Hollow-Cone Spray Modeling for Outwardly-Opening Piezoelectric Injector

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Linear instability sheet atomization (LISA) breakup model has been widely used for modeling hollow-cone spray. However, the model was originally developed for inwardly-opening pressure-swirl injectors by assuming toroidal ligament breakups. Therefore, LISA model is not suitable for simulating outwardly opening injectors having string-like structures at wide spray angles. Furthermore, the varying area and shape of the annular nozzle exit makes the modeling difficult. In this study, a new spray modeling was proposed for outwardly opening hollow-cone injector. The injection velocities are computed from the given mass flow rate and injection pressure regardless of ambiguous nozzle exit geometries. The modified Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) breakup model is used with adjusted initial Sauter mean diameter (SMD) for modeling breakup of string-like liquid film spray. Liquid spray injection was modeled using Lagrangian discrete parcel method within the framework of commercial CFD software CONVERGE, and the detailed model was implemented by user defined functions. It was found that the new model predicted the liquid penetration length and local SMD accurately for various fuels and chamber conditions.

I. Introduction

SPRAY atomization of liquid fuels drew increased interest recently for the demand of high efficiency and low emission engines. Finely atomized spray has increased droplet surface area and enhances fuel evaporation and mixing.^{1,2} Furthermore, latest gasoline direct injection (GDI) and gasoline compression ignition (GCI) engines require precise control of fuel injection and atomization to manipulate equivalence ratio without throttle losses for diesel-like high thermodynamic efficiencies and reduced nitrogen oxides (NOx) and soot emissions.^{3,4}

Due to the demand of precise injection control, an outwardly-opening hollow-cone injector controlled by accurate piezoelectric actuator was developed for modern GDI engines although inwardly-opening pressure-swirl injectors have been widely used.⁵ However, understanding the detailed spray characteristics of this promising injector is still challenging and few modeling studies are available.

In the hollow-cone spray modeling under framework of Lagrangian discrete parcel method, the linear instability sheet atomization (LISA) model developed by Schmidt et al.⁶ is the only available model to represent the breakup of annular liquid films. The model has been widely used for hollow-cone spray modeling by combining Taylor analogy breakup (TAB) as a secondary breakup after primary LISA breakup. However, LISA model was originally developed for inwardly-opening pressure-swirl injectors and it assumes toroidal ligament breakups. This LISA-TAB model was further applied to the outwardly-opening injector by assuming slug flow,⁷ although the mechanism is different. Das⁸ simulated outwardly-opening hollow-cone spray using TAB model by specifying the gap height as the initial droplet size, but the liquid penetration measurement showed large deviations from experiment except initial period. Pischke et al.⁹ proposed a combined LISA-KH-TAB model by adding KH model as a secondary breakup for high Weber number conditions because TAB model produces unreasonably fine droplets at that condition.

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The LISA model has been the most common approach for simulating the liquid sheet breakup of hollow-cone spray, and shows good agreement on the traditional inwardly-opening pressure-swirl injector having toroidal ligaments by transverse swirling motions. However, recent experimental studies on the modern outwardly-opening piezoelectric injector reported hollow-cone spray with string-like structures instead of toroidal ligaments.¹⁰ The mechanism of these string-like structures has not yet been clearly understood, and no appropriate models has been proposed to predict such a string formation and accurate droplet sizes.

In this study, the outwardly-opening hollow-cone injector was modeled by CONVERGE¹¹, a commercial CFD software specified for simulating spray and engines, under the framework of Lagrangian discrete parcel method. A new spray injection model for the injector was proposed by implementing the modified KH-RT model with adjusted injection velocity and initial SMD calculation using user-defined function (UDF) features. The developed model is compared with the built-in LISA model and experimental study, and validated using two different fuels under various chamber conditions.

II. Numerical Method

A. Spray injection modeling

The numerical modeling of outwardly-opening hollow-cone spray in a constant volume chamber is conducted by CONVERGE¹¹ with the proposed new spray injection model using user-defined functions. In the present study, the Lagrangian discrete parcel method is used for spray modeling by introducing parcels (groups of droplets) of liquid into the gas phase because it is beyond the current computational scope to conduct complete direct numerical simulations of multi-phase interaction between gas and many small spray droplets. Figure 1 shows the difference between inwardly-opening and outwardly-opening hollow-cone injectors. Both of them produce annular liquid film. However, outwardly-opening injector produced string-like structures while inwardly-opening makes toroidal structure by transverse flow motions.

Figure 1. Schematic drawings of hollow-cone injectors and liquid film structures. (a) Inwardly-opening pressure-swirl injector with toroidal liquid film structure. (b) Outwardly-opening injector with string-like liquid film structure.

To model liquid fuel spray accurately, we need to know details of the nozzle flow including mass flow rate, velocity profiles in time and in space at nozzle exit, amount of cavitation, spray angle and thickness, nozzle exit area and shapes, and so on. However, there exist cycle-to-cycle variations, and the chamber condition has huge influence on the nozzle flow itself. It is difficult to measure the flow features in the engine operational condition. For practical modeling, many parameters of nozzle flow are assumed known or fixed, and the nozzle flow is estimated based on the reference case and a few key parameters.

Previous modelings on outwardly-opening hollow-cone injectors assumed slug flow at nozzle exit. Therefore, the nozzle exit area and the annular gap height are assumed known. However, small gap height and varying nozzle exit area and shape cannot guarantee slug flows at the nozzle exit. In most experimental studies, the mass flow rate and injection pressure are the only available information. The key feature of the present study is computing spray injection velocity and initial liquid film thickness using unsteady Bernoulli equation and mass conservation by assuming the temporary varying nozzle exit area and shape unknown. In addition, the string-like structures are modeled with modified KH-RT breakup model and adjusted SMD values by imagining attached many solid-cone-like spray.

The details of nozzle flow and the inside structure of the injector is mostly unknown. However, the injection velocity can be estimated by unsteady Bernoulli equation and nozzle's discharge coefficient (C_D). The injection velocity (V_{inj}) can be computed from the liquid density (ρ_l), streamline length (L_0), and pressure difference (Δp) between the injection (p_{inj}) and chamber pressure (p_c):

$$p_{inj} - p_c = \rho_l \frac{dV_{inj}}{dt} L_0 + \frac{\rho_l}{2} \left(\frac{V_{inj}}{C_D} \right)^2. \quad (1)$$

Where, the streamline length is assumed as 2 mm like typical injectors and the discharge coefficient (C_D) is estimated as 0.75 according to the experimental results.

When the mass flow rate ($\dot{m}$) is known, the initial sheet thickness of the liquid film (t_0) can be obtained from the injection velocity (V_{inj}) and nozzle diameter (d_n) according to mass conservation equation by:

$$\dot{m} = \pi \rho V_{inj} t_0 (d_n - t_0). \quad (2)$$

Previous approaches assume that the liquid film thickness is known, and then calculate the injection velocity from mass flow rate and liquid film thickness. In this study, however, the liquid film thickness is estimated at a little distance from the nozzle exit after the nozzle flow is fully developed, which is reasonable approach when the gap height is small. Typical gap height of outwardly-opening injectors is less than 30-40 μm , which is much smaller than nozzle diameter of solid-cone.

The calculated liquid sheet thickness is a starting point in our spray modeling regardless of breakup or collision models. To utilize the modified KH-RT breakup model, the initial SMD should be known. The initial liquid sheet thickness (t_0) of Eq. (2) can be considered as an initial SMD. However, it does not comply with the liquid jet stability analysis in the Kelvin-Helmholtz instability because the spray is a circular liquid film with the initial thickness of t_0 . In this model, the spray is considered many small solid-cone injections along a circular liquid sheet, and this favors the experimentally observed string-like structure of hollow-cone spray.

Assuming that the cylindrical liquid blobs are attached each other, the initial SMD (D_0) for the KH-RT breakup model is computed by

$$\frac{\pi}{4} [d_n^2 - (d_n - 2t_0)^2] = \frac{\pi}{4} D_0^2 \frac{\pi (d_n - t_0)}{D_0}. \quad (3)$$

By simplifying the equation, the initial SMD can be computed by

$$D_0 = \frac{4}{\pi} t_0. \quad (4)$$

For the liquid jet stability analysis to be valid, the cylindrical liquid blobs must be detached from each other, but Eq. (4) serves as a low limit of SMD for the implementation of non-LISA breakup models for a hollow-cone spray.

For turbulence modeling, the RANS-based renormalization group (RNG) k- ϵ model is utilized. As a breakup algorithm of liquid spray, the modified Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model is mainly used without an *ad hoc* breakup length¹², and compared with the built-in linear instability sheet atomization (LISA) breakup model¹¹. The dynamic drag model was implemented by determining the droplet drag coefficient dynamically, accounting for variations in the drop shape through a drop distortion parameter for accurate spray modeling. The effect of the turbulent flow on spray drops is modeled using O'Rourke's turbulent dispersion model by accounting a fluctuating velocities. For collision model, no-time-counter (NTC) method are utilized with extended Post and Abraham's inclusion of collision regimes. For spray evaporation, Frossling's evaporation model is implemented.

B. Problem description

The liquid spray is injected into the quiescent air in a cylindrical constant volume chamber with a diameter of 150 mm and height of 106.5 mm. The base mesh size is 4 mm, and the minimum cell size of 0.125 mm is obtained with 5 levels of adaptive mesh refinement based on the temperature and velocity gradients. In addition, 5 levels of fixed embedding are implemented around nozzle exit are for better accuracy. Figure 2 shows the computation domain with an example of adaptive meshes and injection mass profiles for different cases of Table 1.

Figure 2. The simulated domain and injection profiles. (a) Computational domain of a constant volume chamber. The mesh refinement for the spray region is also shown. (b) Injection duration and estimated mass flow rate profile.

The experimental data as well as the operating conditions can be found in ARAMCO's internal data and Pischke's study⁹. The BMW Siemens piezoelectric outwardly opening hollow-cone GDI injector was utilized in their spray characterization. The injection pressure (p_{inj}) is 100 bar, and the actuation duration is 0.30 ms. The actual injection duration is longer than actuation period, and opening and closing transient periods are estimated from experimental data. Two different liquid fuels are tested; PRF 95 mixture of 95%-vol iso-octane and 5%-vol n-heptane, and PRF 65 mixture of 65%-vol iso-octane and 5%-vol n-heptane. The closed chamber is filled with quiescent air. The injector diameter is 4 mm and the maximum needle lift is 0.035 mm. Three cases with different type of fuels and chamber conditions of Table 1 are simulated and compared with experiments.

Table 1. Modelled spray cases with two different fuels and various chamber conditions.

	liquid fuel	chamber pressure, p_c	chamber temperature, T_c	spray angles
case 1	PRF95	5 bar	300 K	95 ± 15 deg
case 3		10 bar	600 K	95 ± 15 deg
case 3	PRF65	1 bar	298 K	100 ± 15 deg

III. Results and Discussion

Before validating the present spray injection model for the outwardly-opening hollow-cone injector, the influence of injection distribution models were tested first and compared with each other to find an appropriate injection distribution model. It is known that Rosin-Rammler distribution produces narrower distribution than Chi-squared distribution, and represent experimental measurement better in solid-cone spray modeling. In the hollow-cone spray, however, the initial droplet size is less than 0.04 mm, which is much smaller than typical solid-cone spray having 0.2-0.3 mm of initial droplet diameters. In these smaller initial droplet sizes, the difference of injection distribution can be negligible. Figure 3 shows that the narrower distribution of Rosin-Rammler, wider distribution of Chi-squared, and no-distribution of constant droplet size model produce almost identical spray penetration length. In this study, the constant droplet size will be used because thin liquid film is injected from the same height of annular gap of nozzle exit.

Figure 3. Comparison of axial spray penetration length between different injection distribution models; no distribution, Chi-squared distribution, and Rosin-Rammler distribution.

With the chosen injection distribution model, the proposed spray injection model is simulated and compared with the built-in LISA model. Figure 4 shows the comparison of liquid penetration length between the modified KH-RT and the LISA breakup models. For the LISA breakup model, Taylor analogy breakup (TAB) is added as a secondary breakup model after the primary sheet breakup. In the beginning, both breakup models produce almost identical liquid penetration lengths, but the present modeling shows longer penetration length than built-in LISA. Both of them are in the range of experimental data. However, we measured 98% of liquid mass location along axial direction in the simulation, and it would be the high limit of spray penetration in the experiments. It can be concluded that the new model matches much better experimental data. The global SMD plot of Figure 4(b) shows bigger difference between models. Built-in LISA produces smaller droplets than the new model from the beginning, and TAB breakup model makes unreasonably small droplets less than 0.003 mm as known. These smaller droplets enhance evaporation and make shorter penetration length than experiment.

Figure 4. Comparison of axial spray penetration length between built-in LISA+TAB model and the present injection approach with a modified KH-RT model (a) Axial liquid spray penetration length and (b) Temporal evolution of global Sauter mean diameter.

For detailed comparison of spray features, the local SMD along radial direction are calculated and compared with experimental data at the distance of 10 mm from the nozzle exit. Most studies report only global SMD, and local SMD comparison is quite challenging because the modeling should simulate the details of spray structure accurately. Figure 5 shows the comparison with experimental measurement at radial direction of 10 mm and 20 mm. For more accurate comparison, droplets smaller than $1\text{ }\mu\text{m}$ were omitted when calculating SMD because the experimental equipment cannot capture them. The comparison shows the overall trends match well at different location in time. Small differences may be from the breakup modeling and primarily from the variation of spray angle in the experiment. Another reason is that the experimental study measured at a point for the given radial location while simulation calculated average value at the same radial location. Even with these differences, the comparison indicates that the present approach is able to model the spray structure of the outwardly opening hollow-cone injector with details.

Figure 5. Comparison of local Sauter mean diater (SMD) along radial direction at the distance of 10 mm from the nozzle exit. Experimental data are measured at one point for the given radial location and numerical modeling data are averaged at the given radial location.

As a further validation of the new spray models, two more cases in Table 1 are simulated and compared with experiments, as presented in Figure 6. Cases of various fuels and chamber conditions show good agreements with experiments. For case 3 of PRF65, the experiment measured the penetration by 0.5 ms, and match well simulations. In case 2 (10 bar and 600 K), the increased evaporation due to higher pressure and temperature causes shorter spray penetration length. The increased evaporation can be proved in Figure 6(b), where case 2 shows much smaller liquid mass due to evaporation. In the beginning, the liquid mass is similar because droplets are large. As times goes, however, droplets become smaller by breakup process, and then evaporates. This liquid mass plot supports faster evaporation and shorter penetration length of case 2 in Figure 6(a). In addition, the lower injection velocity by smaller pressure difference contributes shorter penetration length. One of the noticeable feature is that case 3 (PRF65, 1 bar, 298K) shows small liquid spray tip fluctuations represented by error bar in the Figure 6(a). Smaller air density reduces breakup effect and drag, and it results in longer penetration with less spray tip fluctuation. Even for the case 3, the new model match well by the end of measurement. The results validate the present model successfully for various fuels and chamber conditions. Figure 7 shows 3-D spray structure of the outwardly opening hollow-cone injector for case 1. One of the noticeable features is a counter-rotating vortex ring-like structure by the injection of the thin liquid sheet. This vortex is clearly observed in Figure 8, and it makes a big donut-like torus.

Figure 6. Validation of the present spray modeling for three different cases; case 1 (PRF95, 5 bar, 300 K), case 2 (PRF95, 10 bar, 600 K), and case 3 (PRF65, 1 bar, 298 K) (a) Comparison of axial liquid spray penetration length with experimental data (b) Comparison of liquid mass of PRF95 for different chamber conditions.

Figure 7. Temporal evolution of 3-D spray structures with vortices.

Figure 8. Velocity vector plot at $t = 0.4$ ms in case 1 (PRF95, 5 bar, 300 K). The injection of thin liquid sheet develops counter-rotating vortices.

IV. Conclusions

The new spray injection model was proposed for modern outwardly-opening piezoelectric hollow-cone injector. The numerical simulation was conducted by CONVERGE, a commercial CFD software specified for spray and engine simulations, and the new model was implemented using UDF functions. In an outwardly opening hollow-cone spray, the difference of injection distribution model can be negligible due to smaller initial droplets sizes. The new model was validated successfully by comparing spray penetration length and detailed spray features of local SMD distribution using two different fuels under various chamber conditions. It was found that the new approach models the string-like liquid film structure of the injector successfully, and shows better agreement with experiments than built-in LISA-TAB model having toroidal ligament breakups.

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