

Evaluation of Spray/Wall Interaction Models under the Conditions Related to Diesel HCCI Engines

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ABSTRACT

Diesel homogeneous charge compression ignition (HCCI) engines with early injection can result in significant spray/wall impingement which seriously affects the fuel efficiency and emissions. In this paper, the spray/wall interaction models which are available in the literatures are reviewed, and the characteristics of modeling including spray impingement regime, splash threshold, mass fraction, size and velocity of the second droplets are summarized. Then three well developed spray/wall interaction models, O'Rourke and Amsden (OA) model, Bai and Gosman (BG) model and Han, Xu and Trigui (HXT) model, are implemented into KIVA-3V code, and validated by the experimental data from recent literatures under the conditions related to diesel HCCI engines. By comparing the spray pattern, droplet mass, size and velocity after the impingement, the thickness of the wall film and vapor distribution with the experimental data, the performance of these three models are evaluated. The results indicated that the predicted mean droplet diameters by HXT model are in better agreements with measurements due to the consideration of the gas density. However, the film thickness and fuel vapor distribution near the wall region are not significantly affected by the spray/wall interaction models, and all the models present inaccurate predictions relative to the experimental results.

INTRODUCTION

Because of low fuel consumption and good performance, diesel engine is very popular for the automotive applications in recent years. However, as the emission regulation becomes more and more stringent, diesel engine is required to drop the NO_x and particulate matter (PM) emissions significantly. As the promising technique

with the potential for significant reduction in NO_x and PM emissions while maintaining the high thermal efficiency, Homogeneous Charge Compression (HCCI) engine has achieved considerable attentions [1].

Unlike the conventional diesel combustion, the charge is well mixed and very lean in the diesel HCCI engine. In order to achieve the homogeneous fuel/air mixture in the combustion chamber, early injection is commonly applied to diesel HCCI engine [2-4]. However, the early injection is easy to produce spray impingement on the cylinder wall, which leads to power loss and high emissions [5]. It is revealed by Reveille et al. [6] that the wall impingement was unavoidable when the multiple injections with early injection timing was used. Siewert [7] experimentally observed that the liquid spray that misses the piston bowl was directly linked to the increases in HC, CO and smoke emissions and reduction in the thermal efficiency.

A large number of spray/wall interaction models have been developed in recent years. However, Kim et al. [8] indicated that none of these models were based on experiments conducted under high injection pressures with high ambient temperature and pressure conditions, and they compared the performance of Naber and Reitz [9] model and O'Rourke and Amsden model [10] under premixed compression ignition operating conditions. It was found that the spray/wall interaction model played a more important role as the injection timing was advanced, and O'Rourke and Amsden model [10] showed better agreement with the experimental data. Kong [11] reviewed the spray impingement criteria, and indicated that the improvements of the spray impingement model was required to accurately simulate modern diesel premixed charge compression ignition (PCCI) combustion with early injection times.

The aim of this paper focuses on the review of spray/wall interaction models and evaluation of their performance under the conditions related to diesel HCCI engines. The necessity of this study is believed to be following three reasons. Firstly, most of spray/wall interaction models are based on the experiments conducted by injecting a single water drop on a flat wall under the atmospheric environment, which is far from the operating conditions of diesel HCCI engines, so they should be validated before further application. Secondly, with the development of the test equipment, more experimental data is provided which could help to understand the process of impingement. Thirdly, the vapor distribution in the impingement process, which is important for the combustion of diesel HCCI engines, is seldom studied by previous studies.

In the following sections, the current spray/wall interaction models are reviewed firstly. The model formulations in three spray/wall interaction models which are compared in this study are then given. The comparisons between the experimental data and the predictions of these three models are presented next. Finally, the conclusions are drawn.

REVIEW OF CURRENT SPRAY/WALL INTERACTION MODELS

One of the first spray/wall interaction model was developed by Naber and Reitz [9]. Three regimes, i.e. stick, reflect and jet which assumes the droplets move tangentially along the surface like a jet are considered in their model. Several limitations exist in this model. The first one is that the splash regime which is important in affecting wall spray and vaporization is ignored. And the model doesn't account for the energy and momentum losses and the formation of a liquid film adhering to the wall. It was also found that the conditions for occurrence of each regime in the model of Naber and Reitz were not suitable for the conditions for engines [12]. This model was further improved by Gonzalez, Borman and Reitz [13], in which the normal droplet velocity in the reflection regime was computed by a correlation from the experiments.

Watkins and Wang [14] extended the model developed by Naber and Reitz [9] by considering the momentum and energy losses due to the droplet-wall interaction. Contrasting with the jet regime in Naber and Reitz model in which the tangential velocity after impact is equal to the approaching speed of the droplet and the drop size remains unchanged, it is improved that the tangential velocity is the same as that before impingement, the normal velocity is set to zero and the drop size is reduced by a factor of four in the new model. Watkins and Wang [14] also extended the collision model of O'Rourke and Bracco [15] in such a way that the droplets tend in a stochastic manner to move away from areas of high droplet concentrations. It should be noted the way of modifying the collision to satisfy the predictions of the impingement is some arbitrary, and Watkins and Wang [14] also showed that the new model

gave good predictions for the cases of normal spray impactions, but it was not so good for angled injection on relatively far walls. Park and Watkins [16] found that the collision model presented by Watkins and Wang [14] led the droplets to eject from the spray for free spray which is in contradiction to experimental data, and they implemented this collision model only in the near-wall region.

Mundo, Sommerfeld and Tropea [17, 18] derived a new spray/wall interaction model based on their experimental investigations with single drop impinging on dry surfaces [19] and slightly rough surfaces covered by a thin liquid film [17]. Two regimes of deposition and splash are distinguished in their model, and splash criteria is defined by a new critical threshold which incorporates both the kinematic impingement parameters and fluid properties of the impinging droplet. The diameter, velocity, and number of the secondary droplets are all dependent on the impingement parameters. They also compared the model of Naber and Reitz [9], the model of Wang and Watkins [14] and the new model, and found that the model that accounts for the splash regime and the individual kinetics of each impinging droplet fit the experiments better.

Senda et al. [20, 21] presented a spray/wall interaction model including the fuel film formation for applications to diesel and spark ignition (SI) engines. The deposition and the splash regimes are included in the new model. The corrections investigated by Mundo et al. [19] are used to describe size distribution and the splashing angle of the second droplet, and the velocity magnitude of the second droplet is assessed by the energy conservation relationship between incoming droplet on the wall and the splashed droplets away from the wall.

Bai and Gosman [22] presented a more detailed model with formulations to determine the impingement regimes and the regime transition criteria, and describe the post-impingement droplet characteristics. In the dry wall case, three regimes of stick, spread and splash are included, and the rebound, spread and splash are considered in the wetted wall case. The transition criterion between different regimes is the Weber number. The rebound velocity in the rebound regime, and the ratio of the splashed mass to incoming mass, the sizes, velocities and ejection angles of the second droplets in the splash regime are determined by the empirical relations which are consistent with the experimental data. The energy conservation is also satisfied in evaluation of the second velocity in the splash regime. This model is refined by Bai, Rusche and Gosman [23] in order to improve the accuracy of the predictions for gasoline spray impingement. The transition criterion is slightly adjusted to account for the interference effects of neighboring previously-impacting droplets in the new model. For the splash regime, the sizes of the secondary droplets are evaluated from a probability density function (PDF) instead of the uniform probability previously assumed, and a more realistic energy budget for splashing

droplets is made to ensure more accurate evaluation of the secondary droplet velocity magnitudes.

Following by Bai and Gosman [22], Stanton and Rutland [24] developed another spray/wall interaction model with consideration of four regimes including stick, rebound, spread and splash. The transition criteria are based on experimental results. In the rebound regime, the velocity of the rebounded droplet are the same as that of Bai and Gosman [22]. The quantities of the second droplets in the splash regime are based on the experimental work conducted by Yarin and Weiss [25] and Mundo et al. [19]. The energy balance is performed on the determination of the magnitude of the secondary velocity. A limitation of this model is that it is not defined for dry walls. Lindgren and Denbratt [26] indicated that the Weibull distribution equation which is used to determine the second droplet size distribution in the model of Stanton and Rutland [24] was not defined for negative coefficients, and it makes that there is an upper limit for the Weber number.

A new spray spray/wall interaction model was presented by Trujillo et al. [27] with the validations by the experiments of spraying fuel on a flat surface with different angles of incidence. The effect of surface roughness is incorporated into the model by affecting the splash threshold and the sizes of second droplets. The velocities and size distributions of secondary droplets in the splash regime are based on the experimental investigation of Mundo et al. [19]. The direction of the second droplet velocity in the wall plane is expressed by the angular distribution presented by Naber and Reitz [9].

O'Rourke and Amsden [10] realized a full spray/wall interaction model into the KIVA code. Only two regimes of stick and splash are included in this model. The splash criterion is obtained to accounts for the effect of film thickness. Similar to the model of Stanton and Rutland [24], the properties of the second droplet in the splash regime are chosen to conform to the experimental results of Yarin and Weiss [25] and Mundo et al. [19] and an energy consistency results. The direction of the tangential velocity of the second droplet is taken from the results of Naber and Reitz [9].

The model of O'Rourke and Amsden [10] was improved by Han et al. [28, 29]. Another two regimes of rebound and spread are added into the new model, and similar transition criteria used by Bai and Gosman [22] are employed. The splash threshold is updated to take account of the effects of surface roughness and the film. It was found that the O'Rourke and Amsden model [10] overestimated the effect of film thickness to the splash criterion, and the new proposed splash threshold agreed better with the experimental data. Because aerodynamic factors play an important role in the splash process, the ambient gas density is included to calculate the size of the second droplet. Compared to the O'Rourke and Amsden model [10], a simpler function is introduced to model the tangential velocity magnitude of the second droplet which agrees with the experimental results better,

and the normal velocity is also revised to account for the effect of the incident angle. Han et al. [28] indicated that a considerable underprediction of the second droplet size and mass deposition rate using the deviation based on a single drop impingement scenario directly. Therefore, an effective impingement hypothesis is proposed to account for the effect of multiple drop interactions by introducing the "impingement effectiveness factor". Then the factor is used to modify the secondary drop size and mass deposition.

Lee et al. [30, 31] presented a extended spray/wall interaction model, in which the regime transition criterion is the same as the model of O'Rourke and Amsden [10] from the experimental data of Mundo [19], the total splash mass is determined by the work of Bai and Gosman [22], the velocity magnitude of second droplets in the splash regime is deduced from the energy conservation law and the experimental results from Yarin and Weiss [25]. The results indicate that the splash mechanism is effectively described by the new model.

Grover and Assanis [32] implemented a new model into the KIVA-3V code, and the mass, tangential momentum and energy of an impinging droplet are conserved in the model. The splash criteria for dry or wet wall are taken from the related experimental results [19, 33]. The size of the second droplets are the same as that of Han et al. [28], and the in the case of splash, the tangential momentum of the impinging droplet is divided between the splashing parcels and the wall-film parcels according to the assumption of Bai and Gosman [22]. The new model incorporates a viscous dissipation model, and distinguishes between the energy lost to viscous dissipation and wall film formation. However, because the TAB breakup model [34] is used in the validation for the new spray/wall interaction model, the arrival time of the spray is slightly offset. The TAB breakup model significantly underpredicts the diameter of the droplet which further influences the interaction of the wall and the spray, so this model should be validated by more experimental data before being widely used.

The features of the spray/wall interaction models which are reviewed above are summarized in Table 1. It can be seen that the structure of various spray/wall interaction models are very similar although their details are different. In order to fully describe the process of wall/spray interaction, some basic issues are needed to be addressed in the model including the types of impingement regime, the transition criteria from one regime to another and the post-impingement characteristics.

In fact, the spray impingement is an extremely complicated process, in which the drop shows different characteristics depending on the velocity, size and temperature of the incident droplet; the viscosity and surface tension of the fluid; the temperature and roughness of the impinged wall as well as the wall film thickness and gas boundary conditions. Especially when

the surface temperature exceeds the Leidenfrost temperature at which the drop will rebound or slide along the wall without wetting the wall. However, it is found that the Leidenfrost temperature is significant higher than the combustion chamber surface temperature under the conditions of gasoline [28] and diesel [11] engines. Thus, only the treatment of a liquid film is included for all the spray/wall interaction models. In diesel engine conditions, Bai and Gosman [22] identify

four typical impingement regimes including stick, rebound, spread and splash, and this assumption is widely used among other models. It is assumed that the droplet adheres to the wall in the 'stick' regime when impact energy is very low for a wetted surface. For a droplet with higher energy, it will rebound off the surface. As the impact energy goes on increasing, the droplet spreads out to form a wall film. When the impact energy is high enough, the 'splash' will occur.

Table 1. Summary of features in different spray/wall interaction models

	(1) Naber and Reitz [9, 13]	(2) Watkins and Wang [14]	(3) Mundo et al. [17, 18]	(4) Senda et al. [20, 21]	(5) Bai and Gosman [22, 23]
Interaction Types	Stick Rebound Jet	Rebound Deposition	Deposition Splash	Deposition Splash	Stick Rebound Spread Splash
Regime Transition Criteria	Weber	Weber	$K=Oh \cdot Re^{1.25}$	Weber, Laplace	Weber Laplace
Considered Wall Conditions	-	-	-	Smooth and Rough	Dry and Wetted
Rebounding Droplet Velocities	No change on the magnitude	Empirical	-	-	Empirical
Splashing Droplet Mass	-	-	Empirical	Empirical	Empirical
Splashing Droplet Sizes	-	-	Empirical	Empirical	Empirical
Splashing Droplet Velocities	-	-	Empirical	Empirical Energy Constraints	Empirical Energy Constraints

Continue

	(6) Stanton and Rutland [24]	(7) Trujillo et al. [27]	(8) O'Rourke and Amsden [10]	(9) Han et al. [28, 29]	(10) Lee et al. [30, 31]
Interaction Types	Stick Rebound Spread Splash	Stick Splash	Deposition Splash	Stick Rebound Spread Splash	Deposition Splash
Regime Transition Criteria	Weber	$K=Oh^{-2/5}We$	Weber E, $K=Oh \cdot Re^{1.25}$	Weber,	$K=Oh \cdot Re^{1.25}$
Considered Wall Conditions	-	Dry and Wetted Roughness	Film Thickness	Film Thickness Roughness	-
Rebounding Droplet Velocities	Empirical Same as (5)	-	-	Empirical Same as (5)	Empirical
Splashing Droplet Mass	Empirical	Empirical	Empirical	Empirical	Empirical
Splashing Droplet Sizes	Empirical	Empirical	Empirical Energy Constraints	Empirical	Empirical
Splashing Droplet Velocities	Empirical Energy Constraints	Empirical Energy Constraints	Empirical Energy Constraints	Empirical	Empirical Energy Constraints

The regime transition criterion in the spray/wall interaction model is used to determine which regime will happen under a specified environment. However, the experimental results indicate that there is often no exact border

between two regimes, and two regimes always mix together [33]. Therefore, most of models use the empirically-derived relationship to describe the transition criterion. Watkins and Wang [35] suggested a very simple

way in which the Webber number is used as the transition criterion. Mundo et al. [17, 18] used the nondimensional impact parameters $K=Oh\cdot Re^{1.25}$ to determine whether splashing or deposition occurs. O'Rourke and Amsden [10] derived a splash criterion in which the effect of the film on the splash threshold is considered. Han et al. [28, 29] further improved this criterion of O'Rourke and Amsden [10] by according for both the influence of surface roughness and the film thickness, and indicated that the new correlation agreed well with experimental data.

The most complicated issue for the spray/wall interaction model is the post-impingement characteristics including mass fraction, size and velocity of the droplet after being rebounded or splashed. For the rebound regime, most of the models use the correlations proposed by Bai and Gosman [22] to determine the rebound velocity components. In the splash models, the size and the velocity of the second droplet are always based on directly curve-fitting impingement experimental data. In terms of second droplet size, Bai and Gosman [23] give it by a Chi-squared distribution and Stanton and Rutland [24] determine it by a Weibull distribution. O'Rourke and Amsden [10] use a Nukiyama-Tanasawa PDF function to describe the size distribution, and Han et al. [28, 29] further improved this distribution. The formulations for the second droplets in most of the models are fitted by the experimental results produced by Mundo et al. [19], Yarin and Weiss [25], as well as Cossali and Marengo [33], and then some additional mass, energy and momentum constraints are added to the corresponding models. However, it should be pointed out that some of these experiments are the studies for single-drop impingement, so Stanton and Rutland [24] add the splashing threshold with an additional term to account for the effect multi-drop impaction, and Han et al. [28, 29] uses 'impingement effectiveness factor' to modify the secondary drop size and mass deposition fraction.

Another issue must be addressed here is that the wall film dynamics model will also affect the predictions of spray/wall interaction model, because film shape and thickness play an important role in the transition criterion and the post-impingement characteristics, and it will be discussed later.

MODEL FORMULATION

CFD CODE

The computational fluid dynamics (CFD) code is KIVA-3V [36] in present study. Spray is represented by a particle method, several submodels are included in the code to account for spray atomization, breakup, collision, evaporation and spray/wall interaction [36]. The interaction of the spray and the gas flow is accounted for through coupling source terms in the governing equations. The fuel model is the Diesel fuel model DF2 ($C_{12}H_{26}$ Cummins model). The standard k- ϵ turbulence model was used in the simulations of this study.

The KH-RT (Kelvin-Helmholtz Rayleigh-Taylor) model which is based on a linear stability analysis of liquid jets [37, 38] was used to describe the breakup process of the spray, and our previous study indicated that all the Evaporation parameters including spray penetration, droplet diameter and velocity, and vapor distribution were well reproduced by the KH-RT model [39]. The collision model developed by Nordin [40] with the improvement of grid independence was integrated into the KIVA-3V code. Evaporation and drop drag force were simulated by the models provided by KIVA-3V. The cavitation and turbulence effect inside nozzle were not considered here, all the initial diameters are identical to the nozzle orifice diameter. The wall film model is based on the research of O'Rourke and Amsden [10, 41].

SPRAY/WALL INTERACTION MODEL

In this paper, the following spray/wall interaction models including the Bai and Gosman [22, 23] model, the O'Rourke and Amsden [10] model and the Han et al. [28, 29] model which have been widely used in the recent literatures were implemented in the KIVA code, and they are referred to subsequently as BG, OA and HXT model respectively in the following sections.

In order to explain the predictions of these three models in detail, the transition criterion, the ratio of the splashed mass to incident mass, the sizes, velocities and ejection angles of the second droplets are compared in Table 2, where D , M and w_0 are diameter, mass and velocity of the incident droplet; d , m , w are diameter, mass and velocity of the second droplet in the splash regime; α incident angle measured from the normal; Re_n , We_n and La are Reynolds, Weber and Laplace number of the incident droplet; ρ_l , μ and σ are density, dynamic viscosity and surface tension coefficient of the liquid.

RESULTS AND DISCUSSIONS

The performance of BG, OA and HXT models are evaluated in this section by comparing with the experimental data of spray wall impingement under the conditions related to diesel HCCI engines. The injection timing varies significantly in diesel HCCI engines with early injection, it may be from intake valve close (IVC) to the time near top dead center (TDC), so the experiments selected in this study include both the low and high ambient pressure and temperature conditions.

All the simulations were conducted in a cylindrical domain the grid size varying from 0.6 to 3 mm, and the nozzle center was located at axially at a point 1 mm above the edge center. The mesh refined near the point of injection, using a geometric distribution in both the radial and azimuthal direction. It was found that the spray penetration wasn't influenced by grid size significantly with further grid refinement. The largest time step of 1 μs was used in this study.