

3D Modeling of Particulate Matter from Spark Ignition Engines

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ABSTRACT

A 3D simulation technique to estimate density of particulate matter (PM) from spark ignition (SI) gasoline engines is proposed. The technique is based on a two-equation model consisting of coupled conservation equations of soot particle number and mass and fluid transportation equations.

The nucleation rate of soot particles was obtained from a database built by simulation of elementary reaction with the proposed technique. Two approaches were explored to obtain the nucleation rate. One involves 0-dimensinal SI simulation and the other involves 1-dimensinal flame propagation simulation.

The estimation results were verified with measurement data obtained with a single cylinder SI engine a homogeneous pre-mixed fuel was supplied. It was confirmed that appropriate results could be obtained with the 1-dimensional approach for the nucleation rate model.

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INTRODUCTION

One of the most urgent problems with tightening emission regulations for automobiles is reducing particulate matter (PM) from gasoline direct injection (DI) engines. Using particulate filters, such as those used in diesel engines, is unfavorable for gasoline DI engines from the viewpoint of cost.

Therefore, reducing PM by improving combustion has been explored by optimizing engine hardware specifications, such as fuel injectors, pistons, and gas-flow devices, and optimizing engine control parameters, such as injection timing, valve timing, and rail pressures.

Computational fluid dynamics (CFD) is one of the most useful tools to optimize such specifications and parameters. Some methods for solving the transportation equations of PM with combustion simulation in engine cylinders are well known as for estimating PM emitted from internal combustion engines [1], [2], [3], [4], [5]. The rate at which PM is generated and dispersed has been described using chemical reaction models that represent the nucleation and surface oxidation of PM particles with these methods. The two-equation model [1], [2] or the method of moments [3], [4], [5] is typical of these. However, as most methods are aimed for estimation in diesel combustion, their applicability to spark ignition (SI) engines is not well known. Generally, air-fuel mixture in SI engines is far homogeneous and PM density from SI combustion is quite small compared to diesel engines. Therefore, the PM estimation methods should be modified in accordance with combustion when they are applied to SI engines.

We propose a technique of estimating PM from SI engines to address the above issue, which computes the mass density and particle number density (PN) of PM by using the two-equation model. The nucleation rate, the most significant term for PM estimation, is derived by simulation of elemental reactions of gasoline surrogate fuel. Two approaches were used to estimate the nucleation rate. We describe our technique in detail and its verification results from comparing them with engine data.

ESTIMATION TECHNIQUE OF PM IN SPARK IGNITION ENGINES THROUGH NUMERICAL SIMULATIONS

Outline

Temporal and spatial distributions of soot particles were estimated by solving mass and number conservation equations for PM coupled with a 3D CFD.

We describe the details on our technique in the following sections.

CFD Modeling

An in-house CFD code we developed was used for the in-cylinder 3D simulation. Table 1 outlines this CFD code. The conservation equations of momentum, total energy, and mass for compressible fluid were discretized with the finite volume method (FVM). Ordinary differential equations obtained as a result of FVM were time-integrated with the flux limiter centered (FVM) method.

standard k-ε model was applied as a turbulence model. The discrete droplet method [7] was applied to simulate the movement and evaporation of fuel droplets.

Table 1. Methodology for 3D CFD analysis

Basic equations	Moments, energy and mass conservation for mixture Mass conservation for fuel vapor Mass conservation for burned gas State of gas for mixture
Numerical method for gas flow	Spatial : Finite volume method Temporal : FLIC method Scheme for convection terms : 2nd order total variation diminishing (TVD)
Numerical method for sprays	Discrete droplet method (DDM)
Turbulence model	Standard k-ε model
Grid system	Cartesian coordinates and voxel grid

The CFD code was verified with some experimental data such as those from spray visualization, fuel vapor distributions obtained with laser induced fluorescence (LIF), and gas velocity distribution measured with a laser Doppler velocimeter (LDV) [8] in an engine cylinder. Examples of these data are shown in Figures 1 and 2.

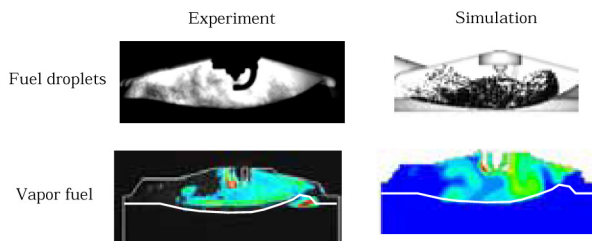


Figure 1. Comparison of experimental and simulation results (fuel droplets are in transmitted light image and vapor fuel is in LIF image in experiments).

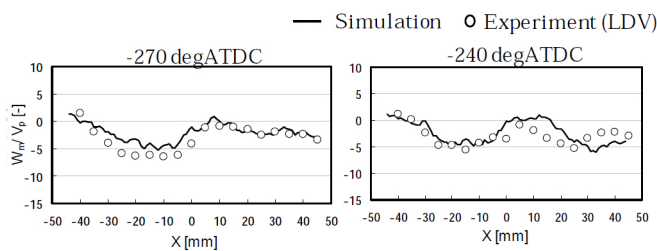


Figure 2. Comparison of in-cylinder gas velocities

Combustion Modeling

A mass conservation equation for burned gas (Equation (1)) was solved to handle a composition change following combustion.

$$\frac{\partial \rho \tilde{C}}{\partial t} + \frac{\partial u_j \rho \tilde{C}}{\partial x_j} = \frac{\partial}{\partial x_j} D_c \frac{d \tilde{C}}{d x_j} + \bar{\omega}_i, \quad (1)$$

Where C is the burning fraction, ρ is mixture density, D_c is eddy diffusivity, and ω_i is the burning rate.

It is well known that combustion can be categorized into two forms. One is premixed combustion; burning after the fuel and air are mixed. The other is diffusion combustion in which oxidant is provided into fuel by diffusion from outside the flame. There is a possibility that both forms of combustion occur in engines.

In this study, the gross burning rate was obtained from the sum of the as premixed burning rate ω_p and diffusion burning rate ω_d

$$\bar{\omega}_i = \theta \bar{\omega}_p + (1 - \theta) \bar{\omega}_d, \quad (2)$$

where θ is the flame form parameter. Premixed combustion and diffusion combustion can be combined seamlessly by introducing the parameter. The flame form parameter was obtained from Equation (3) proposed by Yunoki et al. [9]

$$\theta = \max \left(0, \min \left(1, \frac{1}{2} \frac{|\nabla \tilde{C}|}{|\nabla f| + \varepsilon} - 1 \right) \right), \quad (3)$$

where ε is a small value to prevent a zero divide, and f is the mixture fraction. If the gradient of mixture fraction is much larger than the gradient of burning fraction, the flame form parameter becomes unity, indicating premixed combustion. Otherwise if the gradient of mixture fraction is much smaller than the gradient of burning fraction, the flame form parameter becomes zero, indicating diffusion combustion.

The premixed burning rate ω_p was obtained using the hyperbolic tangent approximation (HTA) model proposed by Inage et al. [10]

$$\bar{\omega}_p = 8 \rho_u \left(\frac{S_L}{\delta} \right) \tilde{C}^2 (1 - \tilde{C}), \quad (4)$$

where δ is laminar flame thickness, S_L is laminar burning velocity, and ρ_u is unburned gas density.

Laminar flame thickness is expressed by Equation (5).

$$\delta = \frac{4 \lambda_m}{\rho_u C_{pm} S_L}, \quad (5)$$

where λ_m and C_{pm} are heat conductivity and specific heat, respectively, at mean temperature of unburned gas and burned gas.

Laminar burning velocity is expressed by Equation (6) [11].

$$\begin{aligned}
 S_L &= S_{L0} \left(\frac{T_u}{T_0} \right)^\gamma \left(\frac{P}{P_0} \right)^\beta (1 - 2.1\gamma) \text{ [m/s]} \\
 S_{L0} &= (B_M + B_2(\phi - \phi_M)^2) / 100 \text{ [m/s]} \\
 \gamma &= 2.18 - 0.8(\phi - 1) \\
 \beta &= -0.16 + 0.22(\phi - 1)
 \end{aligned}
 \quad (6)$$

where T_u is unburned gas temperature, T_0 is reference temperature (298 K), P_0 is reference pressure (101.3 kPa), γ is dilute gas fraction, and ϕ is equivalence ratio. Also, B_M , B_2 and ϕ_M are model constants that depend on the fuel.

The diffusion burning rate was obtained using the flamelet model. With this model, the flame is assumed to maintain a laminar flame structure in the turbulence flow field. The flamelet database was built by elemental reaction simulation to the counterflow of the diffusion flame. Gasoline surrogate fuel used in the simulation contained 90% iso-octane and 10% n-heptane. The elemental reaction equations, consisting of 188 species and 692 reactions, were solved using FlameMaster, a computer program for 1D laminar flame calculations [12].

PM Estimation Modeling

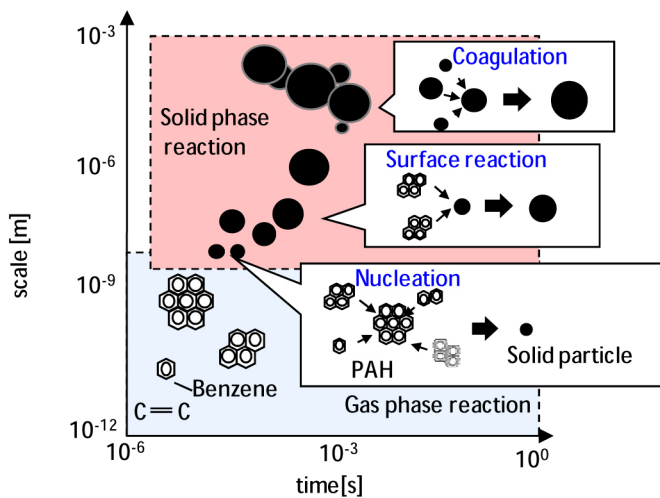


Figure 3. Creation and growth processes of PM

The creation and growth processes of PM-oriented hydrocarbon fuel combustion are shown in Figure 3. The processes are as follows.

The first process is gas-phase reaction. Polycyclic aromatic hydrocarbons (PAHs) are formed in the gas-phase reaction originating from acetylene generated by thermal decomposition of hydrocarbon fuel. The PAHs are the precursors of soot particles.

The second process is solid-phase reaction. The nuclei of PM are created by collision between the precursors (nucleation). Then the particles then grow due to the surface reaction and coagulation.

We applied the two-equation model [1][2] for the solid-phase modeling. The PM density distribution is estimated by solving the conservation equations for PM number and mass with this model. The conservation equations for number density and mass density of PM are expressed by Equations (7) and (8), respectively.

$$\frac{dN}{dt} + \frac{du_j N}{dx_j} = \frac{d}{dx_j} D_N \frac{dN}{dx_j} + R_N + G_N \quad (7)$$

$$\frac{dM}{dt} + \frac{du_j M}{dx_j} = \frac{d}{dx_j} D_M \frac{dM}{dx_j} + R_M + W_M, \quad (8)$$

where N [1/m³/s] is particle number density (PN), M [kg/m³/s] is particulate mass density (PM), R_N [1/m³/s] and R_M [kg/m³/s] are source terms of nucleation, G_N [1/m³/s] is a source term of coagulation, and W_M [kg/m³/s] is a source term of surface reaction. The following modeling was devised for nucleation source terms and surface reaction source term.

- A database of PN, particulate mass density, and nucleation rate built with detail reaction simulation was applied to calculate nucleation source terms in 3D simulation.
- The surface reaction source term was calculated from PM and density of acetylene, OH radical, and oxygen. Required species density was estimated with the flamelet model by using the species database.

The purpose of this modeling is to satisfy both high accuracy and low simulation load. Figure 4 shows the basic procedure of the PM simulation using the database. The nucleation rate R_c is calculated using 0-dimensional or 1-dimensional elementary reaction simulation and is stored to the database as a function of equivalence ratios, temperatures, pressures, and progress variables. In the 3D CFD, the R_c according to the physical values, such as equivalence ratio or temperature, of each simulation cell are read from the database.

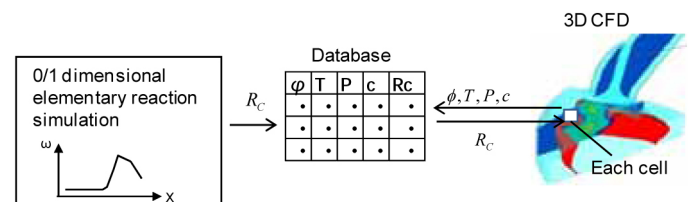


Figure 4. Basic procedure of PM simulation using database

Two methods of applying the database were devised for nucleation source term estimation. One method involves applying the database with the assumption that a simulation cell is filled with homogeneous gas (Model A). The other method involves applying the database with the assumption that a cell is divided into burned gas and unburned gas by the premixed flame (Model B).

Since PM generation is assumed to occur inside an entire cell under homogeneous reaction with Model A, it requires 0-dimensional elementary reaction simulation to build the database. This is a quite