

Detailed Diesel Combustion and Soot Formation Analysis with Improved Wall Model Using Large Eddy Simulation

Beini Zhou, Masahiro Horikoshi, Akira Kikusato, Jin Kusaka, and Yasuhiro Daisho
Waseda University

Kiyotaka Sato and Hidefumi Fujimoto
Mazda Motor Corporation

ABSTRACT

A mixed time-scale subgrid large eddy simulation was used to simulate mixture formation, combustion and soot formation under the influence of turbulence during diesel engine combustion. To account for the effects of engine wall heat transfer on combustion, the KIVA code's standard wall model was replaced to accommodate more realistic boundary conditions. This was carried out by implementing the non-isothermal wall model of Angelberger et al. with modifications and incorporating the log law from Pope's method to account for the wall surface roughness. Soot and NO_x emissions predicted with the new model are compared to experimental data acquired under various EGR conditions.

CITATION: Zhou, B., Horikoshi, M., Kikusato, A., Kusaka, J. et al., "Detailed Diesel Combustion and Soot Formation Analysis with Improved Wall Model Using Large Eddy Simulation," *SAE Int. J. Engines* 9(1):2016.

INTRODUCTION

The need to comply with increasingly stringent emissions regulations and fuel economy standards has created pressure to downsize and turbocharge existing diesel engines. Computational fluid dynamics (CFD) has emerged as a powerful tool for this purpose, enabling the development of diesel engines with higher efficiency and lower emissions. Direct numerical simulation (DNS) is one of the most accurate CFD methods. While DNS can describe organized vortex structures in turbulent flows, the computational time and cost of predicting diesel spray characteristics using this technique is excessive. Consequently, engine simulation must be used in conjunction with some alternative turbulence model in practical applications.

There are two established methods for turbulence modeling: (1) Reynolds Averaged Navier-Stokes (RANS), which is based on ensemble- and time-averaged governing equations; and (2) Large eddy simulations (LES). In RANS, the averaging used in RANS model means that detailed information on the instantaneous unsteady characteristics of the turbulent flow is lost. Therefore, RANS simulations are not proper method, especially for studying highly transient flows such as those in engine cylinders. Consequently, LES is becoming more popular as a practical alternative to DNS for the analysis of in-cylinder turbulent phenomena.

Multiple groups have recently reported studies on the numerical analysis of diesel engines using LES. Celic et al. [1] were among the first to apply LES techniques to engines; their group implemented a Smagorinsky-based turbulence model into the KIVA code [2] and

used it to model intake and compression flows. Their results showed that LES models can capture instantaneous large-scale flow structures and predict turbulence statistics more accurately than some alternative methods. Sone et al. [3] used LES to model the fuel-air mixing process in a direct injection spark ignition engine with wide cycle-to-cycle variations. Their results showed that the method can capture very unsteady, anisotropic fuel-air mixing processes as well as dynamically evolving fine-scale vortical and scalar structures. Rutland and his group [4, 5, 6, 7, 8, 9] have performed a great deal of research on the combustion modeling of internal combustion engines with the LES approach. Their dynamic structure model works very well in engine applications and provides reliable estimates of the subgrid turbulence kinetic energy (TKE), which can be used to support combustion, scalar mixing, and spray models.

Many soot models have been developed over the last few decades, from simplistic phenomenological models to complicated kinetic approaches. The two-stage empirical soot model of Hiroyasu [10] is widely used for its simplicity and convenience. In the Hiroyasu model, soot formation involves an initial formation step followed by an oxidation step. The mass rate of soot formation is assumed to be directly proportional to the amount of fuel vapor, and the Arrhenius constants for formation and oxidation are derived from experimental data. However, in reality soot formation is a very complex physical phenomenon that involves both gas phase chemical processes and physical processes such as particle dynamics. To capture this complexity, Fusco et al. [11] proposed an eight-stage phenomenological soot model for studying diesel combustion. This model is based on eight global reaction steps including particle

inception, particle coagulation, surface growth, and surface oxidation, as well as global reaction steps for intermediate species formation and oxidation. In addition, Tao et al. [12] coupled a phenomenological soot model with a detailed chemical kinetic mechanism incorporating Polycyclic Aromatic Hydrocarbon (PAH) chemistry for gas phase soot precursor formation and oxidation. This approach proved to have important advantages over alternative methods for predicting diesel flame structures while also providing information on useful variables such as the identity of the soot precursor species, the soot particle number density, and the soot particle size.

Engine wall heat transfer has important consequences for the performance of internal combustion engines. However, its analysis is very challenging because its effects depend on turbulent motion and the combustion process in the cylinder as well as the thermal boundary layer contacting the cylinder wall surface. During the engine's operating cycles, the unsteady and transient behavior of the turbulent motion in the cylinder creates variations in the heat fluxes between the fluid and walls. It is therefore important to accurately predict the heat transfer through the combustion chamber's walls. The standard KIVA wall model [2] is that of Launder and Spalding [13], which assumes an incompressible flow with a constant density and viscosity across the thermal boundary layer. Han et al. [14] subsequently proposed a model with a modified temperature wall function to describe compressible flows. Angelberger et al. then introduced a model that accounts for variations in the density and viscosity of the gas in the boundary layer [15]. Unfortunately, all of these models are RANS-based and may therefore be of limited utility in LES simulations.

This paper presents the results of LES simulations using three different wall models. All of the simulations were performed using a reduced chemical mechanism coupled to a phenomenological soot formation model dealing with complex chemistry for gas phase soot precursor formation and oxidation. The diesel fuel surrogate mechanism [16] developed at Chalmers University of Technology, comprising 74 species and 320 reactions, was used to simulate evaporative n-dodecane evaporative sprays and diesel fuel combustion. The phenomenological soot formation model was developed at Waseda University based on the model of Tao et al. [12]. The present model framework has four fundamental steps: particle inception via the five-membered ring PAH species acenaphthylene, surface growth via the addition of C_2H_2 , surface oxidation by the hydroxyl radical and O_2 attack, and particle coagulation, are used to predict the change of the soot mass and particle number density.

NUMERICAL APPROACH

The CFD methodology used in this study is based on the KIVA4 [17] code with improved subgrid turbulence, liquid spray, chemical combustion, wall function and soot models. This section briefly reviews the governing equations and modeling methods for LES simulations implemented in the KIVA4 code.

Large Eddy Simulation Equations

Applying the filtering operator to the conservation equations of species, momentum and energy equations, LES equations for two-phase flows in accordance with the KIVA4 formulation are as follows:

Continuity equation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = \bar{\dot{\rho}}^s \quad (1)$$

Momentum conservation equation:

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j - \bar{\tau}_{ij} - \tau_{ij}^{sgs}) = \bar{F}_i^s \quad (2)$$

Energy conservation equation:

$$\frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{e}}{\partial x_j} + \bar{p} \frac{\partial \tilde{u}_j}{\partial x_j} + \frac{\partial \bar{h}_j^{sgs}}{\partial x_j} + \frac{\partial \bar{q}_j}{\partial x_j} - \bar{\sigma}_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} - \theta^{sgs} = \bar{Q}^s \quad (3)$$

Species conservation equation:

$$\frac{\partial \bar{\rho} \tilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{Y}_m \tilde{u}_j - \bar{D}_m \frac{\partial \tilde{Y}_m}{\partial x_j} + \varphi_{j,m}^{sgs}) = \bar{\dot{\rho}}_m^s \quad (4)$$

The subgrid stress tensor is modeled using the resolved strain rate and a subgrid eddy viscosity. The Boussinesq eddy viscosity approximation is defined as:

$$\tau_{ij}^{sgs} = -2\nu_t \left(\tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} K^{sgs} \delta_{ij} \quad (5)$$

where the filtered rate of strain tensor is defined as:

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (6)$$

the subgrid eddy viscosity is calculated using a mixed-time scale model proposed by Inagaki et al. [18] and is expressed as:

$$\nu_t = C_m K^{sgs} T_s \quad (7)$$

$$T_s = \left(\frac{\Delta}{\sqrt{K^{sgs}}} \right)^{-1} + \left(\frac{C_t}{S} \right)^{-1} \quad (8)$$

where Δ is the LES spatial filter size based on the local grid size, and the coefficients C_m and C_t are set to 0.05 and 10 respectively according to Inagaki et al. [18]. The subgrid kinetic energy K^{sgs} is obtained by solving the equation proposed by Menon et al. [19]. The magnitude of the rate of strain tensor is defined as:

$$\tilde{S} = 2(\tilde{S}_{ij}\tilde{S}_{ij})^{1/2} \quad (9)$$

Phenomenological Soot Model

A phenomenological soot model [20, 21, 22, 23] is used to predict soot emissions in this work. The reaction scheme used in this model is specified in Table 1. The principle framework of the present soot model is based on the detailed approach of Tao et al. [12]. Four competing processes (soot inception, surface growth, surface oxidation and soot coagulation) are combined to determine the rate of change of the soot mass and particle number density. The model's key components are equations (1) and (2); it is described in more detail below.

$$\frac{d[C(s)]}{dt} = \omega_{nuc} + \omega_{sg} - \omega_{O_2} - \omega_{OH} \quad (10)$$

$$\frac{dN}{dt} = \frac{dN_{nuc}}{dt} + \frac{dN_{coag}}{dt} \quad (11)$$

If the soot mass concentration and the particle number density are known, the particle diameter is given by

$$d_p = \left(\frac{6}{\pi} \frac{C_s}{\rho_{soot} N} \right)^{1/3} \quad (12)$$

Table 1. Reaction mechanism in the soot model

Step	Reaction	$k = A T^b \exp(-E/RT)$		
		A	b	E
		cm/(mol s)		kcal/mol
Nuc	$A_2R_5 \Rightarrow 12 C(s) + 4 H$	2.15e+04		5.0
Sg	$C(s) + C_2H_2 \Rightarrow 3 C(s) + H_2$	3.00E+04	0.55	12.1
Sg	$C_{soot}H + O_2 \Rightarrow C_{soot-2}H + 2 CO$	Nagle & Strickland-Constable model		
Sg	$C_{soot}H + OH \Rightarrow C_{soot-1}H + CO + H$	Neoh et al. model, $\gamma = 0.13$		
Coag	$\kappa C_{soot} \Rightarrow C_{soot}$	Modified Smoluchowski equation		

Particle Inception/Nucleation

The first critical step in soot formation is soot particle inception or nucleation.

$$\frac{dN_{nuc}}{dt} = \omega_{nuc} \frac{dN_A}{C_{min}} \quad (13)$$

$$\omega_{nuc} = 12k_{nuc} [A_2R_5] \quad (14)$$

Soot particles are assumed to be dry, graphite-like particles containing only carbon atoms. Based on this assumption, the incipient soot particles are assumed to have a diameter of 12.5 nm, which corresponds to about 100 carbon atoms. [12]

Surface Growth

Soot particle surface growth is assumed to be C_2H_2 -assisted:

$$\omega_{sg} = 2k_{sg} P_{C_2H_2} \left(\alpha \frac{\chi}{N_A} A_s N \right) \quad (15)$$

In this equation, χ is the active site density defined by Surovikin's coefficient [24] while α is an inactivation factor representing the fraction of the surface area that is available for surface growth reactions. It is computed using the expression of Kazakov et al. [25]:

$$\alpha = \frac{1}{2} \left[\tanh \left(\frac{8186}{T} - 4.57 \right) + 1 \right] \quad (16)$$

Surface Oxidation

The concentrations and effects of two oxidants are considered in this work. Oxidation by O_2 attack is modeled using the Nagle-Strickland-Constable model [26], which assumes the existence of two reaction pathways involving different reactive sites that are associated with different rates of surface chemistry. Oxidation by OH radicals is described using the model of Neoh et al. [27]. A value of 0.13 is assumed for the collision efficiency of OH radicals with the soot surface.

Particle Coagulation

Soot particle coagulation is an important process that occurs before the exhaust stroke. In this work it is modeled using the modified Smoluchowski equation:

$$\frac{dN_{coag}}{dt} = \frac{6}{5} \kappa f_v^{1/6} N^{11/6} \quad (17)$$

The rate constant of coagulation is computed as

$$\kappa = \frac{5}{12} \left(\frac{3}{4\pi} \right)^{1/6} \left(\frac{6k_B T}{\rho_p} \right)^{1/2} G C_a \quad (18)$$

where f_v is the particle volume fraction, k_B is the Boltzmann constant, ρ_p is the particle density, G is the spherical particle factor, C_a is the self-preserving size distribution factor, and T is the ambient temperature.

Wall Functions

This section outlines the three wall function models used in this work. The first is the standard wall shear stress model included in the KIVA code, which is simulated with RANS-based techniques and the LES approach. The second is the non-isothermal wall model of Angelberger et al. [15], and the third is an improved two layer rough wall model for LES. Results obtained using all three models are compared.

The Standard KIVA Wall Model

This model uses RANS techniques to determine wall shear stresses and heat losses. Its law-of-the-wall velocity equations are summarized below.

$$F = \begin{cases} \frac{y^+ Pr_l / Pr_t}{\kappa \ln y^+ + B + 11.05(Pr_l / Pr_t - 1)} & (y^+ > 11.05) \\ 1.0 & (y^+ < 11.05) \end{cases} \quad (19)$$

Where Pr_l and Pr_t are the Prandtl numbers in the laminar and turbulent fluids, which are equal to 0.74 and 0.9, respectively. For smooth walls, the Karman constant κ and B are set to 0.4327 and 5.5, respectively. More detailed information on the model's derivation is presented reference [2]. The corresponding formulation of the wall heat flux is:

$$q_w = \frac{\rho C_p u_\tau F(T_g - T_w)}{Pr_l y} \quad (20)$$

where ρ is the gas density, T_g is the gas temperature, T_w is the wall temperature, and y is the distance from the wall. The friction velocity u_τ is calculated from the mean turbulent kinetic energy at a point in the logarithmic zone:

$$u_\tau = c_\mu^{1/4} K^{1/2} \quad (21)$$

where c_μ is a constant set to 0.09.

Since the turbulent kinetic energy is replaced by the subgrid-scale turbulent kinetic energy in LES models, [equation \(21\)](#) can be rewritten to obtain a formulation suitable for use in LES:

$$u_\tau = c_\mu^{1/4} K^{sgs^{1/2}} \quad (22)$$

The Non-Isothermal Wall Model

Angelberger et al. [15] proposed a non-dimensional wall distance η^+ , velocity ψ^+ and temperature θ^+ :

$$d\eta^+ = \frac{v_w}{v} y^+, d\psi^+ = \frac{\rho}{\rho_w} y^+, d\theta^+ = \frac{\rho}{\rho_w} T^+ \quad (23)$$

The corresponding velocity and temperature wall laws are:

$$\psi^+ = \begin{cases} \eta^+ & (\eta^+ \leq 10.8) \\ 2.44 \ln \eta^+ + 5.0 & (\eta^+ > 10.8) \end{cases} \quad (24)$$

$$\theta^+ = \begin{cases} Pr \eta^+ & (\eta^+ \leq 13.2) \\ 2.075 \ln \eta^+ + 3.9 & (\eta^+ > 13.2) \end{cases} \quad (25)$$

The wall heat flux is given by

$$q_w = \frac{\rho_w C_p u_\tau T_w \ln(T_g/T_w)}{\theta^+} \quad (26)$$

where ρ_w is the mean gas density in the near-wall first computing cell and the friction velocity u_τ is computed using [equation \(22\)](#).

The Two Layer Rough Wall Model

Pope's log law [28] is used to model rough wall surfaces. The non-dimensional stream-wise velocity u^+ is defined as follows:

$$u^+ = \frac{1}{\kappa} \ln\left(\frac{y}{s^+}\right) + \tilde{B}(s^+) \quad (27)$$

where s^+ is the roughness length in viscous units and s is the dimensional roughness. The parameter $\tilde{B}$ varies with s^+ but attains a constant value B_c equal to 8.5 in the fully rough limit. $\tilde{B}$ was defined as the following:

$$\tilde{B} = \begin{cases} B + \left(\frac{1}{\kappa}\right) \ln s^+ & (s^+ < 5.83) \\ \tilde{B}_{max} & (5.83 \leq s^+ < 30.0) \\ B_c & (s^+ \geq 30.0) \end{cases} \quad (28)$$

where $\tilde{B}_{max} = 9.5$. The roughness of the wall surface is set to 0.045 mm as commercial steel in this work.

The friction velocity u_τ is defined as

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad (29)$$

The strategy employed in this work is to first compute τ_w as if the flow is locally laminar and to then use the laminar value as an initial guess for the non-laminar value.

Other Numerical Models

KIVA4 uses the Lagrangian drop and Eulerian-fluid methods to describe two-phase flows. The KH-RT model [29] with velocity interpolation [30] is used to describe the fuel atomization process during spray modeling. The collision and coalescence model used in