \cdot \frac{d_f}{a \cdot \tan(\theta/2)}.
\]

(7)

The effective diameter of the orifice (dₜ) represents the reduction of useful area when flow through the orifice becomes choked. Eq. (7) demonstrates how the effective area can be found, where Cₐ is the coefficient of area contraction and d is the physical diameter of the orifice.

\[
d_f = \frac{1}{\sqrt{C_A}} \cdot d.
\]

(7)

The equation (8) shows the liquid length \(L^+\) expression based on SIEBERS (1999). The actual liquid length is determined by multiplying the dimensionless liquid length by the length scale of the liquid spray. In Eq. (8), b is an empirical constant (0.41), and B is obtained by a thermodynamic balance.

\[
L^+ = b \cdot \left(\frac{2}{B} + 1\right)^2 - 1.
\]

(8)

The liquid length relation depends on the ratio of mass flows of air and fuel represented by the term B, which itself is a balance of two thermodynamic relations (SIEBERS, 1999). The Eq. (9) shows these relations.
Where $v_a$ is the compressibility of air at the conditions of $T_2$ and $P_{a_2}$, $v_f$ is the compressibility of the vaporized fuel at the conditions $T_2$ and $P_{f_2}$. $P_{f_2}$ is the partial pressure of air at thermodynamic equilibrium, $P_{f_2}$ is the partial pressure of the fuel at thermodynamic equilibrium, $T_2$ is the temperature reached by the fuel and air at thermodynamic equilibrium. $M_f$ is the molar mass of the fuel, $M_a$ is the molar mass of air, $h_{a_1}$ is the initial enthalpy of the entrained air, $h_{a_2}$ is the final enthalpy of the entrained air at thermodynamic equilibrium, $h_{f_1}$ is the initial enthalpy of the fuel, and $h_{f_2}$ is the final enthalpy of the fuel at thermodynamic equilibrium.

Restricting the final state of the fuel to saturated vapor and assuming the final mix of fuel and air to be in thermodynamic equilibrium, allows an iterative approach to finding the final temperature of the air-fuel mixture. After an initial guess for $T_2$ is made, the vapor pressure of the fuel can be found, as well as can the other properties of the vaporized fuel in the hypothesized thermodynamic state. The partial pressure of the air can be found by subtracting the partial pressure of the fuel from the total cylinder pressure, at the guessed temperature $T_2$. At that point, it is possible to determine all the other properties of the air at the chosen state. If the two halves of Eq. (9) are not equal, a new guess is made, utilizing a binary search with a continually narrowing search area.

**Lift-Off Length**

The Lift-Off length (LO) is the distance from the injector to the point along the Diesel spray where the diffusion flame sheaths the spray and the air can no longer be entrained into the spray. The Lift-Off length, although coupled to the liquid length, also depends strongly on the thermodynamic and reactive properties of the fuel. The relation that calculates the Lift-Off, set in Eq. (10), is based on the expression of SIEBERS et al. (2003).

$$LO = (0.25).L + C \left( \frac{U_0 \cdot Z_{st} \cdot D_T}{S_{LO(st)} \cdot \tan(0/2)} \right).$$

Where $L$ is the liquid length, $U_0$ is the injection velocity of the fuel, $Z_{st}$ is the stoichiometric fuel mixture fraction, $D_T$ is the thermal diffusivity of the air-fuel mixture, $S_{LO(st)}$ is the laminar flame speed of the stoichiometric mixture, $C$ is an empirical constant, dependent on ignition delay characteristics of fuel, with a value of 3.5, and tan (0/2) is the tangent of the spray half angle. The value of the stoichiometric fuel mixture fraction ($Z_{st}$) is defined by PETERS (2000) in the Eq. (11), where $R_1$ is the ratio of mass of oxygen to mass of fuel for stoichiometric mix, $R_2$ is the ratio of mass of fuel on fuel stream (normally 1 for pure fuels), and $R_3$ is the ratio of mass of oxygen in the oxidizer stream (0.232 is used for air). This fraction ($Z_{st}$) remains constant for a given fuel.

$$Z_{st} = \left(1 + \frac{R_1 \cdot R_2}{R_3} \right)^{-1}.$$  

Thermal diffusivity ($D_T$) is defined also by PETERS (2000) in Eq. (12), as an indicator of how quickly the heat of reaction is passed downstream, to heat the incoming reactants to a temperature appropriate to propagate the reaction.

$$D_T = \frac{\lambda}{\rho \cdot C_p}.$$  

Where $\lambda$ is the thermal conductivity of the material, $\rho$ is the density of the material, and $C_p$ is the specific heat of the material. The laminar flame speed for the stoichiometric mixture of air and fuel ($S_{LO(st)}$ in m/s is calculated from the temperature of mixture in K ($T_a$) and the pressure of the mixture in bar ($P$), using the empirical relation expressed in Eq. (13). The relation was developed by BRADLEY et al. (1998), from measurements taken of a 10 % n-heptane and 90 % iso-octane mixture, but was found to be useful for similar hydrocarbon fuels.

$$S_{LO(st)} = 48 \cdot \left( \frac{T_a}{358} \right)^{0.101} \cdot P^{-0.282}.$$  

**Equivalence Ratio**

The equivalence ratio of the initial reaction ($\phi$) can be determined from the Lift-Off length (LO). Under the assumption of an ideal spray model, the mass of air entrained into the fuel spray is a function of the distance from the injector tip. SIEBERS & HIGGINS (2001) developed the Eq. (14) for the equivalence ratio, during their investigation of Lift-Off length, where $x^+$ is the characteristic length scale. Assuming no air can be entrained once the spray is sheathed in the diffusion flame, the Lift-Off length becomes the determining factor for the maximal mass of air entrained.

$$\phi = \left( \frac{100}{1 + 16 \cdot \left( \frac{LO}{x^+} \right)^2 - 1} \right)^{10 \div 3}.$$  

**Soot Model**

The soot model is based on modified versions of rate equations developed by HIROYASU & KADOTA (1976) for soot formation and soot oxidation. The Eq. (15) shows the net soot rate formula used (PATTERSON et al., 1994).

$$\dot{m}_s = \dot{m}_{sf} - \dot{m}_{so}.$$  

Where $\dot{m}_s$ is the net mass rate of soot formation, $\dot{m}_{sf}$ is the mass rate of soot formation, and $\dot{m}_{so}$ is the mass rate of soot oxidation. The net mass rate of soot formation is integrated with respect to time over the combustion event, to determine the total mass of soot at any moment in the cylinder. Based on the work of KAZAKOV & FOSTER (1998), once quenching conditions are met, mainly temperature of formation drops below 1000 K, soot calculations end, and the model is immediately reset for the next combustion event.

**Soot Formation**

KHAN & GREEVES (1974) indications are, that under high temperature and short reaction time conditions, encountered in a Diesel combustion chamber, the overall mechanism of soot formation may be characterized by an Arrhenius type equation. Equation (16), based on the expression of PATTERSON et al.
(1994), defines the soot formation rate \( \frac{d \text{msf}}{dt} \), where \( C_{\text{BS}} \) is the base soot formation constant, \( \phi \) is the equivalence ratio of the initial reaction, \( m_f \) is the mass of fuel available to soot reaction, \( P \) is the cylinder pressure, \( E_{\text{sf}} \) is the activation energy of the soot formation reaction (12500 cal/mol), \( R \) is the universal gas constant (1.9872 cal/gmol K), and \( T \) is the temperature in the soot formation region.

\[
\frac{d \text{msf}}{dt} = C_{\text{BS}} \cdot \phi \cdot m_f \cdot P^{0.5} \cdot \exp \left( - \frac{E_{\text{sf}}}{RT} \right). \tag{16}
\]

The empirical base soot formation constant adapts the model to a specific engine and fuel type. The temperature in the soot-formation region is determined by first establishing the temperature of the rich reaction products and how they are affected by the diffusion flame and pressure. To establish the temperature rise due to the rich reaction, a simplified one-way reaction is utilized (TURNS, 1996). The heats of formation and mass fractions are used in Eq. 17 through 19 to determine the temperature of the products. Reactants are n-heptane, used as a single component fuel to simulate Diesel, and air, taken to be an oxygen and nitrogen mix. Reaction products for an ideal reaction are assumed to be carbon dioxide, carbon monoxide, water, excess fuel (12) and nitrogen. The equivalence ratio \( \phi \) is determined from the spray model, and the mass fractions of products are interpolate, from tabulated data of STANJAN (Chemical Equilibrium Solver, v 3.96 - Stanford University, 1995), for different equivalence ratios.

\[
H_R = m_f \left( h_f^0 + T_{\text{ini}} \cdot C_p f \right) + m_{O_2} \cdot T_{\text{ini}} \cdot C_p O_2 + m_{N_2} \cdot T_{\text{ini}} \cdot C_p N_2. \tag{17}
\]

\[
H_P = m_{CQ} \left( h_{CQ}^0 + T_{\text{fin}} \cdot C_p CQ \right) + m_{CO} \left( h_{CO}^0 + T_{\text{fin}} \cdot C_p CO \right) + m_{N_2} \cdot T_{\text{fin}} \cdot C_p N_2 + m_{H_2O} \left( h_{H_2O}^0 + T_{\text{fin}} \cdot C_p H_2O \right) + m_f \left( h_f^0 + T_{\text{fin}} \cdot C_p f \right). \tag{18}
\]

\[
H_R = H_P. \tag{19}
\]

Where \( m_x \) is the mass fraction of species \( x \), \( h_x^0 \) is the heat of formation of species, \( C_p x \) is the specific heat of species, \( T_{\text{ini}} \) is the initial temperature of reactants, \( T_{\text{fin}} \) is the final temperature of products, \( H_R \) is the energy released in the combustion products, \( H_P \) is the total energy of reactants, and \( H_{R} \) is the total energy of products.

Soot can only be formed when unburned fuel is available in the soot formation cloud. To determine the mass of fuel that is unburned and thus available to form soot, a simple thermodynamic relation based on the mass conservation is performed in Eq. (20).

\[
\dot{m}_f = \dot{m}_f - \frac{E_R}{LHV_f}. \tag{20}
\]

Where \( \dot{m}_f \) is the mass flow of fuel available in soot cloud, \( \dot{m}_f \) is the mass flow of fuel injected, \( E_R \) is the energy released in the cylinder, and the LHV\(_f\) is the lower heating value of the fuel. The mass of fuel injected into the cylinder is determined by integrating the mass flow of fuel during injection with respect to time. The energy released is found by integrating the heat release rate of the combustion event with respect to time.

\[
\frac{d \text{msf}}{dt} = C_{\text{SO}} \cdot m_f \cdot Y_{O2} \cdot P^{1.8} \cdot \exp \left( - \frac{E_{\text{so}}}{RT} \right). \tag{21}
\]

The base soot oxidation constant is, once again, empirically determined to adapt the oxidation rate to a specific engine and fuel type. Soot oxidation occurs in and around the diffusion flame. The diffusion flame is the area where a turbulent flame front has developed from the mixing of fresh air, with incompletely reacted products of the rich initial reactions. This turbulent flame front is often considered to be occurring near a stoichiometric condition (DEC, 1997). Thus, the molar fraction of oxygen in the region of oxidation is assumed to be equal the molar fraction of oxygen on the reactant side of a stoichiometric mixture of air and n-heptane. The temperature of the soot oxidation region is established in a similar way to that used for the soot formation region. However, the simplified reaction is assumed to occur at an equivalence ratio of 1, to simulate the stoichiometric conditions assumed in the diffusion flame (DEC, 1997). Eq. 17 through 19 again predict the temperature of the combustion products. The temperature of the reactants is assumed to be that of the soot formation region, until all of the fuel in the soot formation is burned.

**Model Validation**

The model was compared to experimental data to determine the validity of predictions made. The experimental data used for the comparisons was obtained from two sources:

- A research single-cylinder Diesel engine from the work of KWEON et al. (2002), adapted from an in-line six-cylinder 14 liters engine, at the Engine Research Center of the University of Wisconsin-Madison (USA).
- A vehicular six-cylinder, 12 liters, Diesel engine, at the DaimlerChrysler Technological Development Center in Brazil.

**Single Cylinder Research Engine**

The specification of the single-cylinder engine employed in the experiments of KWEON et al. (2002) is given in Table 1. Table 2 displays run conditions for six soot mass measurements of CARB 8 mode emissions test of KWEON et al. (2002). The six data set were generously provided by Prof. Dr. David E. Foster, of the University of Wisconsin-Madison (USA), for model comparisons. The cylinder pressure signal of the low load points, corresponding to points number 4 (25% load, peak torque speed) and 8 (10% load, idle speed) was deteriorated, and the particulate mass of these points were not predicted by the model.
Table 1. The research single-cylinder engine specification (KWEON et al., 2002).

| Engine model       | Cummins N14 single cylinder |
|--------------------|------------------------------|
| Type               | Diesel, direct injection, 4 stroke |
| Combustion chamber | Quiescent                     |
| Combustion chamber diameter | 97.8 mm               |
| Number of intake valves | 2                         |
| Number of exhaust valves | 2                   |
| Injection system   | Electronic, Unit Injector (UIS) |
| Displacement       | 2.333 dm³                   |
| Bore/Stroke        | 139.7 mm / 152.4 mm          |
| Connecting rod length | 304.8 mm            |
| Number of nozzle orifices | 8                      |
| Nozzle orifices diameter | 0.200 mm              |
| Discharge coefficient of the orifices | 0.86                  |
| Aspect ratio of the orifices | 4.1 (length/diameter of orifices) |
| Temperature of the fuel injected | 305 K                   |
| Spray angle        | 152°                        |
| Compression ratio  | 13.1                        |

Table 2. Summary of operating conditions of CARB test cycle (KWEON et al., 2002).

| CARB mode | 1 | 2 | 3 | 5 | 6 | 7 |
|-----------|---|---|---|---|---|---|
| Speed (min⁻¹) | 1800 | 1800 | 1800 | 1200 | 1200 | 1200 |
| Load (%) | 100 | 75 | 50 | 100 | 75 | 50 |
| Intake pressure (kPa) | 179.3 | 179.3 | 179.3 | 175.2 | 179.3 | 177.9 |
| Intake temperature (°C) | 49.0 | 48.3 | 48.3 | 48.3 | 49.0 | 48.1 |
| Equivalence ratio | 0.69 | 0.50 | 0.34 | 0.82 | 0.69 | 0.41 |
| Indicated specific fuel consumption (kg/ihp-h) | 0.172 | 0.146 | 0.140 | 0.168 | 0.160 | 0.141 |
| Indicated mean effective pressure (MPa) | 1.083 | 0.922 | 0.671 | 1.491 | 1.225 | 0.878 |
| Start of injection (CA aTDC) | -5 | -5 | -5 | -11 | -2 | -2 |
| Injection duration (CA) | 25 | 20 | 13 | 27 | 22 | 15 |

When the model detected the end of each combustion cycle during continuous operation of the engine, the conditions in cylinder were reset for the next cycle to begin. The final mass of soot in cylinder, when quenching conditions are reached, was considered soot emitted from the cylinder into the exhaust. Figure 3 shows an example, for the mode 7 of KWEON et al. (2002) data, of the predicted time-history of the soot mass in the combustion chamber. The same analysis was made for the other test modes.

Prediction of particulate matter that exists at the end of the combustion cycle is ultimately the goal of this modeling project. A single data point (mode 7) is chosen as the adapting point for the six operating conditions simulated from KWEON et al. (2002). Figure 4 shows the comparison of the measured soot-mass per fuel mass (KWEON et al., 2002) to the predicted soot-mass per fuel mass. From the studies of Mc MILLIAN (2002) apud GAUTAM et al. (2004), the uncertainty associated with particulate material measurements using the mini-dilution tunnel varies between 2.8% to 10% of the reading. The value of 10% total uncertainty was chosen for the analyses. Although predicted values do not perfectly match measured values, there is certainly reasonable agreement. Qualitative predictions of the model are valid.

Six Cylinder Vehicular Engine

The new model is tested to determine the validity of predictions also for a complete vehicular engine on test bench. The specification of the six-cylinder engine employed in the experiments is given in Table 3, and the engine on the DaimlerChrysler-Brazil test bench can be seen in Fig. 5. Table 4 lists the conditions of the EURO III (ESC - European Stationary Cycle) at which the engine was operating when measurements of soot mass were taken. The engine was equipped with a cylinder pressure transducer (0-20 MPa), and an injection pressure transducer (0-200 MPa), in the sixth cylinder. A needle-motion sensor, also in the sixth cylinder, monitors the start of injection and the injection duration directly at the injection nozzle. The cylinder pressure signal of the low load points (0% and 25%), corresponding to points number 1 (idle), 7, 9 and 11 was deteriorated, and the particulate mass of these points were not predicted by the model.
Table 3. The vehicular engine specification.

| Engine model | Mercedes-Benz OM457LA |
|--------------|------------------------|
| Type         | Diesel, direct injection, 4 stroke |
| Number of cylinders | 6 (in line) |
| Combustion chamber | Quiescent |
| Combustion chamber diameter | 92.8 mm |
| Number of intake valves | 2 |
| Number of exhaust valves | 2 |
| Injection system | Electronic, Unit Pump (UPS) |
| Total Displacement | 11.967 dm³ |
| Bore/Stroke | 128 mm / 155 mm |
| Connecting rod length | 251 mm |
| Number of nozzle orifices | 6 |
| Nozzle orifices diameter | 0.229 mm |
| Discharge coefficient of the orifices | 0.72 |
| Aspect ratio of the orifices | 4.4 (length/diameter of orifices) |
| Temperature of the fuel injected | 308 K |
| Spray angle | 150° |
| Compression ratio | 17.25 |

Table 4. Summary of operating conditions of EURO III test cycle.

| Points | 2 | 3 | 4 | 5 | 6 | 8 | 10 | 12 | 13 |
|--------|---|---|---|---|---|---|----|----|----|
| Speed (min⁻¹) | 1135 | 1493 | 1493 | 1135 | 1135 | 1492 | 1876 | 1876 | 1876 |
| Load (%) | 100 | 50 | 75 | 50 | 75 | 100 | 100 | 75 | 50 |
| Intake pressure (kPa) | 236.2 | 164.9 | 220.4 | 146.9 | 189.2 | 273.5 | 267.1 | 248.9 | 197.6 |
| Intake temperature (°C) | 29.7 | 27.6 | 32.3 | 24.8 | 26.3 | 39.4 | 45.2 | 41.6 | 34.2 |
| Equivalence ratio | 0.67 | 0.40 | 0.45 | 0.50 | 0.60 | 0.61 | 0.47 | 0.39 | 0.32 |
| Mass-flow of fuel (kg/h) | 50.36 | 30.37 | 45.15 | 25.59 | 37.78 | 60.62 | 67.56 | 55.28 | 37.33 |
| Measurement time in each point (s) | 72 | 90 | 90 | 45 | 45 | 80 | 72 | 45 | 45 |
| Start of injection (CA aTDC) | -11 | -11 | -10 | -11 | -10 | -13 | -12 | -5 | -5 |
| Injection duration (CA) | 28 | 21 | 29 | 19 | 22 | 35 | 38 | 35 | 30 |

For the current study, one primary and one secondary particulate filters for each measurement was used, not only a pair of filters for the complete EURO III test. The system used was the AVL SPC 472 Smart Sampler. As an example, Fig. 6 shows the predicted time-history of the soot mass in the combustion chamber for the point 3. Comparing the particulate-mass time-history of the engines, it can be seen that the single-cylinder engine has a high peak of soot formation. This characteristic is probably related with the very low compression rate of the adapted single-cylinder engine (13.1:1), in comparison with the vehicular complete engine (17.25:1). Again, a single data point (point 3) is chosen as the adapting point for the all other operating conditions simulated. Figure 7 shows the comparison of the measured soot-mass per fuel mass (test bench) to the predicted soot-mass per fuel mass (model). From the work of McMILLIAN (2002) apud GAUTAM et al. (2004), the value of 10% total uncertainty was chosen for the analyses using mini-dilution tunnel. Qualitative predictions of the model, are valid also for the six cylinder vehicular engine.

Figure 6. Predicted time-history of the soot mass for the point 3 of the EURO III test.

Figure 7. Predicted values by the model versus measured values from DaimlerChrysler-Brazil test bench, of particulate mass per mass of fuel.

**Conclusions**

A new phenomenological model has been compared with results from two engines, a single-cylinder research engine and a vehicular six-cylinder engine. The simulation, as shown in above sections, has achieved a reasonable level of fidelity. Qualitative predictions of the model are valid for both, the single-cylinder engine and also the vehicular six-cylinder engine. The model predicts the particulate mass, and also identifies intrinsic differences between the combustion process of the two engines, like the compression ratio. The model also shows a great potential for expansion. A complex chemistry solver could be interfaced at the initial reaction point, to determine a detailed description of exhaust gasses that contribute to particulate emissions.
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