Modeling Low-Pressure Injections in Diesel HCCI Engines

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Abstract
Homogeneous Charge Compression Ignition (HCCI) combustion is being considered as an alternative to conventional engine combustion systems due to its high efficiency and low engine-out emissions. To prepare a homogeneous mixture for diesel HCCI combustion, two types of low pressure (5MPa–20MPa) injectors were considered: a swirl injector and a multi-hole injector. A modified version of the KIVA-3V R2 code, was used to simulate the two types of injections. The Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) hybrid breakup model, which is often used to simulate droplet breakup processes of high-pressure (50MPa–300MPa) diesel injections, was recalibrated and extended for low-pressure, multi-hole injection applications. Two techniques were used to improve the prediction of spray behavior: use of an independent collision mesh with random rotation, and coupling the gas and liquid phases using polar interpolation. The numerical models were validated by comparing simulation results with experiments under different conditions. The simulation results show that the spray structure of the swirl nozzle injection is sensitive to the intake flow field and in-cylinder gas density, while the spray structure of a multi-hole nozzle injection is less influenced by the in-cylinder flow and gas density. The simulation results also show that swirl injectors are more suitable for low ambient pressure (<0.3MPa) conditions because at high pressures (>0.3MPa), the hollow-cone spray collapses into a solid-cone spray. Multi-hole injectors are more suitable for high ambient pressure conditions because at low pressures, the spray penetration is too long, which can cause spray-wall impingement.

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**Introduction**

Future diesel engine technologies will need to incorporate advanced combustion strategies for achieving low emissions while maintaining good fuel economy and power density. It will be necessary to operate seamlessly over broad load and speed ranges when conditions change between different combustion regimes.

HCCI combustion is being considered as an alternative to conventional engine combustion systems. It has the potential to eliminate noxious engine-out emissions while producing higher engine efficiencies.

To prepare a homogeneous mixture, fuel should be injected early into the cylinder to allow enough time for fuel/air mixing. However, when direct injection of fuel into the cylinder during the intake or early compression stroke is used for mixture preparation, the use of conventional high pressure common-rail injection systems is limited by the relatively low in-cylinder gas density due to spray impingement on the cylinder walls [1]. Too much wall impingement can not only deteriorate the quality of the charge mixture, increase fuel consumption and unburned hydrocarbon emissions, but also lead to lubrication oil contamination. Therefore, it is of interest to consider low-pressure injection systems as an alternative.

In this study, the KIVA-3V Release2 code [2] with improved numerical models was used to explore the charge preparation in a diesel HCCI engine using two types of low-pressure injectors: a swirl injector and a multi-hole injector. Several numerical models in KIVA were updated and the improved models were validated by comparing simulation results to experiments. An inhomogeneity concept is also proposed to evaluate the effects of injector type and SOI timing on diesel HCCI charge preparation.

**Numerical Approach**

The CFD code used in the simulations was a version of the KIVA-3V Release2 code with improvements in various physical and chemistry models developed at the Engine Research Center, University of Wisconsin-Madison.

The RNG k-ε model [3] was used for the in-cylinder turbulence simulation. For hollow-cone sprays from swirl injectors, the Linearized Instability Sheet Atomization (LISA) breakup model [4] was used to calculate the primary breakup process of the fuel droplets, and the Taylor Analogy Breakup (TAB) model [5] was used for the secondary breakup calculation. For low-pressure multi-hole sprays, the KH-RT hybrid breakup model, which is used to simulate the droplet breakup process of high-pressure diesel injections, was recalibrated and extended for low-pressure injection applications.

An advanced unsteady vaporization model [6] was applied to predict the droplet evaporation process. A droplet collision model based on the stochastic particle method [7] was used to calculate the droplet collision and coalescence. The effects associated with spray/wall interactions including droplet splash, film spreading due to impingement forces and motion due to film inertia were considered in the wall-film model [8].

**Engine Specifications and Operation Conditions**

The engine considered was a Caterpillar 3401E single cylinder oil test engine (SCOTE). The specifications of the engine are listed in Table 1.

<table>
<thead>
<tr>
<th>Engine type</th>
<th>Caterpillar 3401E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore× Stroke (mm)</td>
<td>137.2 × 165.1</td>
</tr>
<tr>
<td>Engine valve timing (°CA)*</td>
<td>EVC=-355, IVC=-143, EVO= 130, IVO= 335</td>
</tr>
<tr>
<td>Swirl Ratio</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 1. Engine specifications  * In this paper, °CA means °CA ATDC

Six engine modes have been proposed to simulate the Federal Test Protocol (FTP) cycle [9]. Mode 2 (25% load, 821rev/min, naturally aspirated) and Mode 5 (57% load, 1737rev/min, boosted) were selected for the study.

Two types of injectors were considered in this study. The swirl injector was a Siemens hollow-cone spray injector with 90° spray cone angle and 250 micron nozzle diameter. The multi-hole injector was a Bosch 6-hole solid-cone spray injector with 90° included angle and 170 micron nozzle diameter. 10MPa injection pressure was used for both injectors.

**Hollow-Cone Spray at High Ambient Pressure**

One way to prepare a homogeneous mixture is to inject the fuel early into the cylinder using a low-pressure hollow-cone spray injector. However, it was found that an unrealistic spray structure was predicted using KIVA at high ambient pressure (0.3MPa) using a Cartesian mesh, as shown in Figure 1(a). To understand the reasons, for simplicity, a hollow-cone injection into a quiescent high-pressure atmosphere was tested using a regular Cartesian mesh. In this case, a “four-leaf clover” spray was predicted as shown in Figure 1(b). However, this problem does not appear in a cylindrical mesh or with injections at atmospheric pressure. This is due to the grid dependency of the O’Rourke collision model, and also due to the gas and liquid phase coupling method used in KIVA, according to Nordin, Schmidt and other researchers [10, 11]. This problem was solved using a combination of techniques also proposed by these researchers: use of a cylindrical collision mesh and by coupling the gas and liquid phases using polar interpolation. These techniques were adopted in this study and the details are described as follows.
Figure 1. Unrealistic structures of hollow-cone sprays at high ambient pressure (0.3MPa) in Cartesian mesh computations using KIVA

Cylindrical collision mesh with random rotation

The “four-leaf clover” spray structure shown in Figure 1(b) was found to be mainly due to the mesh dependency of the O’Rourke collision model [7] used in KIVA. O’Rourke assumes that the probability of a droplet, $i$, colliding with any other droplet, $j$, is given by:

$$ p_{i,j} = \frac{\sigma_{i,j} v_{i,j} \Delta t}{V} $$  \hspace{1cm} (1) 

Only droplet parcels located in the same computational cell are allowed to collide, and the incidence of collision is proportional to the relative velocity $v_{i,j}$ between the pair parcels, as shown in Eq. (1). Those parcels which have velocities perpendicular to each other have the highest probability to collide if the nozzle location coincides with a cell node. This is illustrated in Figure 2, where parcel ‘d’ is not in the same computational cell as parcel ‘a’ and ‘b’, so it is not allowed to collide with them. Parcels ‘a’ and ‘b’ are in the same cell and their velocities are perpendicular, so they have the highest probability to collide and if coalescence occurs, the resulting parcel ‘c’ moves in the direction shown in the figure, according momentum conservation. This explains why the ‘four-leaf clover’ structure is observed.

At low ambient pressure, such as atmospheric pressure, the problem still exists. However, it is not so noticeable. This is probably because at low pressure, the spray is not as dense as it is at high pressure, so droplet collision doesn’t occur as frequently as at high pressure.

In a cylindrical mesh, the problem should also exist and an ‘n-leaf clover’ structure is predicted. However, when there is enough resolution in the azimuthal direction (i.e., $n$ is big enough), the problem also becomes unnoticeable even at high ambient pressure. Therefore, a ‘pseudo’ cylindrical collision mesh, which is coaxial with the spray and independent of the KIVA mesh, was used. An example of the collision mesh is shown in Figure 3 [11]. The cylindrical collision mesh is based on a cylindrical coordinate system that is coaxial with the spray. It is called a ‘pseudo’ mesh because the mesh is not actually generated in the code. The mesh is established only hypothetically, and each cell can be identified by an identification array (i, j, k), where i, j, and k are integers that correspond to the three cylindrical coordinates. Using the ‘pseudo’ mesh concept, not only is computer memory saved, but also the programming effort and computational time is reduced. Another merit of using this concept is that the mesh has no boundary and it is not needed to calculate the extent that the spray reaches every time step.

To further reduce non-axisymmetry of the predicted spray structure, the collision mesh was rotated at a random angle around the spray axis every time step. Similar to the standard O’Rourke collision model, only parcels in the same collision cell, instead of a KIVA cell, are allowed to collide.

Use of a randomly rotated cylindrical collision mesh significantly improves the spatial resolution of the spray and reduces grid dependency. However, since the method is based on the assumption that there is only one spray, it must be refined for multiple sprays. Indeed, for multiple sprays the method has been found to work better than computations performed without an independent collision mesh.

Figure 2. Parcels which have velocities perpendicular to each other in the same injection cell have the highest probability to collide if the nozzle is located on a cell node

Figure 3. A cylindrical collision mesh is used that is independent of the Cartesian gas phase mesh [11]
Gas and liquid phase coupling—polar interpolation

After introducing the randomly rotated cylindrical collision mesh, the results were found to be greatly improved. However, there was still some non-axisymmetry predicted in the spray structure. The remaining grid dependency was found to be mainly due to numerical errors associated with the gas and liquid phase coupling method used in KIVA [10, 11]. Therefore, an interpolation method was introduced to improve the accuracy of the calculation. The goal of the interpolation is to calculate the momentum transfer between the gas and liquid phases more accurately by providing more accurate gas phase velocities at the point where the parcel is located.

In KIVA, the gas phase velocity of the cell node nearest to a parcel is simply taken as the gas phase velocity at the point where the parcel is located, and it is used to calculate the relative velocity between the gas and liquid phases. This is a simple but potentially inaccurate method. A better approach is to take a weighted average (interpolation) of the gas phase velocities from all eight nodes of the gas phase cell in which the droplet resides, as shown in Eq. (2) [10, 11]. The velocities are weighted by the inverse of the distance from the nodes to the drop location raised to the power n, where n was selected to be 3 (mass weighting):

\[
\bar{V} = \frac{\sum_{j=1}^{8} \bar{V}_{j} r_{j}^{-n}}{\sum_{j=1}^{8} r_{j}^{-n}} \tag{2}
\]

This velocity is used to calculate the momentum transfer from the gas phase to the liquid phase. The same weightings are used to distribute the momentum transfer from the liquid phase to the gas phase (source terms).

This interpolation can be done in a Cartesian coordinate system, i.e., the weighted averages of the Cartesian components of the velocities are calculated. However, since the spray is polar in nature, it is better to use polar interpolation [11] instead of Cartesian interpolation. In the polar interpolation method, a cylindrical coordinate system coaxial with the spray is established first. Cartesian components of the velocities of the eight nodes are transformed to the corresponding polar components. Then the weighted averages of the eight nodes’ polar velocities are calculated. Finally, the averaged polar velocities are transformed back to Cartesian velocities, which are the Cartesian components of the gas phase velocity at the droplet location.

The advantage of using polar interpolation over Cartesian interpolation can be illustrated using Figure 4. For simplicity, a 2-D mesh is depicted. The left bottom spot represents the spray axis of symmetry and the upper spot represents a droplet parcel. Considering a spray injected into a quiescent atmosphere, since the spray is axisymmetric, the gas phase entrained velocity at any location should point at the spray axis, as shown in Figure 4. Using Cartesian interpolation, the resulting velocity may not point at the axis, as the arrow ‘b’ shows. However, using polar interpolation, all the interpolated velocities have no tangential component, which guarantees that the resulting velocity also has no tangential component, i.e., the resulting velocity also points at the axis, as the arrow ‘a’ shows. Since polar interpolation represents the nature of the spray better than Cartesian interpolation, it is suggested and used in this study.

**Figure 4.** Advantage of using polar interpolation over Cartesian interpolation (a: polar interpolation result. b: Cartesian interpolation result)

**Improved results**

Simulation results using the combination of the above two techniques: collision mesh and polar interpolation, are shown in Figure 5. Compared to the results in Figure 1, significant improvements were achieved using these techniques, and the results are seen to be approximately axisymmetric and physically reasonable.

**Figure 5.** Structures of hollow-cone sprays at high ambient pressure (0.3MPa) in Cartesian meshes using KIVA with collision mesh and polar interpolation.
Low-Pressure Multi-Hole Injection

Low-pressure multi-hole injectors have been mainly developed for use on Gasoline Direct Injection (GDI) engines to replace swirl injectors as spray-guided GDI combustion systems are receiving more attention than wall-guided GDI combustion systems. One major advantage of the multi-hole injector over a swirl injector is that the spray does not collapse at high ambient pressure conditions, as does the swirl spray.

Model Description

Low-pressure multi-hole injection has a similar spray pattern as compared to conventional high-pressure diesel injection sprays. The main difference is the fuel injection pressure, which is relatively low (5~20MPa) compared to conventional diesel common-rail injections (50~300MPa). Therefore, the atomization processes are different for these two types of injections and different droplet breakup models must be potentially applied. In conventional diesel injection, the high injection pressure leads to high droplet velocities and therefore inclusion of RT accelerative instabilities is necessary. In high-pressure injection, most of the droplet breakup occurs in the catastrophic breakup regime (We>1000) and breakup models based on a competition between KH and RT instabilities should be considered. While for low-pressure injection, RT instability is not as important because of the low injection velocities and accelerations. Most breakup occurs in the stripping regime (100<We<1000) where KH instability plays the major role in droplet breakup [12].

Accordingly, the KH-RT hybrid breakup model, which has been used for high speed jets, was recalibrated to extend its application to low speed jets in the present study. Though RT instability is still included in the model, it was observed that it rarely occurs in low speed injections, which is consistent with the argument above. Therefore, only the KH breakup model constants were recalibrated to extend the application of the KH model from high speed jets to low speed jets, and to match Nauwerck and Mitroglou’s experimental data [13, 14]. The wave length constant of the KH model was recalibrated to be 0.2 (vs. 0.6 for high speed jets), and the breakup time constant was recalibrated to be 15 (vs. 40 for high speed jets).

The polar interpolation technique was also found to be important for low-pressure multi-hole injection simulations. Figure 6 shows improvements of the prediction of the spray structure of low-pressure multi-hole injections after using the polar interpolation technique. Unrealistic spray structures (shown circled in Figure 6(a)) are eliminated by using polar interpolation, as shown in Figure 6(b).

At high ambient pressures, a solid-cone spray is much denser and collision occurs more frequently than at low ambient pressures. In a cylindrical collision mesh, the collision mesh size around the spray axis can be too small, which prevents collisions from occurring and this causes an under-prediction of SMD. A Radius of Influence (ROI) method [15] was used to prevent this problem. The radius of influence for the collision calculation was chosen to be 2mm. In the ROI method, one parcel is allowed to collide with another only if this parcel resides within the radius of influence of the other one. This ensures that the effective collision mesh size remains adequate.

Model validation

Since several models were updated, the new code was validated using the experimental data of Sun [16] and Mitroglou [13] and Nauwerck [14].

Model validation for swirl injection

Simulation results of hollow-cone sprays at different times after the Start-of-Injection (SOI) (1, 2, 3, 4, and 5 ms), under different ambient pressures (0.1, 0.3, 0.9 and 1.1 MPa) and using different injection pressures (4.3, 5.3 and 7.7 MPa) are compared with the experiments in Figure 7. It can be seen that both the spray structures and the spray tip penetrations predicted by the simulations match the experiments very well at the different ambient and injection pressures. Both experiment and simulation shows that, as the ambient pressure increases, the spray collapses, and the spray angle and the spray penetration decrease. As the injection pressure increases, the spray becomes denser, the spray angle decreases and the spray penetration increases. With this validation by the experiments, it was determined that the code can be used in swirl injection simulations with more confidence.
(a) $P_{\text{amb}}=0.1\,\text{MPa}, P_{\text{inj}}=5.3\,\text{MPa}$

(b) $P_{\text{amb}}=0.3\,\text{MPa}, P_{\text{inj}}=5.3\,\text{MPa}$

(c) $P_{\text{amb}}=0.9\,\text{MPa}, P_{\text{inj}}=5.3\,\text{MPa}$

(d) $P_{\text{amb}}=1.1\,\text{MPa}, P_{\text{inj}}=5.3\,\text{MPa}$
Model validation for multi-hole injection

Figures 8 to 10 show the corresponding validation results of the low-pressure multi-hole spray model. Figure 8 shows a comparison of SMD between experiments [14] and simulations at different injection pressures. It can be seen that both experiments and simulations show decreased drop size with increased injection pressure. The predicted SMD matches the experiments very well at the different injection pressures. Figure 9 shows a comparison of the liquid spray tip penetration length between the experiments [13] and simulations at different injection and ambient pressures. Figure 10 compares the spray structures of the cases shown in Figure 9. The results show that not only are the spray structures well predicted under the different conditions, but the simulated spray penetration also matches the experiments very well. It can be seen that as the injection pressure increases, the spray penetration also increases due to the increased spray momentum. Unlike swirl injection sprays, which collapse at high ambient pressures, the spray structure of a multi-hole nozzle injection almost does not change and only the spray penetration is reduced significantly with increased ambient pressure. This is a favorable feature for diesel HCCI operation, because spray-wall impingement might be reduced or avoided by operating the engine under boosted conditions, or by injecting the fuel during the compression stroke.

From the results shown in Figures 8 to 10, it can be concluded that the recalibrated KH model predicts the behavior of low-pressure multi-hole nozzle injections very well under a wide range of operating conditions.

Figure 8. Comparison of SMD between experiments and simulations at different injection pressures
Inhomogeneity

An inhomogeneity concept was proposed to evaluate the quality of fuel/air mixtures in the engine simulations. In this case, the fuel chemistry is deactivated, i.e., only fuel spray evaporation and mixing is considered. The calculation ends at -10°CA, which is close to when ignition normally occurs in HCCI engine combustion. At -10°CA, the equivalence ratio in each computational cell is calculated using the concentration of C, H and O atoms; as

\[
\Phi = \frac{2[C] + 0.5[H]}{[O]}
\]  

Then the statistical mean equivalence ratio in the whole computational domain is calculated using the gas phase mass in each cell as a weighting factor

\[
\bar{\Phi} = \frac{\sum_{i} \Phi_i \delta m_i}{\sum_{i} \delta m_i}
\]

The standard deviation of the equivalence ratio in the computational domain is defined as

\[
SD = \sqrt{\frac{\sum_{i} \delta \Phi_i^2 \delta m_i}{\sum_{i} \delta m_i}}
\]
Finally, the normalized standard deviation of the equivalence ratio, which is called inhomogeneity, is calculated by

\[ \text{NSD} = \frac{\text{SD}}{\Phi} \]  

(6)

The inhomogeneity value (NSD) is thus an indicator of the mixture quality: the higher the inhomogeneity, the less homogeneous the mixture. Since fuel chemistry is not considered, computer time is greatly reduced and the approach can be used for mixture preparation optimization, especially for HCCI combustion, since, to achieve HCCI combustion, charge inhomogeneities should be minimized. According to the authors’ previous experience of using the inhomogeneity definition, when its value reaches below about 0.25, an adequately homogeneous mixture is achieved in the cylinder and HCCI combustion is optimized.

**SOI Sweep Study Results and Discussion**

The performance of both the swirl injector and the multi-hole injector was evaluated at the Mode 5 and Mode 2 operating conditions through several SOI timing sweep studies. Only single injections were considered in this study.

**SOI sweep at Mode 5**

Mode 5 is a boosted, high-speed and medium-load engine operating mode. The in-cylinder pressure at the SOI and the EOI for both injectors is plotted in Figure 11 as a function of the SOI timing.

![Figure 11](image)

**Figure 11.** In-cylinder pressure at the SOI and the EOI at Mode 5

1. **SOI sweep of swirl injection**

The effects of SOI timing on diesel HCCI charge preparation were investigated at Mode 5 using the swirl injector. The SOI timing was varied from -330°CA to -120°CA.

![Figure 12](image)

**Figure 12.** Wall-film fuel amount and inhomogeneity as a function of SOI timing using the swirl injector at Mode 5

Figure 12 shows the wall-film fuel fraction and inhomogeneity as a function of SOI timing. The wall-film fuel fraction was defined as drops liquid that have impinged on wall surfaces and are located in wall cells, divided by the total amount of fuel injected. Both wall-film fuel fraction and inhomogeneity were calculated at -10°CA.

From Figure 12, both variables are seen to decrease as the SOI timing is retarded from intake TDC, to reach a minimum value at SOI timings around BDC, and to increase again with further delay of the SOI timing. There is thus an optimum SOI timing around BDC for the minimization of spray-wall wetting and charge inhomogeneity.

When the fuel is injected during the early intake stroke, as shown in Figure 13(a), the intake flow is very strong and the spray is blown off course, and hits the cylinder liner. As the SOI timing is delayed to around BDC, as shown in Figure 13(b), the intake flow is not so strong because the valves are about to close and the piston velocity is close to zero. The spray is less deflected by the intake flow. The minimum inhomogeneity is achieved and there is relatively little wall-film fuel (3.3%). However, the inhomogeneity (0.81) is still well above the desired value (0.25) for HCCI combustion. When the fuel is injected during the compression stroke, as shown in Figure 13(c), though the intake flow effects are minimal, the spray collapses due to the higher gas density caused by the piston compression and finally the spray hits the piston. The collapsing spray also confines the fuel droplets in a small spatial range in the cylinder, which deteriorates the fuel/air mixing. From Figures 11 to 13, it can be seen that when the ambient pressure is higher than about 0.3MPa, apparent collapse of a swirl nozzle spray can be observed, which leads to spray-wall impingement and deterioration of fuel/air mixing. Therefore, swirl injectors are
only suitable for low ambient pressure conditions (<0.3MPa).

Figure 13. Spray structures of swirl injections at Mode 5

2. SOI sweep of multi-hole injection

A similar SOI timing sweep study was conducted using the multi-hole injector at Mode 5 and the results are shown in Figures 14 and 15.

From Figure 14, when the SOI timing is before BDC, the wall-film fuel amount does not change much. As the SOI timing is delayed in the compression stroke, the wall-film fuel amount decreases very quickly and the inhomogeneity first decreases and then increases again. The optimum SOI timing is between -120ºCA and -140ºCA with the mixture inhomogeneity close to the suggested value (0.25).

Figure 15 shows the structure of the sprays with the different SOI timings. Unlike for swirl injection, multi-hole injection does not have a deflected spray when the SOI occurs in the intake stroke (Figure 15(a)) and the spray does not collapse when the SOI occurs in the compression stroke (Figure 15(c)). The spray structure is almost preserved at the different SOI timings, though the spray penetration of the different spray plumes is not the same due to the influence of the intake flow, as depicted in Figure 15(a). Due to the tumble motion which is formed during the intake stroke, the spray plume on the left of the image has a longer tip penetration than the one on the right. However, the tumble gradually disappears during the compression stroke. Therefore, the effect becomes less obvious for fuel injection during the compression stroke (Figure 15(c)).

During the intake stroke, both the in-cylinder pressure and the spray structure does not vary much, and therefore the wall-film fuel amount does not change much. During the compression stroke, as the SOI timing is retarded, the in-cylinder pressure increases very quickly (Figure 11), and the spray penetration is reduced, so the wall-film fuel amount decreases very quickly. When the SOI timing is later than -120 ºCA, the in-cylinder pressure is higher than 0.3MPa during the entire injection process and the wall-film fuel amount becomes negligible. From the above discussion, multi-hole injectors are suitable for injections under high ambient pressure (>0.3MPa) conditions.

Comparing Figure 12 and Figure 14, it can also be seen that, although the wall-fuel amount is comparable for the two injectors, the inhomogeneities of the mixture generated by the multi-hole injector is significantly lower than that generated by the swirl injector due to the avoidance of a collapsing spray.

Figure 14. Wall-film fuel amount and inhomogeneity as a function of SOI timing using the multi-hole injector at Mode 5
SOI sweep at Mode 2

Mode 2 is a naturally aspirated, low-speed and low-load engine operating mode. The in-cylinder pressures at the SOI and the EOI for both injectors are plotted in Figure 16 as a function of SOI timing. Similar SOI sweep studies were conducted using both injectors at Mode 2 as at Mode 5. However, only SOI timings after the stock engine IVC were considered at Mode 2 because the duration-of-injection (DOI) at Mode 2 is significantly lower than that at Mode 5 (in crank angle).

1. SOI sweep of swirl injection

A 2-D mesh was used to save computer time since the influence of the flow field has been found to be small at these conditions. The SOI sweep results are shown in Figure 17 and 18. As expected, when the SOI is later than -110 °CA and the in-cylinder pressure reaches above 0.3MPa before the EOI (see Figure 16), the spray collapses, as shown in Figure 18(b), and the spray-wall impingement amount and inhomogeneity increases very quickly. An SOI around -120 °CA seems to be the optimum with almost no wall-film fuel and with an inhomogeneity only about 0.3. From Figure 18(a), it can be seen that the air entrainment effect associated with vertex at the spray tip helps the swirl injection to reduce the spray penetration. These results further prove the conclusion that swirl injectors are suitable only for low ambient pressure conditions (<0.3MPa).
2. SOI sweep of multi-hole injection

A 60° sector mesh was used in this study considering the fact that the nozzle had six holes. Figures 19 and 20 show the predicted SOI timing sweep results using the multi-hole injector at Mode 2. As can be seen, an optimum injection timing was found to be around -80°CA, where both the wall-film fuel amount and inhomogeneity was relatively low. However, from Figure 19, it can be seen that even the lowest wall-film fuel amount is above 30%.

With relatively early injection, the spray hits the cylinder liner (Figure 20(a)) due to the low gas density. As the SOI timing is delayed, the spray penetration is reduced due to the increased in-cylinder pressure. As the SOI timing is later than -80°CA, the in-cylinder pressure during injection becomes higher than 0.3MPa. However, with the delayed SOI, the maximum allowed spray penetration without wall-wetting is also decreased because the spray starts hitting the piston surface (Figure 20(b) and 20(c)). That is why the wall-film fuel amount does not change much with SOI timings later than -100°CA, while it might be expected to decrease monotonically.

At mode 2, all the cases simulated had significant amounts of spray-wall impingement. This supports the conclusion that multi-hole injectors are suitable for injections under high ambient pressure (>0.3MPa) conditions. However, the spray-wall impingement amount could be reduced at Mode 2 by optimizing the injection or engine operating parameters, such as using lower injection pressure and/or higher boost pressure, as shown in Figure 21. Figure 21 shows that using a reduced injection pressure (5MPa) and a higher boost pressure (0.15MPa), spray-wall impingement could be avoided at an optimum SOI timing around -100°CA with a relatively low inhomogeneity (0.4).
Conclusions

In this study, numerical simulations of two types of low-pressure sprays, swirl and multi-hole nozzle sprays, were conducted using the KIVA-3V Release2 code with improved numerical models. An inhomogeneity concept is introduced to evaluate the effects of injector type and SOI timing on charge preparation in a diesel HCCI engine.

The following conclusions can be drawn from the simulation results:

1. To improve the numerical accuracy of spray predictions, spray models must be improved to remove mesh dependencies. In the present study, the models were also validated using experimental data.

2. The spray structure of swirl nozzle injections is sensitive to the intake flow details and the in-cylinder gas density, while the spray structure of a multi-hole nozzle injection is less influenced by the in-cylinder flow and gas density.

3. Swirl injectors are suitable for low ambient pressure (<0.3MPa) conditions because at high pressures (>0.3MPa), the spray collapses. Multi-hole injectors are suitable for high ambient pressure conditions because at low pressures, the spray penetration is too long, which causes spray-wall impingement.

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Nomenclature

- $p$: probability of collision between two parcels
- $\sigma$: collision cross-section between two parcels
- $v$: relative velocity between two parcels
- $\Delta t$: time step
- $V$: volume
- $\vec{V}$: velocity vector
- $r$: distance between a droplet and a cell node
- $\Phi$: equivalence ratio
- $\bar{\Phi}$: average equivalence ratio
- $\delta m$: gas phase mass in a computational cell
- $SD$: standard deviation of equivalence ratio
- $NSD$: normalized SD of equivalence ratio

Subscripts

- $i,j$: parcel or cell index

References