Large-eddy spray simulation under direct-injection spark-ignition engine-like conditions with an integrated atomization/breakup model

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Abstract
In this work, a hybrid breakup model tailored for direct-injection spark-ignition engine sprays is developed and implemented in the OpenFOAM CFD code. The model uses the Lagrangian–Eulerian approach whereby parcels of liquid fuel are injected into the computational domain. Atomization and breakup of the liquid parcels are described by two sub-models based on the breakup mechanisms reported in the literature. Evaluation of the model has been carried out by comparing large-eddy simulation results with experimental measurements under multiple direct-injection spark-ignition engine-like conditions. Spray characteristics including liquid and vapor penetration curves, droplet velocities, and Sauter mean diameter distributions are examined in detail. The model has been found to perform well for the spray conditions considered in this work. Results also show that after the end of injection, most of the residual droplets that are still in the breakup process are driven by the bag and bag–stamen breakup mechanisms. Finally, an effort to unify the breakup length parameter is made, and the given value is tested under various ambient density and temperature conditions. The predicted trends follow the measured data closely for the penetration rates, even though the model is not specifically tuned for individual cases.

Keywords
Large-eddy simulation, fuel sprays, atomization, breakup, spray modeling, direct-injection spark-ignition, gasoline engines

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Introduction
Performance and operation of direct-injection spark-ignition (DISI) engines rely heavily on the fuel injection and subsequent fuel–air mixing quality, especially for the spray-guided DISI combustion systems.\textsuperscript{1} The fuel injector is the most critical part of DISI fuel systems, and its design needs to meet more stringent requirements than that of the port-fuel injector. Modern DISI injectors have a multi-hole design similar to that used in diesel engines. Unlike the hollow-cone swirl-type injectors, the spray characteristics of this configuration have been proven to have less dependence on ambient conditions. It also has the flexibility to direct spray plumes at desired locations to help meet the combustion system requirements.\textsuperscript{2}

Atomization, or primary breakup, refers to the disintegration of liquid jet or liquid core into ligaments and droplets at the nozzle exit. Atomization provides initial conditions for droplet breakup and the subsequent fuel–air mixing process. In general, higher injection pressure results in faster atomization. However, it has been found that higher injection pressure does not necessarily lead to smaller droplet sizes in diesel sprays.\textsuperscript{3} This suggests that droplet breakup and collision are more important determining factors of the mixing process. A recent study by Baumgarten\textsuperscript{4} found that the disintegration of high-pressure diesel sprays begins inside the nozzle-hole, hence the liquid core does not exist. For modern DISI injectors, the relatively small length-
to-diameter (L/D) ratios and volatile fuel components promote complex turbulent flows and phase-change phenomena such as cavitation and flash boiling, which suppress the formation of the liquid core. Therefore, liquid fuel near the injector exit may contain only droplets and ligaments. The highly turbulent two-phase internal flows also make the modeling of atomization a particularly difficult challenge.

One way to overcome the challenge of atomization modeling is to perform direct numerical simulations (DNS) to resolve the atomization completely. These can be achieved by Eulerian representation of the turbulent two-phase flow with an interface tracking approach such as the volume of fluid (VOF) or level set (LS) methods. However, the computational requirements for DNS are extremely challenging so that its practical applications are still under development. Therefore, phenomenological approaches using Lagrangian representations of liquid fuel still remain the most popular methods for atomization modeling in engine applications. A reasonable approximation is to inject fuel parcels with a characteristic size equal to the nozzle orifice diameter (i.e. the blob method). Other reported work also utilizes a prescribed probability density function (PDF) for the initial parcel size distribution to mimic the atomization process. In this approach, however, the PDF must be guessed and tuned to match spray characteristics further downstream of the injector exit. Modeling efforts focused on the atomization induced by internal turbulence and cavitation were also reported and encouraging results were obtained. One issue of these methods is that one-dimensional (1D) modeling of the internal flow is usually needed, which requires detailed information about the nozzle geometry. Moreover, only one atomization mode (e.g. cavitation, turbulence, or flash boiling) is normally considered.

Compared to the diesel counterpart, DISI injectors operate at much lower system pressure, resulting in several times lower liquid velocity at the nozzle exit. Gasoline fuel also has a lower density and viscosity than diesel fuel. As a result, the governing nondimensional numbers in droplet breakup, such as the Weber number and the Ohnesorge number, are generally smaller in gasoline sprays. The Weber number and Ohnesorge number are defined as $We = \frac{\rho L U d_d^2}{\sigma}$ and $Oh = \frac{\mu_d}{\sqrt{\rho_d d_d \sigma}}$, where $\rho$, $\mu$, and $\sigma$ are the gas-phase density, droplet diameter, liquid-phase viscosity, and surface tension, respectively. This difference is demonstrated in Figure 1, where a map of droplet breakup regimes as functions of $We$ and $Oh$ is plotted. In the map, the $We$-$Oh$ diagrams of typical gasoline and diesel sprays are enclosed with dashed and dotted lines, respectively. As Figure 1 shows, there is only a small overlap between diesel and gasoline sprays, implying that the governing breakup mechanisms are vastly different. Most diesel droplets break owing to either catastrophic or sheet-thinning mechanisms. However, gasoline sprays shift to the lower left region in the map and a unique breakup mechanism, namely, the bag breakup, becomes more pronounced.

The droplet breakup regimes depicted in Figure 1 have been extensively studied by various researchers. Selected references on this topic are those of Pilch and Erdman, Krzeczkowski, Faeth et al., Liu and Reitz, Reitz and Lee, Opfer et al., Theoanous et al., Gelfand, Jain et al., and Girin. Detailed descriptions of each breakup regime can be found in the above references or a recent review by Guildenbecher et al. It has been generally accepted that the transitions among different breakup regimes are continuous functions of $We$ and $Oh$. Some experimental studies also show that the transitions are nearly independent of $Oh$ for $Oh$ less than 0.1. In Table 1, the droplet breakup regimes identified in various studies are reported along with the transition $We$. Note that the inconsistencies in reported $We$ values among listed studies are primarily due to the experimental uncertainties (non-sphericity of droplets and uncertainties associated with velocity measurements) and the fact that the transitions are continuous processes.

Most of the earlier research on large-eddy simulation (LES) of DISI sprays was conducted by combining spray models with a LES turbulence closure. Some of these studies have utilized the Taylor analogy breakup (TAB) models. While this approach can give satisfactory results under certain DISI operating conditions, it has a few shortcomings such as the somewhat arbitrary breakup criteria and the assumption of instantaneous breakup. Recently, Van Dam and Rutland explored the possibility of applying a diesel-type breakup model to DISI gasoline sprays. The Kelvin–Helmholtz/Rayleigh–Taylor (KH-RT) breakup model was validated against DISI spray experiments in a constant volume chamber over a wide range of ambient conditions. A functional relationship between the
KH-RT model parameters and the liquid-gas density ratio was found after carefully calibrating the KH-RT model. Although this functional relationship was found to give good vapor contours compared to Schlieren images, discrepancies were noted for both liquid and vapor penetration rates. The addressing of bag breakup in DISI engines is even more scarce in the literature, even though various numerical models have been reported. Chryssakis and Assanis proposed a unified approach for both diesel and gasoline engine applications. In their model, the droplet breakup has been divided into four regimes, namely, the bag, multi-mode, shear, and catastrophic regimes. Sub-models or correlations have been proposed in this unified approach to describe each breakup regime. The model has been found to perform well under both diesel and gasoline engine conditions. However, the validation was carried out at non-evaporating conditions. The application of this model under high-temperature high-pressure engine-like conditions has yet to be demonstrated.

This work is aimed to develop a physically representative breakup model for DISI gasoline sprays. The model, termed as the “integrated atomization/breakup (IAB) model,” builds on previous modeling efforts by incorporating a bag breakup model developed by the authors and addressing the breakup issues of droplets at relatively low We conditions. The model does not treat atomization and droplet breakup as separate processes. Instead, liquid ligaments and droplets are assumed to form immediately at the nozzle exit, and two sub-models are employed to describe the subsequent atomization/breakup processes. A revised breakup length concept is also employed to account for different penetration rates near and far from the nozzle. However, this concept should not be confused with the liquid core length, which normally implies that liquid jet or ligaments within this length experience atomization only. This conceptual difference was also noted by Beale and Reitz. In their work, certain parcels within the breakup length are also assumed to experience droplet breakup. The IAB model has been incorporated into the LES framework developed at the Engine Research Center, University of Wisconsin–Madison, and implemented in the three-dimensional (3D) CFD code OpenFOAM-2.3.x. Validation of the model has been performed by comparing LES predictions with experimental data. In the remaining of this article, detailed discussions of the model and results will be provided as follows. Section “IAB model” presents the formulations of the IAB model. Sections “Spray experiments for comparison” and “Simulation setup” discuss the spray experiments for validations and the numerical setup. In section “Results and discussion,” we discuss both the numerical and experimental results. Finally, concluding remarks and future directions are made in section “Summary and conclusion.”

IAB model

The IAB model relies on the well-known KH-RT hybrid model to describe the atomization of liquid fuel and breakup process of liquid ligaments and droplets in the plume-sheet thinning, sheet-thinning, and catastrophic breakup regimes depicted in Figure 1. Note that even though this model was developed based on linear stability theories (hence not physically suitable for the multi-mode breakup), it has been found to perform reasonably well for diesel sprays, which also experience multi-mode breakup. Besides, multi-mode breakup resembles a combination of bag and sheet-thinning breakup and hence constructing a numerical model for this specific regime is still impractical. Therefore, the multi-mode breakup regime is not treated separately in the IAB model. The IAB model also utilizes a phenomenological bag-breakup model to describe the breakup process in the bag and bag-stamen regimes. The KH-RT sub-model will be briefly reviewed first, followed by the descriptions of the bag sub-model and the IAB model implementation.
The KH-RT sub-model

In the catastrophic breakup regime, the dynamic pressure on the droplet surface becomes very large, causing unstable waves to grow on the droplet leading surface. Liu et al.\textsuperscript{42} suggested that those unstable waves may be described by either Rayleigh–Taylor (RT) or Kelvin–Helmholtz (KH) instabilities. RT unstable waves form when a density discontinuity is accelerated toward the lighter end, which eventually penetrates the denser droplet and create several small droplets. KH instabilities occur at the droplet periphery where the relative velocity is the largest. Wavelengths of KH instabilities are much shorter compared to those of RT, leading to micro-size droplets being continuously stripped from KH waves.

The KH-RT hybrid model refers to the one developed by Su et al.\textsuperscript{43} based on the work of Reitz and Diwakar\textsuperscript{44} and Reitz.\textsuperscript{45} The model was later improved by Ricart et al.\textsuperscript{40} by introducing the RT breakup length to account for different penetration rates within and beyond a certain distance from the nozzle exit. The model was divided into two sub-models, namely, the KH breakup model and the RT breakup model. The former was derived based on a linear stability analysis of a cylindrical liquid surface subjecting to an infinitesimal perturbation.\textsuperscript{35} The dispersion relation between the growth rate of this perturbation and its wavenumber was determined. Curve-fits of the numerical solutions were further generated for the maximum wave growth rate of this perturbation and its wavenumber.

The KH-RT hybrid model builds on the idea that only the KH breakup is activated if the distance between liquid parcels and the nozzle exit is within a pre-calculated breakup length, $L_B$. Beyond that length, both KH and RT unstable waves compete to break the droplet. In the revised model by Ricart et al.\textsuperscript{40} and Tsang,\textsuperscript{46} the breakup length is computed as

$$L_B = 9.12C_d d_{noc} \sqrt{\frac{\rho_i}{\rho_g}}$$

where $d_{noc}$ is the nozzle diameter and $C_d$ is a model parameter. Although the breakup length is conceptually considered as a global parameter, its value may be different among fuel parcels depending on the local fuel–air density ratios. In this study, the breakup length is calculated according to the following formula

$$L_B = 9.12 \sqrt{\frac{C_d d_{noc}}{\sin(\theta)}} \sqrt{\frac{\rho_i}{\rho_g}}$$

Figure 2. Schematic of the bag breakup process\textsuperscript{23} (a) bag growth, (b) bag rupture, and (c) torus breakup. A bi-modal droplet size distribution may be observed after the bag rupture and torus breakup.
where \( C_a \) is the area contraction coefficient, \( \alpha \) is a model parameter, and \( \theta \) is the plume direction (i.e. the spray axis angle). Note that there is no typical range for \( \alpha \), as setting it to a large positive number will effectively disable \( L_B \), leading to faster breakup and lower penetration. Contrarily, RT breakup will be disabled if \( \alpha \) is zero. In our experience, equation (4) works well for \( \theta \) in the range between 25° and 55°. Although it has not been tested for \( \theta \) beyond this range as there are limited experimental data for validation, it is expected to work reasonably well. Equation (4) is proposed based on the mixing-limited vaporization model of Siebers,\(^{47} \) where \( L_B \) projected to the injector centerline is proportional to the characteristic liquid length defined in Siebers.\(^{47} \) Although the model was developed for diesel sprays, it can be applied to multi-plume DISI sprays with some success.\(^{48} \) In equation (4), the product of the square root of the area contraction coefficient and the nozzle diameter equals the effective nozzle diameter. The impact of plume interactions is considered by taking the sine of the plume direction.

**The bag sub-model**

The physical mechanisms involved in bag breakup are very complicated. Experimental studies can hardly measure the local droplet and gas flow fields that lead to the formation and disintegration of the bag structure. However, it is generally observed that a thin hollow membrane-like bag forms at the front stagnation point of the deformed droplet and continues to be blown downstream. The bag bursts first, leaving a few small fragments and a liquid torus ring. The latter will eventually break into a few child droplets.\(^{19} \) A phenomenological model for the bag and bag–stamen breakup is developed based on the experimental observations of Chou and Faeth.\(^{19} \) In this model, the breakup process is divided into three stages as illustrated in Figure 2: (a) deformation and bag growth stage, during which the droplet deforms from its initial spherical shape into a liquid disk and forms a continuously growing thick membrane-like bag; (b) bag rupture stage, where the bag bursts into a liquid torus ring and many micro-size droplets; and finally, (c) torus breakup stage, where the torus ring breaks into a few child droplets. Two characteristic sizes are expected, one corresponding to the bag rupture and the other to the torus breakup. As a consequence, a bi-modal droplet size distribution may be observed.\(^{28,36} \)

During the first stage of the breakup process, the rate of droplet deformation or bag growth can be quantified by the ratio of the cross-stream diameter \( d_b \) to the initial droplet diameter \( d_d \). A semi-theoretical model has been developed by the authors to describe the deformation and bag growth process.\(^{41} \) Droplet dynamics were analyzed by subjecting a liquid droplet to an inviscid, incompressible ambient flow. The solution of the resulting equations gives the following expression to describe the droplet deformation and bag growing process, which relates the diameter ratio with a non-dimensional time \( t' \) and the initial droplet Weber number, \( W_{e_0} \)

\[
\frac{d_{b}}{d_{d}} = f(t', W_{e_0})
\]

\[
= \exp \left[ C_{bag,g} t^2 \sqrt{\left( 1 - \frac{6}{W_{e_0}} \right)} \right], \quad 0 < t' < \tau_{bag}
\]  

(5)

where \( t' \) is the ratio of elapsed time \( t \) to a non-dimensional characteristic time proposed by Nicholls and Ranger,\(^{49} \) \( T^* = \frac{d_d (\rho_l / \rho_g)^{0.5}}{U_{ref}} \). Equation (5) is valid only when the non-dimensional time is smaller than \( \tau_{bag} \), which is defined as the non-dimensional time when the bag ruptures. A model parameter \( C_{bag,g} \) is also introduced in equation (5), whose value is determined by curve fitting of the experimental data from Kulkarni.\(^{26} \)

\[
C_{bag,g} = \left[ 0.2983 - \frac{0.2691}{1 + \left( \frac{W_{e_0}}{14.013} \right)^{13.629}} \right]
\]

(6)

Chou and Faeth\(^{19} \) observed that the bag rupture starts at approximately \( t' = 3 \), while Opfer et al.\(^{23} \) identified the rupture to happen at about \( t' = 2 \). In this study, the onset time of bag rupture \( \tau_{bag} \) is determined using a correlation based on the experimental data from Opfer et al.\(^{23} \)

\[
\tau_{bag} = \frac{C_{bag,r}}{1 + \frac{0.018}{W_{e_0}^{0.5}}}
\]

(7)

where \( C_{bag,r} \) is a model parameter with a nominal value of 0.8. The coefficient of determination (i.e. \( R^2 \)) of this correlation is 0.999, and the corresponding root mean square error (RMSE) is 0.037. Predicted onset times using equation (7) are plotted in Figure 3 as a function of \( W_e \), for \( Oh \) less than 0.1. The plotted results also include experimental data from Opfer et al.,\(^{23} \) Krzeczkowski,\(^{14} \) Dai and Faeth,\(^{20} \) and VOI predictions from Jian et al.,\(^{26} \) Liang et al.,\(^{50} \) and Khosla et al.\(^{51} \) The \( W_e \) range spans from the bag to sheet-thinning breakup regimes. As Figure 3 shows, the qualitative trend of the onset time is well captured by the correlation. The RMSE of equation (7) increases to 0.24 if the VOI results are also taken into consideration. The experimental data from Krzeczkowski\(^{14} \) and Dai and Faeth\(^{20} \) seem to be outliers, which may be attributed to the vague definition of \( t' = 0 \) among different studies. In this work and the VOI studies reported in Figure 3, \( t' = 0 \) is defined as the time when the droplet enters the disruptive gas field. In the shock tube experiments by Dai and Faeth,\(^{20} \) \( t' = 0 \) may be defined as the time when the diaphragm ruptures. The cross-flow measurement results from Krzeczkowski\(^{14} \) lie even further away from plotted data. The reason of this rather large deviation is unknown to the authors.
It is important to know the relative volume fraction of the bag and the remaining liquid torus in order to estimate the child droplet size. Chou and Faeth showed that the liquid bag may contain about half of the initial droplet volume. Assuming the bag thickness is the volume fraction of the liquid bag when it ruptures. Child droplets formed after the bag rupture are assumed to have a size proportional to the bag thickness, \( \delta l = C_{bag,rc} h_{bag} \), where \( C_{bag,rc} \) is an adjustable constant with a nominal value of one.

After the bag rupture, the remaining liquid torus ring is assumed to continuously expand outwardly in the cross-stream direction with a constant rate, \( \delta l(t^\prime, W_0) = \delta l(t^\prime, W_0) \). The torus eventually breaks into a few child droplets due to RT-related instabilities. Thus, the breakup in this stage is tracked by the RT breakup sub-model. Finally, if \( W_{ecrit} < W < W_{ebag} \), the revised KH-RT model is used. If \( W > W_{ebag} \), the bag breakup as the first breakup regime. If \( W_{ecrit} < W < W_{ebag} \), the phenomenological bag breakup sub-model is used.

### Model implementation

A flowchart of the IAB model is provided in Figure 4. Note that the choice of sub-model depends on the droplet Weber number. If \( W < W_{ecrit} \), no breakup is assumed to happen since the droplet is in the oscillation/deformation breakup regime. This oscillation breakup does not happen in every instance, and even when it occurs, the overall breakup time is much longer compared to the other mechanisms listed in Table 1.

### Spray experiments for comparison

The standard Spray G condition specified by the Engine Combustion Network (ECN) is used in this work to evaluate the IAB model. The ambient conditions correspond to a non-reacting early injection case in DISI engines. The Spray G injector has eight symmetrically spaced holes, each with a nominal plume direction of 37°. Table 2 lists the injector specifications and operating conditions. More details can be found on the ECN website. Another data set used for spray model validation, termed as the General Motors (GM) DISI sprays, are taken from the work of Parrish and operating conditions. More details can be found on the ECN website.

**Table 2. Operating conditions and injector specifications of ECN Spray G and GM DISI sprays.**

| Data type | ECN Spray G | GM DISI spray |
|-----------|-------------|---------------|
| Ambient gas density (kg/m³) | 3.5 | 3, 6, 9 |
| Ambient gas composition (–) | N₂, CO₂, H₂O | N₂ |
| Ambient gas temperature (K) | 573 | 400, 500, 600, 700, 800, 900 |
| Ambient gas pressure (bar) | 6.0 | 3.56–24.04 |
| Ambient gas velocity (m/s) | ~0 | ~0 |
| Fuel temperature (K) | 363 | 400 |
| Injector orifice diameter (mm) | 0.172 | 0.140 |
| Injection pressure (MPa) | 20.0 | 20.0 |
| Injection duration (ms) | 0.78 | 0.865 |
| Injected fuel mass (mg) | 10.0 | 10.0 |
| Plume direction (°) | 37 | 25 |

ECN: Engine Combustion Network; DISI: direct-injection spark-ignition; GM: General Motors.
Parrish and Zink. Measurements were conducted under late injection DISI engine-like conditions. Isooctane was injected into a high-temperature pressure vessel by a multi-hole DISI injector. The injector has eight symmetrically spaced holes, each with an inlet orifice diameter of 0.140 mm. The measured plume direction of this injector is $25^\circ$. Continuous flow of nitrogen passing through the vessel is used to provide evacuation of fuel vapor and residual droplets. Test conditions and details of the injector are also listed in Table 2.

Figure 5 summarizes the ambient conditions for both ECN Spray G and GM DISI spray experiments. Note that for GM DISI sprays, the spray characteristics were acquired with ambient temperatures ranging from 400 to 900 K at intervals of 100 K. At each temperature, three test conditions corresponding to ambient densities of 3.0, 6.0, and 9.0 kg/m$^3$ were set by adjusting the ambient pressure. Four conditions, represented by circles on the figure, are selected to calibrate the IAB model and to obtain an optimal value of the IAB model parameter, $\alpha$.

Volume-illumination Mie-scatter and Schlieren images were taken at both institutions to understand the macroscopic spray characteristics such as the penetration rates and envelopes of both liquid and vapor phases. Phase Doppler interferometry (PDI) measurements were also conducted for Spray G to measure the droplet velocity and Sauter mean diameter (SMD) distributions. More information about the optical diagnostic devices and the difference between the experimental setups can be found in Parrish and Manin et al.
Simulation setup

The OpenFOAM CFD code is used as the computational framework for running LES spray simulations.39 A one-equation non-viscosity dynamic structure turbulence model39 is used for turbulence modeling, wherein the transport equation of the sub-grid scale (SGS) turbulent kinetic energy, \( k_{\text{sgs}} \), was modified to include the LES spray term.60 The energy dissipation term of the \( k_{\text{sgs}} \)-transport equation also includes a parameter whose value is scaled with a characteristic length in order to reduce the mesh sensitivity of vapor-phase penetration.61 Other spray-related sub-models are listed in Table 3, along with the corresponding references. The initial parcel diameter is assumed to equal the effective nozzle diameter. Other spray boundary conditions such as the rate of injection (ROI) profiles, initial temperature, and plume direction and plume cone angles are taken from experimental measurements.48,56,58

The vapor region in simulations is determined using a threshold of 0.1% local mixture fraction, as recommended by ECN65 for standard Schlieren comparisons. Vapor penetration is then defined as the furthest axial distance between the injector tip and the vapor boundary. The liquid region is determined using a line-of-sight (LOS) integrated surface area method. For volume-illumination Mie-scatter imaging, the light intensity is roughly proportional to the frontal droplet surface area of incident light encounters.56 To mimic this computationally, the total droplet surface area in each cell is calculated and then projected along the camera LOS direction, resulting in a two-dimensional (2D) map of the integrated droplet surface area. The liquid–gas boundary is then defined using a threshold of roughly 3% of the maximum integrated droplet surface area. This mimic Mie-scatter (MMS) method is not in line with the ECN67 standard. The reason behind this choice is that even though both diffused back-illumination (DBI) and Mie-scatter measurement results are provided for Spray G, only Mie-scatter imaging data are available for GM DISI sprays. While the ECN-recommended projected liquid volume (PLV) method is suitable for DBI measurements, the MMS method offers a more physically consistent way to compare against Mie-scatter imaging. The predicted penetration results by those two models are very similar during the initial stage and the quasi-steady state of injection. However, the predicted liquid length (i.e., the maximum liquid penetration) and liquid residence time are different, which is expected since DBI and Mie-scatter imaging measurements also show noticeable differences.57 The liquid residence time is defined as the time after start of injection (ASOI) when the liquid penetration drops to zero.57 A detailed discussion about both methods is documented in Appendix 1.

Prior to the simulations, a mesh resolution study is carried out on a 100 \( \times \) 100 \( \times \) 100 mm cubic mesh composed of hexahedral cells. The base mesh has a uniform cell size of 1.0 mm. Two additional meshes were generated with non-uniform node spacing to capture the near-nozzle flow details at a minimal computational cost. Static mesh refinement was employed in both meshes, where the smallest cell sizes are 0.5 and 0.375 mm, respectively. Cell sizes of 0.1875 mm and smaller are not tested since the liquid volume fraction of the mesh cells can exceed 60% in the near nozzle area, which is beyond the 10% rule-of-thumb for Lagrangian spray simulations. Figure 6 shows an \( x-y \) cut-plane of the 0.375 mm mesh, in which a gradually increased node spacing is noticeable from the injector location to the mesh boundaries. Note that particular attention is paid to the representation of the injector tip in all three tested meshes, as shown in the embedded sub-figure. The injector tip is aligned with the mesh boundaries to prevent false entrainment of ambient gas.34 Wall boundary conditions are applied to the injector tip surfaces in each mesh. The total number of cells is approximately 1.1, 1.0, and 1.6 million for 1.0, 0.5, and 0.375 mm meshes, respectively. The number of injected parcels is set to be 400,000 for all three meshes.

| Spray process          | Model                                |
|------------------------|--------------------------------------|
| Heat transfer          | Ranz and Marshall62                  |
| Evaporation            | Froßling correlation (OpenFOAM implementation)63 |
| Droplet collision      | No collision                         |
| Droplet drag           | Spherical drag42                     |
| Turbulent dispersion   | Discrete Random Walk64               |

Table 3. Spray processes and the corresponding models.
Some studies have argued that the number of injected parcels should increase as the mesh refines in order to achieve convergence. However, the number of injected parcels in this work is comparable to the one reported in Senecal et al. for the same level of mesh refinement. As will be discussed later, the number of injected parcels is sufficient that running multiple realizations has little impact on the global spray characteristics such as liquid and vapor penetrations. Therefore, multiple realizations (five as suggested by Sphicas et al.) were only run for the Spray G conditions in favor of the SMD and droplet comparison. Each realization has a different random number seed in the injection model so that the initial velocity vectors are different.

Figure 7 shows the liquid and vapor penetration results under the standard Spray G conditions. Also plotted are experimental data using Mie-scatter imaging and Schlieren from Sandia National Laboratory (SNL) and Istituto Motori. For liquid penetrations shown in Figure 7, the results converge when the cell sizes are smaller or equal to 0.5 mm. The estimated liquid residence time is the same among all three meshes. The 1.0 mm mesh predicts slightly higher liquid penetration compared to the other two after 0.6 ms ASOI, but the difference is not significant, and the predicted trends follow each other closely. For the vapor penetrations shown in Figure 7, both 1.0 and 0.5 mm meshes predict very similar results throughout the simulation, and the 0.375 mm mesh predicts slightly higher vapor penetration after 0.5 ms ASOI. Results from all three meshes match the Schlieren data from Istituto Motori reasonably well, but fail to match the SNL data. Figure 8 presents the SGS turbulent kinetic energy, along the plume centers at 0.5 ms ASOI. It is seen that is larger with finer mesh within 3 mm from the injector tip. This is expected since the liquid volume fraction increases as the cell size decreases, which leads to larger spray source term in the transport equation and hence higher generation. The differences among three plotted curves become smaller at distances of 5 mm and further, implying that the SGS turbulence field is properly resolved. Overall, the LES results do not show great sensitivity to the mesh sizes. The 1.0 mm mesh is therefore used for the remaining part of this work due to its uniformity and reduced computational cost.

Results and discussion
Prior to the discussion of spray breakup modeling, the bag formation and bag growth processes are analyzed. Evaluation of the IAB model is then performed by comparing its predictions with experimental data and simulation results using the KH-RT model. Targeted spray characteristics include penetration rates, droplet velocity, and SMD profiles. Subsequently, further discussion focusing on the IAB breakup characteristics is provided. Finally, an attempt to correlate the optimal
breakup model parameter values with the ambient conditions is made, and the found value is tested under a wide range of DISI spray conditions.

**Analysis of the bag characteristics**

Bag growth plays a crucial role in the bag breakup process as it determines the breakup length scale. To analyze the evolution of bag over time, initially spherical droplets are assumed to enter a constant flow field so that the initial $We$ equals a specific value. The non-dimensional diameter ratios are then analyzed using equations (5)–(7). Available experimental data from Chou and Faeth,19 Krzeczkowski,14 and Kulkarni36 are used for validation purpose. The measurements were carried out with different experimental setups and working fluids. A typical setup includes a droplet generator, a wind tunnel or a shock tube, and optical diagnostic systems for velocity and droplet size measurements.

Figure 9 presents the temporal evolution of measured and predicted cross-stream bag diameters at various $We$ and $Oh$ numbers: (a) $We_1 = 13$, (b) $We_1 = 14$, (c) $We_1 = 15$, (d) $We_1 = 18$, and (e) $We_1 = 20$. The data reported on both $x$ and $y$ axes have been normalized by the non-dimensional breakup time, $T^*$, and the initial droplet diameter, $d_{db}$, respectively.

Figure 9 shows that all studies qualitatively agree with one another with increasing $We$ number. In both experiments and predictions, the diameter ratio starts to increase slowly during a short period ($t^* < 0.6$) after the droplet enters the disruptive gas field, indicating the transition from a spherical droplet to a relatively thin liquid disk. A liquid bag then forms at the center of the deforming disk and grows rapidly due to the pressure difference inside and outside the bag. The fast growth of the liquid bag also causes the thicker torus ring attached to the open end of the bag to expand in the cross-stream direction. Finally, after the bag rupture, the remaining torus ring continues to expand with a constant velocity until it breaks due to RT instabilities. Note that the rate of cross-stream expansion is the largest when the bag is present, which is in agreement with the findings in Chou and Faeth.19 The diameter ratios in Figure 9(e) differ between experiments and predictions. This is attributed to the difficulties in experimental measurements. While the torus ring is assumed to be of circular shape in equations (5)–(7), it is often heavily curled or distorted in experiments, especially at relatively larger $We$ number.19,23 Results also show that the droplet $Oh$ number has little effect on the bag growth for the $Oh$ range considered in this analysis.

It is important to understand how the bag develops beyond the scope of experiments illustrated in Figure 9. Therefore, the predicted cross-stream diameter ratios for $We$ from 6 to 56, covering a wide range of the bag
and bag–stamen breakup, are computed and plotted in Figure 10. On each curve, the onset time of bag rupture is also overlaid as an asterisk. At $W_e = 6$, the droplet undergoes deformation with no bag develops on its surface. Further increasing of $W_e$ promotes a rapidly expanding liquid bag as expected. However, the onset time of bag rupture decreases as $W_e$ increases, leaving a shorter time for the torus ring to gain momentum from the growing bag. The competitive contributions from the above two factors give a complex behavior of the cross-stream diameter ratio. Before the bag ruptures, the growth rate increases monotonically with $W_e$, but the difference becomes less noticeable at higher $W_e$ number. After the bag ruptures, the liquid torus expands with a constant rate, whose value initially increases then decreases with larger $W_e$. This behavior confirms that the size of the liquid torus is not excessively larger than the initial droplet diameter. It also suggests that the bag structure is unlikely to develop at very high $W_e$ numbers.

**Initial calibration: liquid and vapor penetration curves**

Both the IAB and the KH-RT models were calibrated at the baseline DISI conditions illustrated in Figure 5. Liquid and vapor penetrations were selected as the target spray characteristics. Two IAB model parameters, namely, $B_1$ and $a$, were adjusted using a Monte Carlo approach to obtain optimal predictions compared to the measured penetration curves. The same process was conducted for the KH-RT model using the calibration of three model parameters: $B_1$, $C_b$, and $C_t$. Although it requires more efforts to obtain the optimum compared to the IAB model, it is deemed necessary since adjusting $B_1$ and $C_b$ will not match both the liquid and vapor penetrations, as reported by Van Dam and Rutland. Predicted liquid and vapor penetrations are plotted in Figures 11–14 for cases 1–4, respectively. Available experimental data for the penetration measurements are also plotted on each figure, with the shaded area representing the 95% confidence levels.

Figure 11 presents the penetration curves for case 1, the standard Spray G conditions. Numerical results averaged over five realizations are plotted with the corresponding standard deviations as error bars. Both the liquid and vapor penetrations match the measured curves very well during the early period of injection ($t < 0.2 \text{ ms ASOI}$). Then, liquid penetrations become parabolic due to droplet breakup and aerodynamic drag after approximately 0.2 ms ASOI. Simulations show more variability during the quasi-steady stage of injection ($0.5 < t < 0.7 \text{ ms ASOI}$). The maximum standard deviations for the liquid penetrations are 0.6 and 0.5 mm for the IAB and KH-RT models, respectively, indicating that both models are insensitive to the random number seed in the injection model. As one may expect, only by changing the random number seed is not sufficient to represent the uncertainties in spray.

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**Figure 10.** Predicted cross-stream diameter ratio as a function of non-dimensional time at various $W_e$. Asterisks are overlaid on each curve to illustrate the onset time of bag rupture.

**Figure 11.** Liquid and vapor penetration curves for case 1 (standard Spray G condition). The predicted results are ensemble-averaged over five realizations and plotted with error bars representing the standard deviations. The measured vapor penetrations are plotted with the shaded area representing the 95% confidence levels.
and ambient conditions. Indeed, UQ with proper variations in the boundary conditions is needed to obtain realistic results.53 The negligible standard deviations also suggest that the discrete Lagrangian phase has reached a statistical convergence with the current setup of total injected parcels. Better matching to the experimental data is given by the IAB model during this period. The liquid penetration eventually goes to zero due to evaporation. The timing of this transition is estimated to be around 1.2 ms ASOI by Mie-scatter imaging measurement,57 which is well captured by the IAB model. The liquid length is measured to be 30 mm. The IAB model predictions follow the measurements data closely with a liquid length of 28.3 mm. The KH-RT model, however, predicts the spray to penetrate further downstream until it reaches a liquid length of 35 mm.

The experimental vapor penetrations from SNL and Istituto Motori are plotted in Figure 11. Even though both groups use the same injector at the same nominal spray conditions, the exact setup differs. For transient sprays, a small variation in the initial and boundary conditions can result in large changes in penetration rates at later times. Figure 11 shows that the measured vapor penetrations start to deviate from each other after 0.3 ms ASOI. The deviation continues to increase until about 1.0 ms ASOI, after which the measured curves become parallel to each other. The maximum vapor penetrations are 48.6 and 52 mm for the SNL and Istituto Motori measurements, respectively. The predicted vapor penetrations match the Istituto Motori measurements very well. Small differences are observed between the predicted results. However, both models over-predict the penetration rates compared to the SNL data after 0.5 ms ASOI. The maximum standard deviations are 1.3 and 1.1 mm for the IAB and KH-RT models, respectively. Compared to the mean penetrations at 2.0 ms ASOI, the standard deviations are rather subtle. Therefore, in the following discussion, only single realizations are performed for the GM DISI sprays.

Figures 12–14 present the measured and predicted penetration curves for cases 2–4 (GM DISI conditions of 800 K and 3.0, 6.0, and 9.0 kg/m³, respectively). Again, simulations with the IAB model match the experimental data very well at all three conditions for
liquid penetration. Similar to case 1, the spray structures reach quasi-steady states around 0.5 ms ASOI. The liquid length is well captured by the IAB model as well. On the contrary, KH-RT model under-predicts the liquid penetration at both 3.0 and 6.0 kg/m³. The effects of changing ambient density on liquid penetration at the temperature of 800 K are also illustrated in Figures 12–14. Comparing with the result at the ambient density of 3.0 kg/m³, the liquid length decreases by about 33% and 42% at higher densities of 6.0 and 9.0 kg/m³, respectively. The reduction in liquid length at higher ambient density is expected since the aerodynamic drag increases as well. The measured liquid penetrations also show a gradually retracting liquid tip after the end of injection. This behavior is likely attributed to nozzle dribble from the sac volume after the injection or light reflection by the nozzle tip. Unfortunately, present LES framework is unable to simulate dribble from the nozzle sac volume due to a lack of internal flow modeling.

The predicted vapor penetrations in Figures 12 and 13 match the experimental data to within 95% confidence levels except at the very end of simulation for the 6.0 kg/m³ case, where a sudden increase is observed with both models. This is caused by vapor protrusion along the injector axis as documented in a recent UQ study by the authors. The reason of vapor protrusion is unknown at this time, but it is unlikely caused by the breakup models as the timing (3.5 ms ASOI) is about four times larger than the injection duration. In Figure 14, both models tend to over-predict the vapor penetration just before the end of injection. Like the liquid phase, increasing ambient density also causes a reduction in vapor penetration. Overall, the predicted vapor penetrations show little difference between the KH-RT and the IAB model predictions.

The IAB model parameter values from the optimal calibration for baseline cases 1–4 are listed in Table 4. The difference observed in the α values among all four cases is subtle. However, B₁ values are highly different between Spray G and GM DISI sprays. Indeed, B₁ is given a variety of values as reported in Reitz and Beale, Ricart et al., Van Dam and Rutland, and Brulatout. The rather large B₁ range owes to the fact that the initial KH unstable waves rely heavily on the fuel properties, injector geometry, and near-nozzle air entrainment. The rather close α values indicate that the baseline conditions may share the same density ratio dependency of the breakup length. In support of this statement, the nominal breakup length along the plume centerlines at the baseline conditions was calculated using equation (4) and results are shown in Figure 15. Also plotted are the breakup lengths calculated using equation (3) for the optimal KH-RT simulation results discussed previously. The corresponding model parameter values are listed in Table 6 in Appendix 2. The final combination of KH-RT parameter values from the study of Van Dam are also listed in Table 6 for comparison purpose. Note that the plotted results are computed using the nominal ambient densities depicted in Figure 5. In simulations, the ambient density will increase due to evaporation, which in turn leads to reduced breakup length.

Figure 15 shows that as the ambient density increases, the liquid-gas density ratio decreases, which in turn leads to a reduced breakup length in the IAB model. This trend is consistent with the expectation that higher ambient density leads to reduced breakup length.
The breakup length adopted by the KH-RT model exhibits opposite trends between this work and Van Dam and Rutland\textsuperscript{34} for cases 2–4. Van Dam and Rutland demonstrated that the breakup length increases as the density ratio decreases, while in this work, the breakup length is shown to decrease at higher gas-phase densities. This opposite relationship can be explained by the different revisions of the KH-RT model between this work and Van Dam and Rutland.\textsuperscript{34} In this work, the RT breakup model is only activated once a parcel travels beyond the pre-calculated breakup length. The child droplet sizes after breakup are set to be the RT wavelength, $L_{RT}$. In contrast, the KH-RT model revised by Beale and Reitz\textsuperscript{38} was used by Van Dam and Rutland,\textsuperscript{34} in which the RT breakup is also activated even if the parcel is located within the breakup length. However, this generally results in faster breakup, and to compensate for that, the RT breakup time constant, $C_t$, was set to 9.0 for parcels within the breakup length. In addition, the child droplet sizes from RT breakup are selected from a Rosin–Rammler distribution. In general, both KH-RT revisions struggle to predict accurate penetration curves under the GM DISI conditions, as discussed in the previous section and Van Dam and Rutland.\textsuperscript{34} Moreover, the breakup length obtained from the optimal KH-RT simulations for case 1 does not correlate with the other three cases.

**Droplet velocity and SMD profiles**

After the initial calibration targeted at penetration curves, more rigorous validation of the models is conducted focusing on the droplet velocity and SMD distributions. Data are sampled at the standard Spray G condition in the radial direction through the plume centers at 15 mm axial position, a location where the experimental data are available. The ensemble-averaged simulation results of all eight plumes and five realizations at two selected timings, 0.5 ms and 1.5 ms ASOI, are plotted with PDI data in Figure 16. Simulation results are plotted with the standard deviations computed over 40 samples. The experimental data are plotted with the mean values only. At 0.5 ms ASOI, the residual droplets can no longer be detected by the LOS spray visualization measurements, as evidenced by Figure 11, where both measured and predicted liquid penetrations are zeros. However, droplets can still be captured by the PDI system. As Figure 16(b) and (d) shows, the predicted droplet velocity and SMD distributions at 9 mm radial position. The predicted SMD by the KH-RT model is 42 $\mu$m, while the one given by the IAB model is 16 $\mu$m. Better agreement with the experiments is given by the IAB model, despite the relatively large standard deviations at 1.5 ms ASOI. This improvement owes to the fact that droplet velocities are relatively low at 1.5 ms ASOI, leading most of the residual droplets into the bag and deformation breakup regimes, as will be further elaborated later. The bag sub-model is responsible for the breakup description of remaining droplets that are still undergoing breakup process.

**Characteristics of the IAB model**

More insights into the IAB model can be gained by examining the occurrence percentage of each sub-model for the baseline cases. The occurrence percentage is defined as the ratio of the number of liquid parcels driven by each sub-model to the total number of existing liquid parcels. Temporal evolution of these quantities are shown in Figure 17, where it is found that a
decrease in either the ambient temperature or density leads more parcels with We smaller than We_{crit}, making them fall within oscillation/deformation regime. As the ambient temperature increases, the evaporation rate increases as well, which in turn reduces the life span of small droplets and hence the occurrence percentage of deformation mode. We number increases with the ambient density, leading to more droplets in the plume-sheet thinning, sheet-thinning, and catastrophic breakup regimes.

Figure 17 shows that the occurrence percentages of the deformation mode are already large at 0.1 ms ASOI. About 80% of fuel parcels in the domain are driven by this mode for the moderate-temperature case 1. This is caused by the substantial amount of micro-size child droplets resulting from KH-breakup. Moving to the high-temperature GM DISI conditions at the same time, the percentages reduce to 46%, 28%, and 20% for the ambient densities of 3.0, 6.0, and 9.0 kg/m³, respectively. This trend is accompanied by the observation that the KH-RT breakup mode drives more parcels at higher densities. This is expected since droplet We number increases proportionally with the ambient density. In general, the occurrence percentages of KH-RT mode decrease as time proceeds, though they seem to bump up around 0.5 ms ASOI for cases 3 and 4. It is also noted that the KH-RT mode drives more parcels than the bag mode for case 1 before the injection ends at 0.78 ms ASOI. The crossover happens even later for the high-temperature GM DISI conditions. While the injection ends at 0.865 ms ASOI, the bag mode only begins to surpass the KH-RT mode at about 1.0 ms ASOI. The relative dominance of bag mode over KH-RT after the injection also explains why the SMD and velocity predictions of the IAB model are improved at 1.5 ms ASOI, as shown in Figure 16.

As discussed previously, a bi-modal distribution is expected for the bag breakup.\textsuperscript{28,36} However, the number of child droplets from bag rupture may overwhelmingly outnumber that from the liquid torus breakup, making it difficult for this distribution to be observed in experiments.\textsuperscript{36} In simulations with the parcel approach, this limitation can be easily overcome if results are processed based on fuel parcels, as opposed to the fuel droplets discussed in Figure 16. Recall that a parcel is an ensemble of several maybe hundreds of droplets with same properties. In the bag breakup model, child droplets from bag rupture and torus breakup are enclosed by two separate parcels. Figure
Figure 17. Occurrence percentage of the IAB breakup sub-models for baseline cases. (a) Case 1, 573 K, 3.5 kg/m$^3$. (b) Case 2, 800 K, 3.0 kg/m$^3$. (c) Case 3, 800 K, 6.0 kg/m$^3$. (d) Case 4, 800 K, 9.0 kg/m$^3$.

Figure 18. PDF of parcel diameters at 1.1 ms ASOI for test cases 1–4, using (a) IAB and (b) KH-RT models.

18 shows the PDFs of parcel diameters at 1.1 ms ASOI for baselines cases. Results obtained using the IAB and KH-RT models are plotted on the left and right sub-figures, respectively. Note that all remaining parcels in Figure 18(a) are either driven by the deformation mode or the bag mode since the occurrence percentage of the KH-RT mode is less than 1%, as shown in Figure 17(a). It can be seen that most residual parcels are smaller than 25 μm, with the peaks located at around 10 μm. These small parcels likely lie within the deformation regime where parcels no longer break. Moving to larger parcels, two peaks in PDFs are seen in results from the IAB model. The peaks in the middle are likely associated with the liquid torus rings after bag rupture,
while the peaks on the right correspond to the growing bag. This observation supports the bi-modal droplet size distribution. However, the KH-RT model does not show such behavior at larger parcel diameters, as shown in Figure 18(b).

Application to other DISI conditions

Additional evaluations of the IAB model were done by extending the test matrix to more ambient temperature conditions for GM DISI sprays. Rather than providing the optimal calibration results for each case, we intended to develop a unified set of model parameters to reduce the efforts needed for calibrating the IAB model at different DISI spray conditions. Recall that \( \alpha \) values for the density conditions listed in Table 4 are quite close to each other. Assuming the value of \( \alpha \) is a constant for DISI sprays with a specific type of fuel, then a reasonable estimation can be made by averaging the \( \alpha \) values in Table 4. However, no effort is made to correlate \( B_i \) with ambient conditions, since its value appears to be highly dependent on the injector geometry and near-nozzle air entrainment.

Figures 19 and 20 present the liquid and vapor penetration curves for all GM DISI temperature and density conditions listed in Table 3. Simulation results were taken from single realizations with the IAB model parameters \( \alpha = 0.92 \) and \( B_i = 50 \). Experimental data were the average of 25 duplicate measurements. The left columns show the liquid penetration curves, and the right ones show the vapor penetration results. The top rows show results at 3.0 kg/m\(^3\), and the following two rows show the results at 6.0 and 9.0 kg/m\(^3\), respectively. For clarity of presentation, experimental data are only plotted with the ensemble-averaged values.

A general trend found in Figures 19 and 20 is that higher ambient density leads to reduced liquid length due to the enhanced air entrainment, increased aerodynamic drag, and possibly faster droplet breakup. In Figure 19, the density impact is more pronounced at 400 K compared to 500 K and higher. The liquid residence time also shows the largest difference at 400 K, in which an increase in the ambient density will lead to longer liquid residence time. This is expected since the pressure must be elevated to keep the ambient density constant, and the elevation in ambient pressure suppresses evaporation, hence increases the life span of small droplets. The simulations are able to reproduce the shape of the experimental curve at 3 kg/m\(^3\), but fail to even capture the general trends at higher densities.

The predicted vapor penetration curves in Figure 19 agree reasonably well with the Schlieren measurements. At 400 K, the vapor penetration results are under-predicted during the initial period of injection at all three density conditions. One possible reason is that the identical spray initial and boundary conditions at the nozzle exit at each density condition. While in experiments the ambient temperature and pressure influence the spray behaviors such as the plume cone angle and near nozzle air entrainment, in simulations the spray boundary conditions are kept unchanged among all cases since the primary goal of this test is to see if the IAB model can perform well under conditions beyond the scope of cases 1–4. In Figure 20 at 800 K, the predicted vapor penetrations match the experimental data quite well at 3.0 and 6.0 kg/m\(^3\), even though they are not the calibrated results since the parameter \( \alpha \) in equation (4) is changed. At 9.0 kg/m\(^3\), the predicted vapor penetration results are somewhat discouraging. One possible reason is the extra momentum gained from the over-penetrating liquid droplets as shown in the left columns. Other factors such as the turbulence model can also come into play.

The liquid length and liquid residence time are perhaps two important macroscopic spray characteristics in DISI sprays. In general, the liquid length needs to be accurately captured since it affects the wall-impingement and hence the following mixing and combustion processes. The liquid residence time is also of importance as residual droplets can be a potential source of soot. Therefore, a comparison of these two quantities is extracted from Figures 19 and 20 and plotted in Figures 21 and 22. While the calculation of liquid length is straightforward, the definition of liquid residence time is somewhat vague. In experiments, the liquid residence time is defined as the time required for the penetration to fall to half the maximum due to vaporization. \(^{48}\) In simulations, however, the residence time is defined as the time when the liquid penetration falls to zero. The difference caused by this discrepancy is expected to be negligible providing the liquid penetration falls rapidly back to zero in the simulations.

In Figure 21, the predicted liquid length results are plotted as functions of ambient temperature for the three ambient densities. Experimental data from the Mie-scatter imaging are also plotted as symbols for comparison. It is seen that the predictions match the experimental data very well at 3.0 kg/m\(^3\). At 6.0 kg/m\(^3\), the agreement is quite good as well except at 400 and 900 K, where successful predictions are not achieved. At 9.0 kg/m\(^3\), the simulation results only match the experimental data at 700 and 800 K. However, the general trend of reduced liquid length with increasing ambient temperature is still captured by the model.

The results of liquid residence time are shown in Figure 22. First, it is seen that the liquid residence time is independent of the ambient density for temperatures of 500 K and higher. This implies that the ambient air provides enough energy to vaporize the fuel regardless
of changes in the ambient density. At 400 K, the measured liquid residence times change with density, indicating that this independence no longer stands. In general, higher density enhances the air entrainment and hence increases the energy available for evaporation. However, evaporation is suppressed at increased density, since the pressure must be elevated given the temperature is unchanged. It can be seen that the liquid residence time increases drastically as the density increases, suggesting the evaporation plays a more important role than air entrainment. As Figure 22 shows, the measured liquid residence time increases by 32% and 76% when the ambient density increases from 3 to 6 and 9 kg/m³, respectively. However, the predicted residence time only increases by 11% and 26% for the same changes. The lack of sensitivity to the density change at 400 K suggests that the evaporation rate is over-predicted at higher density cases. This can be a
result of either increased droplet area-to-volume ratio caused by accelerated breakup modeling, or inaccurate phase-change rate by the evaporation model, or even a combination of both factors. At the low-temperature condition of 400 K, high pressure is not required to maintain the densities at 3, 6, or 9 kg/m³. The near-nozzle air entrainment is therefore expected to be not as strong as the other conditions. This will result in a smaller plume angle and possibly weaker KH disturbance levels at the nozzle exit. Since the value of $B_1$ was calibrated at much higher temperature and pressure conditions, keeping $B_1$ unchanged is expected to give accelerated breakup.

**Summary and conclusion**

Direct injection diesel and gasoline sprays share many similarities in terms of the injection system and spray...
pattern, yet there are many differences in the thermophysical properties and operating conditions. In the LES of DISI gasoline sprays, in order to more precisely describe the fuel–air mixing, one may need to take into account the effects of these differences on liquid atomization and breakup, which are mainly expressed as different breakup mechanisms of fuel droplets. In this article, an IAB model tailored for DISI gasoline sprays is presented. In the IAB model, atomization of liquid jet near the nozzle exit and the subsequent breakup of liquid fragments and droplets are treated as indistinguishable processes, and the “blob” approach is adopted to represent the liquid fuel regardless of its physical appearance (jet, ligament, or droplet). The breakup simulation has been divided into two regimes, namely, the bag/bag–stamen breakup regime, and the high We number regime. In the first regime, a phenomenological bag breakup model has been developed by the authors to track the breakup process. In the second regime, the breakup modeling is based on the KH-RT model by Reitz and coworkers with a revised breakup length concept.

The initial calibration has been carried out by adjusting the model parameter values to obtain the optimal matching of penetration curves between LES predictions and experiments. The standard Spray G condition defined by ECN and the spray measurements conducted by GM at the ambient temperature of 800 K and three densities of 3.0, 6.0, and 9.0 kg/m³ were used as four baseline cases. The optimal calibration of the KH-RT model has also been conducted and results were compared against the experiments and IAB model predictions. It was shown that the IAB model gives generally better agreement than the KH-RT model at all conditions discussed. The improvements were minor considering both models have been calibrated to give the best-matching results. However, further analysis of the breakup length reveals that the KH-RT model may not fully capture the atomization/breakup processes of DISI sprays. The KH-RT model also requires more efforts to calibrate, and the results may yield different trends of the characteristic breakup length depending on the implementations. However, the IAB model has an overall good performance among the four baseline cases and the resulting breakup lengths meet the expectation that higher ambient density leads to decreased breakup length.

The model has been further assessed by comparing the predicted droplet velocity and SMD distributions with PDI measurements at the standard Spray G condition. It is shown that the IAB model improves the predictions of droplet velocity and SMD distributions during and after the injection, especially in later times. Analysis of the occurrence percentage of each sub-models reveals that the KH-RT sub-model drives more parcels than the bag breakup model before the end of injection. However, the bag breakup mode becomes the dominant mechanism in later times. This is considered to be an important improvement over the KH-RT model since large residual droplets after the end of injection may be a potential source of soot emissions, and hence their breakup needs to be accurately modeled.

An effort has been made to unify the model parameters across the four baseline DISI conditions, and the given parameter values have been used to test the model performance at more GM DISI spray conditions. Changes in ambient temperature and density were studied. The results agree favorably with the experimental measurements, with some discrepancies at the lowest temperature of 400 K that can be explained. In most cases, the agreement is generally good.
considering that the model parameters were not tuned specifically for individual cases.

It is generally accepted that breakup models coupled with accurate spray boundary conditions and even the internal flow characterization are important for accurate prediction of spray behavior in direct-injection engines. For DISI sprays, the relatively small L/D ratios and volatile fuel components can lead to very complex internal turbulent flows and phase-change phenomena such as cavitation and flash boiling. This article presents a rather promising breakup model for DISI sprays. Future work will be focused on incorporating more physically representative sub-models to initialize the spray parcels at the nozzle exit and hence to improve the predictions at low-temperature conditions for GM DISI sprays.

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### Appendix 1

**Estimation of the liquid penetrations**

Line-of-sight liquid-phase measurement techniques, such as volume-illuminated Mie-scatter imaging and diffused back-illumination imaging, are used by GM and ECN to define the liquid region and hence the penetration length. With Mie-scatter imaging, the light signal is proportional to the square of the incident particle diameter. DBI or laser absorption use light extinction (light deflection or absorption) produced by fuel droplets, thus providing a measure related to the cube of droplet diameter. However, the conventional way to determine liquid penetration in most CFD studies is based on the accumulated liquid mass fraction. To reduce the difference between numerical and experimental methods of measuring liquid penetration, line-of-sight integrated droplet surface area method, referred to as the mimic Mie-scatter (MMS) and projected liquid volume fraction methods (PLV) are employed in this work.

Table 5 summarizes the aforementioned three methods for the estimation of liquid penetrations. The accumulated mass method remains the most popular one in the literature, even though it can give misleading results for highly transient sprays. The other two methods require more efforts to use. A detailed description of both methods can be found in Li.51 Here, only the basics are provided. Assuming the x-axis is the camera line-of-sight direction, then the total droplet surface area or droplet volume in each CFD cells is calculated and projected along the x-direction, resulting in a two-dimensional (2D) map of integrated droplet surface area or volume. The liquid–gas boundary is then defined using the thresholds provided in Table 5. Note that for the MMS method, the threshold is roughly equal to 3% of the maximum integrated surface area.

| Name | Description |
|------|-------------|
| Accumulated mass | Axial distance from the nozzle tip where the accumulated liquid mass fraction is 99% |
| Projected liquid volume fraction | Engine Combustion Network recommended method for comparison against DBI measurements. Recommended two thresholds are $2.0 \times 10^{-3}\text{mm}^2\text{-liquid/mm}^2$ ("high" threshold) and $2.0 \times 10^{-4}\text{mm}^2\text{-liquid/mm}^2$ ("low" threshold) |
| Mimic Mie-scatter | Line-of-sight integrated droplet surface method used in this work to compare penetration results against Mie-scatter measurements. The threshold is set to be $7.0 \times 10^{-2}\text{mm}^2\text{-liquid/mm}^2$. |

DBI: diffused back-illumination.

Predicted liquid penetrations for case 1 using the aforementioned methods are plotted in Figure 23. Also plotted are the liquid penetrations measured using Mie-scatter imaging and DBI from Manin et al.57 As Figure 23 shows, the predicted liquid penetrations are very close to each other during the initial period of injection. Small deviations are noticeable after the spray structure reaches the quasi-steady state at 0.5 ms ASOI. The predicted trends follow the measurement curves quite well until the end of injection, 0.78 ms ASOI. The accumulated mass method keeps giving non-zero penetrations throughout the simulation and thus fails to capture the retracting liquid-tip. The MMS and PLV methods, however, predict a rapid dropping of liquid penetration. An interesting finding from Figure 23 is that there are some inconsistencies between the Mie-scatter imaging and DBI measurements, especially for the liquid residence time. This can be related to the fundamental
basics of both measurement techniques, which is beyond the scope of this work.

Note that the MMS method was initially calibrated against the conventional accumulated mass method before the end of injection. The selected threshold ($7 \times 10^{-2}$ mm$^2$/mm$^2$) guarantees that both methods will give similar results up to the end of injection, as shown in Figure 23. Changing the threshold will inevitably alter the predicted liquid penetration. This can be demonstrated by Figure 24, where the predicted liquid penetrations using the MMS method with three different thresholds are plotted. During the initial period of injection, the predicted penetrations show very little differences. The penetration curves start to deviate from one another after 0.3 ms ASOI. Increasing the threshold by $4 \times 10^{-2}$ mm$^2$/mm$^2$ (57% increase) only over-predicts the liquid length by 2 mm (7% increase) compared to the baseline threshold. However, the liquid length drops by 4 mm (13% decrease) if the threshold decreases by the same value. This rather large deviation suggests that the threshold should be set after a careful calibration against either experiments or a well-established method such as the accumulated mass method.

**Appendix 2**

**KH-RT breakup parameter values from the optimum calibration**

Parameter values from the optimal KH-RT calibration for cases 1–4 are listed in Table 6. The final combination of KH-RT parameter values from the study of Van Dam and Rutland is also listed in Table 6 for comparison purpose.

| Case no. | Ambient density (kg/m$^3$) | Ambient temperature (K) | Present work | Van Dam and Rutland |
|----------|---------------------------|-------------------------|--------------|---------------------|
| 1        | 3.5                       | 573                     | $B_1 = 30$   | N/A                 |
|          |                           |                         | $C_0 = 1.0$  |                     |
|          |                           |                         | $C_{RT} = 0.35$ | $B_1 = 20$         |
| 2        | 3.0                       | 800                     | $B_1 = 50$   |                     |
|          |                           |                         | $C_0 = 1.9$  | $C_0 = 1.0$         |
|          |                           |                         | $C_{RT} = 0.1$ | $C_{RT} = 0.1$     |
| 3        | 6.0                       | 800                     | $B_1 = 50$   |                     |
|          |                           |                         | $C_0 = 2.1$  | $C_0 = 1.5$         |
|          |                           |                         | $C_{RT} = 0.1$ | $C_{RT} = 0.1$     |
| 4        | 9.0                       | 800                     | $B_1 = 50$   |                     |
|          |                           |                         | $C_0 = 2.3$  | $C_0 = 2.5$         |
|          |                           |                         | $C_{RT} = 0.1$ | $C_{RT} = 0.1$     |