

Heat Release Analysis of The Scaled and Colliding Sprays Using RANS Approach

Masumeh Gholamisheeri^{1,2}, Daniel Norling¹, Thomas Hällqvist¹

1- Scania CV AB., Södertälje, Sweden

2- KTH Royal Institute of Technology, Stockholm, Sweden

Abstract

This study tries to optimize the heat release rate of a diesel injector that is injecting into a constant volume combustion chamber. This optimization is performed via spray scaling through Reynolds Averaged Navier-stokes simulations (RANS). The spray-A (diesel spray from Engine Combustion Network) has been used as a reference for validation of the simulations. To scale the diesel jet, the injected mass and cross-sectional area of the injector are varied with similar scaling factor. It was found that using a larger injector leads to a longer spray penetration, ignition delay, and burn duration while it helps a more complete combustion. On the other hand, using a smaller orifice improves the burn duration and reduces the heat release, while it causes a slightly higher amounts of unburned hydrocarbons. It was revealed that it is reasonable to use multiple smaller orifices (two half size or four quarter size injectors) in place of one single injector, to improve the burn rate. To achieve a complete combustion, the configuration must be tuned. For clarity, three configurations are considered, parallel, non-coaxial colliding and co-axial colliding sprays for which the distance between the sprays and the inclination of the sprays are varied and tested. The advantages and disadvantages of each configuration is discussed in length.

Keywords: Reynolds Averaged Navier-Stokes (RANS), Spray-A, Heat Release (HR), Diesel Spray, Scaled Jet.

Introduction

Understanding the behavior of spray and corresponding processes in spray formation, mixing and combustion is well established and widely studied over the past few decades. Stringent emission regulations and fuel economy are the two strong motives for the continuous research on injector characteristics and design, spray formation and complex turbulent flows in piston engines. High spatial and temporal resolution optical diagnostics and numerical simulations are required for further increase in performance and reductions in fuel consumption and emissions [1]. Due to the complexity of the fuel spray and combustion, in both experiment and modeling areas, analysis of involved physical phenomena in simplified geometries such as constant volume combustion vessels [2-10] or rapid compression machines [11-14] are inevitable.

Simply, the high-fidelity experimental data are used for validation of the simulation tools [7]. For this reason, Engine Combustion Network (ECN) [15] provides an international collaborative environment where experimental data under well-defined boundary conditions applicable to engine combustion is available [7]. In this platform, various diesel and gasoline sprays are tested experimentally and pressure rise, jet penetration, liquid penetration length, flame lift-off and ignition delay are measured [3, 6]. Among all, a n-dodecane spray flame, called spray-A has been the focus of many studies [7, 16-21] and is used as the initial reference of the current study. To improve the combustion efficiency and performance of diesel engines, one possible solution is to enhance the spray-flow interaction, such as the air entrainment rate. For this reason, scaling the flow rate (i.e. injected mass and nozzle cross sectional area), rearranging the number of nozzles and the size of nozzle holes can be effective. Utilizing a smaller orifice with higher injection pressure facilitates fuel atomization and evaporation, thus reduces the particulate emission in direct injection (DI) engines [22-25]. However, it is reported that the spray properties change with orifice diameter decrease, i.e. tip penetration decreases causing poor spatial distribution [22]. In the above-mentioned studies, the spray properties are the primarily focus of the research and the effect of orifice size on heat release rate is not investigated. In addition, the orifice size effect is investigated in the context of group-hole nozzle, which has several groups of orifices, each group consists of two micro-orifices, parallel and very close to one another [22].

To shed light on the physics of the flow and spray behavior, numerical studies are necessary. For the past few decades, Computational Fluid Dynamics (CFD) investigations provide insight to the multi-scale physical phenomena with comparably lower cost. A wide range of coupled problems are involved in turbulent flames, fluid mechanical properties, transfer phenomena, detailed reaction schemes and fuel injection add to the complexity of the turbulence modeling. Describing the physics of spray, as a vaporizing two-phase flow with varying spatial and temporal scales have been very challenging [26, 27]. Thus, the precise sub-models for atomization, drop drag, vaporization, break-up, coalescence, turbulence dispersion and spray-wall interaction have been developed. Abraham et al. [28] introduced three models to compute the fuel vapor concentration in the vapor-phase of a diesel spray and compared the results with measured concentrations. Their results showed that the computed vapor fraction along the axial centerline, during the transient development of the spray is lower than the measured values. In addition, Lagrangian-drop Eulerian-fluid spray model has better agreement with experimental data in the quasi-steady state region.

The Eulerian-Lagrangian approach has been used and its accuracy has been improved for spray diesel simulations by Lucchini et al. [5]. They tried to deal with interaction between turbulence and spray, by limiting the turbulence length scale to the nozzle diameter where the liquid jet exists. Their results showed that fuel vapor penetration and distribution have insignificant dependency on the grid size in comparison to the liquid phase and in general, the grid size that is 2-10 times greater than the orifice size was shown adequate.

For the purpose of the current study, the idea of scaled sprays is investigated, (i.e. the injector's orifice cross sectional area, A_i , and injected mass, m_i , are scaled with the same scaling factor) and various jet configurations are considered, see Figure 1. Changing the injected mass and cross-sectional area results in the change of mass flow rate with the scaling factor, n^2 . With this method, injection pressure stays constant and injection momentum varies. In addition, since manufacturing very small injector nozzle sizes are not feasible, it is interesting to investigate the effect of various sizes with computational fluid dynamics (CFD), before putting effort in the experiment. The main focus of this investigation is to improve/optimize the heat release rate and achieve a faster and more complete combustion compared to the initial case of spray-A. For this reason, the spray-A configuration along with the boundary and initial conditions of the constant flow test rig experiments [15] is considered for modeling validation. After that, three configurations are tested numerically, scaled sprays, parallel sprays, and colliding sprays as illustrated in Figure 1 and their effectiveness in terms of heat release and burn rate improvement is investigated. The simulations are performed with Converge code [29] using Reynolds Averaged Navier-Stokes (RANS) for turbulence and SAGE for combustion modeling. Further details on the spray sub-models and numerical scheme is provided in Methodology section.

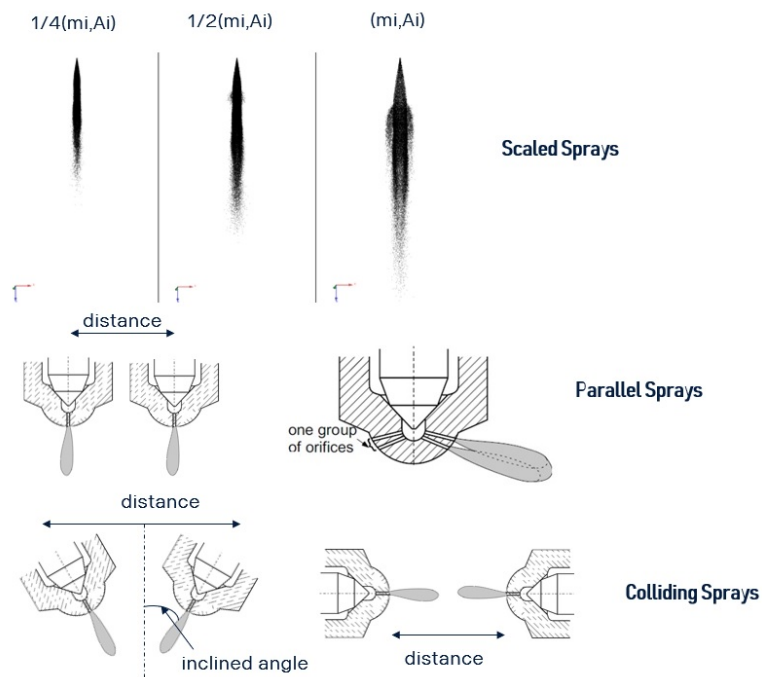


Figure 1- Schematic of various spray configurations.

Physical-Computational Model

The initial physical case considered for validation of the simulation models is spray-A for which experimental pressure, liquid penetration length, flame lift-off and high speed images are available. Experiments are performed in a constant flow combustion chamber [15] at initial pressure and temperature of 6 MPa and 900 K, respectively. Oxygen concentration is 15%, nozzle diameter is $90\ \mu\text{m}$, injected mass is $3.46\text{e}^{-3}\ \text{mg}$, injection duration is $1.5\ \text{ms}$ and n-dodecane ($\text{C}_{12}\text{H}_{26}$) is used as the fuel. Similar to the experimental setup, simulation domain is a constant volume chamber, with $0.108\ \text{m}$ length on each side and the injector is located in the middle of the top surface. With this configuration, the spray-wall interaction is highly unlikely. The computational geometry is shown in Figure 2, highlighting the injected parcels and grid refinement through two cut planes passing in the middle of the geometry.

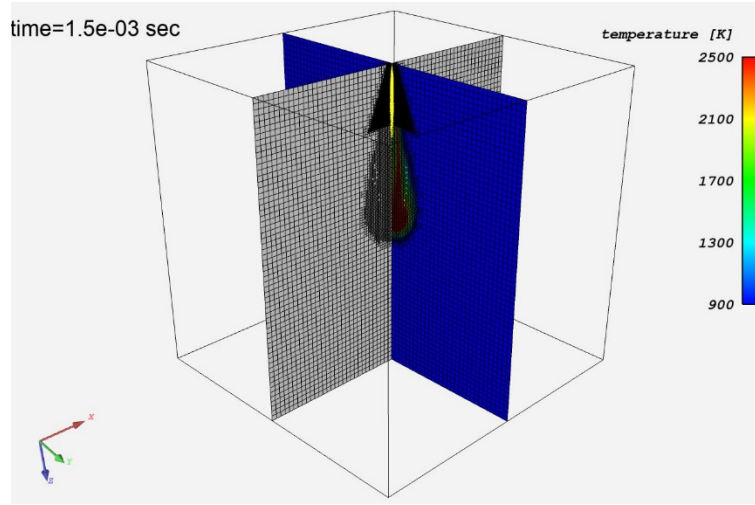


Figure 2- Computational domain of the constant volume combustion chamber, showing the location of the spray and mesh refinement.

The second step after validation of the spray settings and models is to scale the injected mass and cross-sectional area in order to optimize the heat release rate. In the rest of simulations of the present work, no EGR is included (oxygen concentration is 23%). The simulation matrix for this step is provided in Table 1.

Table 1- Simulation matrix for scaling step.

	Mass	Cross Sectional Area
Single injector	m_i	A_i
half	$1/2m_i$	$1/2A_i$
quarter	$1/4m_i$	$1/4A_i$
One-eight	$1/8m_i$	$1/8A_i$
double	$2m_i$	$2A_i$
quadruple	$4m_i$	$4A_i$
otha	$8m_i$	$8A_i$

The third step of the current study is to simulate the dual injectors in different configurations (i.e. parallel injectors, non-coaxial colliding and coaxial colliding) as is shown in Figure 3. The half size injector ($1/2m_i$, $1/2A_i$) from the first step, is chosen as the nominal injector for this step. The simulation matrix is summarized in Table 2.

Table 2- Simulation matrix for colliding sprays.

Configurations	Sprays' axis distance (mm)	Sprays' axis angle	Cross Sectional Area and injected mass
Parallel	0.254	N/A	$1/2m_i$, $1/2A_i$
	3		
	6		
	9		
	12		
	30		
Non-coaxial, colliding	12	30	
		45	
		50	
		60	
		70	
Coaxial colliding	12	N/A	
	18		

The schematic of spray configurations is shown in Figure 3.

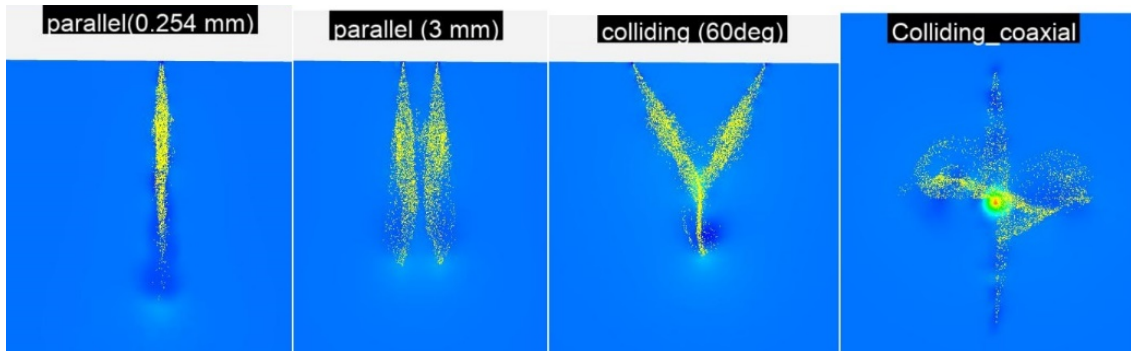


Figure 3- Schematic of some examples of spray configurations based on Table 2.

Methodology

Fuel spray and combustion simulation is performed with Converge [29] using Eulerian-Lagrangian approach for the liquid phase and RNG k- ϵ RANS model for the gas phase. A second order finite volume scheme is used for spatial discretization using modified Pressure Implicit with Splitting Operator (PISO) algorithm to solve for the transport equations. A cut-cell cartesian method is used in Converge that generates the computational grid during the run time [30-32]. To further refine the grid in critical locations inside the domain (i.e. around the injector and alongside the injection trajectory), a fixed embedding is used which refines the grid temporarily and locally. In addition, an adaptive mesh refinement (AMR) is in place that increase the refinement in areas with high gradients of temperature and velocity. The base grid

size is 1.8 mm and refinement scales are 2 and 3 for AMR and embedding, respectively. The grid size after embedding refinement is equal to $\frac{\text{base grid size}}{2^{\text{refinement scale}}}$. This results in cell size of 0.225 mm at the orifice exit and along the injector(s) trajectory.

As mentioned earlier, the spray-A was used for validation of the numerical method and available models. One criterion of adequacy of the grid refinement, hence, the injected parcel numbers, is considered to be the pressure data from ECN. Here, the results of three RANS simulation cases (spray-A) are compared with the experimental data from Sandia and ifpn [15] and the Large Eddy Simulation (LES) results by Gong et al. [4].

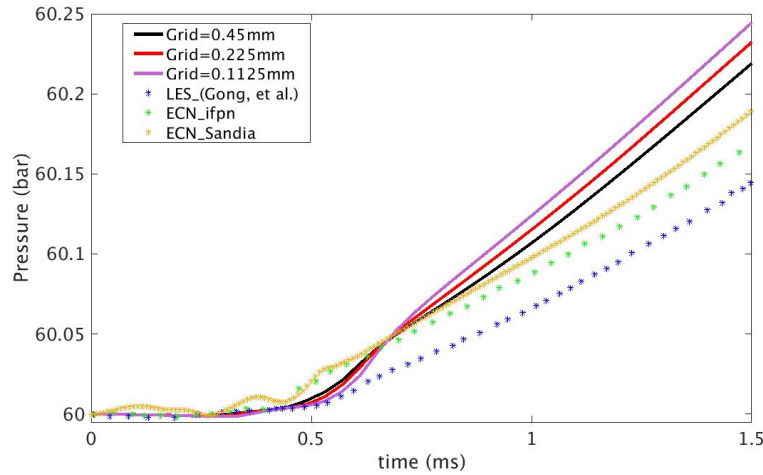


Figure 4- Pressure data, a comparison between RANS, LES [4] and experimental data.

The injected number of parcels has a direct dependency on the grid size at the nozzle orifice and nozzle diameter [29]. If the number of injected parcels are too small, the parcel size is large, and the whole volume of the nearest cells to the injector is occupied by large liquid fuel parcels. In other words, the cell is choked with liquid fuel and no air, hence, the evaporation and ignition is delayed. Note that the parcels are representative of a group of droplets (approximately 100-1000 in number) with similar characteristics such as diameter, velocity, temperature, etc...[30, 33]. Based on the results from Figure 4, the start of ignition is not accurately predicted with neither of the two simulation approaches. In addition, neither LES, nor RANS can provide an accurate burn rate, hence, mixing controlled combustion and pressure rise. Considering that some inaccuracies and uncertainties exist in the experimental measurements [7], the simulations of the current study is performed with the fine grid size of 0.225 mm and approximately $5e^5$ number of injected parcels. The very limited grid dependency of vapor penetration has been shown by Lucchini et. al [5]. They have shown that fuel vapor penetration and distribution have less significant dependency on the grid size, while the liquid phase has more dependency. While the main focus of this research is on the mixing controlled combustion and burn rate and not the liquid phase effect on the ignition delay and evaporation (the phenomena concerning near nozzle simulations), the above-mentioned grid suggestion is shown adequate.

The time steps are chosen dynamically based on the CFL (Courant-Friedrichs-Lewy) limiting criteria for diffusion, velocity and speed of sound. The combustion chemistry is solved using SAGE solver, that treats every cell as a well stirred zero-dimensional reactor [9, 34]. With SAGE, the rate for each elementary reaction in the chemical reaction mechanism is calculated

while the CFD solver solves the transport equations. A reaction mechanism is used for n-dodecane with 163 species and 887 reactions.

The most challenging part of the engine type simulations is the spray simulation and settings. Since the spray experiences various regimes upon leaving the orifice exit, such as Rayleigh, first and second wind-induced break-up and atomization regimes [23, 35], accurate simulation of the break-up, parcel collisions and coalescence is of high importance. Initial break-up in diesel jet fuels normally occurs in atomization zone. Turbulence and collapse of cavitating bubbles are known as the initiatives of the velocity fluctuations in the near nozzle flow field, that destabilize the existing liquid jet [36]. For the purpose of the current study, Kelvin-Helmholtz, Rayleigh-Taylor (KH-RT) break-up model is used and the effect of break-up time constant is investigated. The KH break-up model is based on the liquid jet stability analysis described by Reitz and Bracco [37] for a cylindrical, viscous liquid jet of radius r_0 issuing from a circular orifice at a velocity U into a stagnant, incompressible inviscid gas of density ρ_g . Based on Equation 1, Ω_{KH} and Λ_{KH} are the maximum growth rate of instabilities and the corresponding wavelength, respectively.

$$\tau_{KH} = \frac{3.726C_2r_p}{\Lambda_{KH}\Omega_{KH}}. \quad (\text{Eq.1})$$

On the other hand, the unstable RT waves are thought to occur due to the rapid deceleration of the drops from the magnitude of the drag force [38]. Converge allows to run these models concurrently for which a so-called KH-RT break-up length L_b is used. According to this model, only KH instabilities are responsible for drop break-up inside of the characteristic break-up distance, L_b , and both KH and RT mechanisms are activated beyond this length. Further information can be found in [29]. For the purpose of the current study, the KH break up time constant, (C_2 in Eq. 1) is investigated and pressure results are shown in Figure 5. Note that the chosen time constant is not adjusted for the parameter sweeps in the ECN data base as it has been chosen based on the nominal settings. Consequently, the C_2 parameter is not generic, although reasonably accurate for the current case of study. For a bigger time constant, ignition delay increases and the start of pressure rise does not agree with the experiments. As a result, the $C_2=16$ is chosen for current simulations. It should be noted that this model is mainly responsible for the initial break up of the injected parcels, and that is the reason most of the curves shown in Figure 5 are agreeing in the initial stage of the pressure rise. To achieve a better agreement, other parameters must be taken into account, for instance, turbulence model parameters, contraction coefficient of the orifice and so on. For evaporation, collision and wall interaction, Frossling [39], NTC [40] and rebound/slide wall interaction [41, 42] models are used.

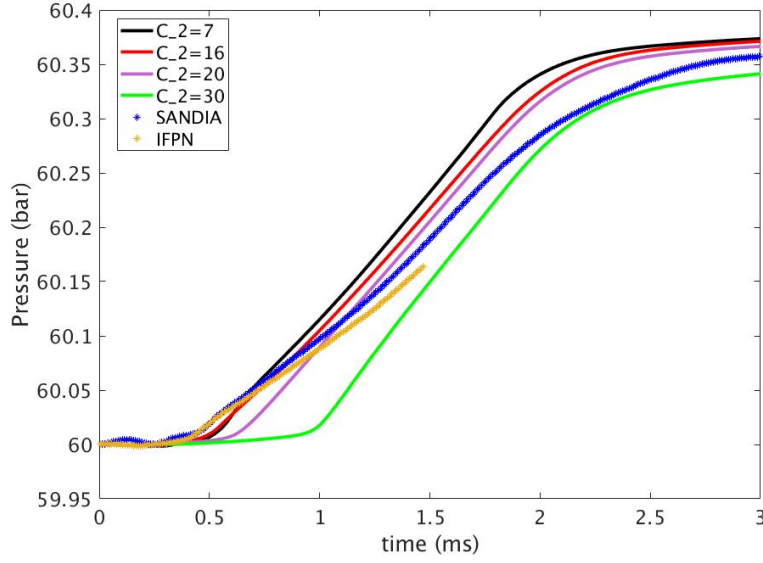


Figure 5- Pressure comparison for simulations with various break-up time constant and experimental measurements from ECN [15].

Results

Spray-A validation

As mentioned earlier, in the first step, simulation's pressure data is compared to the experimental measurements for spray-A. Results are shown in figure 4. Due to the uncertainties in experimental procedure and measurements [7], as well as the numerical errors in RANS simulations, achieving the accurate burn rate is not feasible. However, the error in peak pressure is below 0.02%. In addition, the start of ignition is in good agreement with the experimental data, showing the adequacy of reaction mechanism. It is worth mentioning that the reference LES analysis [4] provided in Figures 4 and 5, has slightly different settings compared to the current simulations, as it was performed with RIF combustion model [43] and the simulation was performed in open foam [44]. The smallest grid cell size for LES simulations is similar to the current RANS simulations (0.225 mm), however, the number of injected parcels was different than the corresponding RANS data.

To calculate the heat release rate for the combustion of an internal combustion engine, first law of the thermodynamics is applied to the confined volume inside the cylinder. With this description, thermal energy (dQ_n/dt), work ($-PdV/dt$), internal energy (dU/dt) and sensible enthalpy of the fuel ($\dot{m}_f h_{s,f}^*$) are included,

$$\frac{dQ_n}{dt} = P \frac{dV}{dt} - \dot{m}_f h_{s,f}^* + \frac{dU}{dt}. \quad (\text{Eq.2})$$

Since the injected fuel temperature is similar to the standard temperature, the sensible enthalpy of the fuel is negligible. Having the assumption of the ideal gas with homogeneous temperature and pressure, the apparent net heat release rate yields to,

$$\frac{dQ_n}{dt} = \frac{\gamma}{\gamma-1} P \frac{dV}{dt} + \frac{1}{\gamma-1} V \frac{dP}{dt}. \quad (\text{Eq.3})$$

In the constant volume spray chamber, the volume change is zero, and apparent rate of heat release is merely a function of pressure difference.

The heat release rate (HRR) results for variation of KH break-up time constant is shown in Figure 6. As it was also shown by pressure data (see Figure 5) the ignition delay increases with higher break-up time constant and the appropriate number for the current spray is found to be 16. In addition, to reach the correct injection pressure, the nozzle discharge coefficient is set to 0.89. Regardless of the discrepancies in RANS approach, results showed acceptable agreement with experiments after tuning the break-up time constant, discharge coefficient, nozzle cone angle (set to 25) and the grid study.

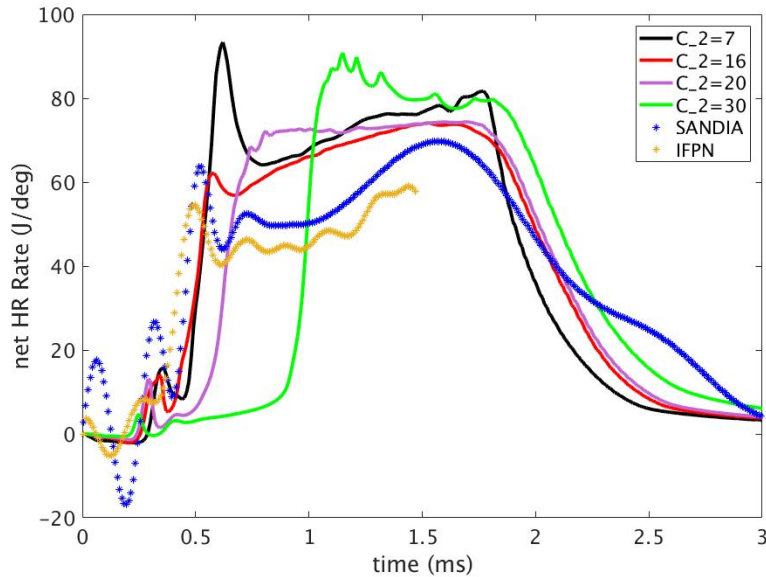


Figure 6- Heat release rate comparison for simulations with various break-up time constant and experimental measurements from ECN [15].

Scaled Sprays

In this section, the concept of the scaled sprays is investigated. Figure 7 demonstrates the HRR results for the simulation cases provided in Table 1. As expected, the pre combustion peak, ignition peak and the combustion duration reduce with the smallest spray size (i.e. lower amount of fuel and smaller orifice size (scaling factor < 1.0)), and in the same manner, they increase with larger orifices and higher increasing amount of fuel (scaling factor > 1.0). However, it is interesting to compare spray-A results with the scaled sprays while the amount of injected mass is constant. For this reason, the HRR plots are inversely scaled (i.e. the HRR is multiplied by the inverse of scaling factor for every individual simulation) to preserve the amount of injected mass. In other words, multiplying the HRR data of the second case in Table 1 (half) with the scaling factor of 2, is as if the two half size injectors exist in the domain.

Figure 8 shows that using smaller sprays, such as two half size injectors or four of quarter size injectors can improve the burn rate and decrease the combustion duration significantly. While the results of larger orifices are not encouraging as they prolong the burn duration comparing to the spray-A.

To be confident about the complete combustion, CO mass concentration is scaled and compared to spray-A. Results are shown in Figure 9. As it is demonstrated, with smaller orifices, the amount of unburned CO is higher than the original size spray-A, (approximately twice) that is an indication of incomplete combustion. However, the achievement in fast combustion (HRR

analysis) is more prominent which makes the higher CO mass concentration of less importance, although not disregarded completely.

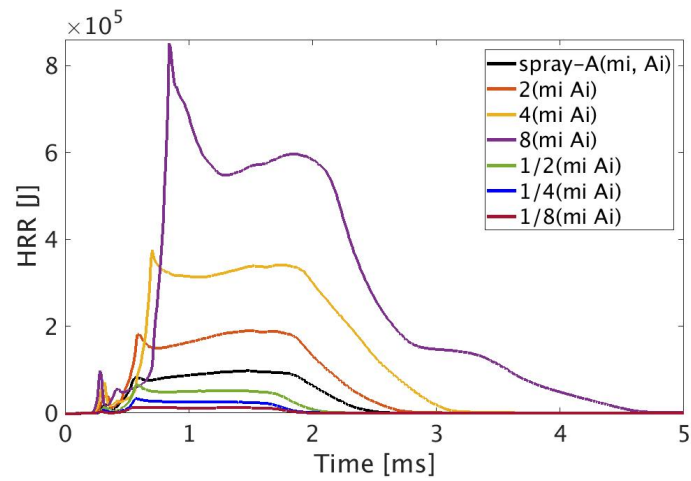


Figure 7- Heat release rate comparison for scaled sprays and spray-A.

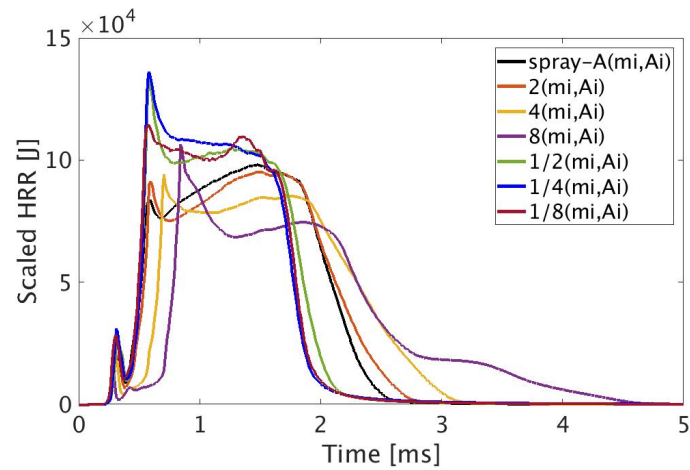


Figure 8- Inversely scaled heat release rates for scaled sprays.

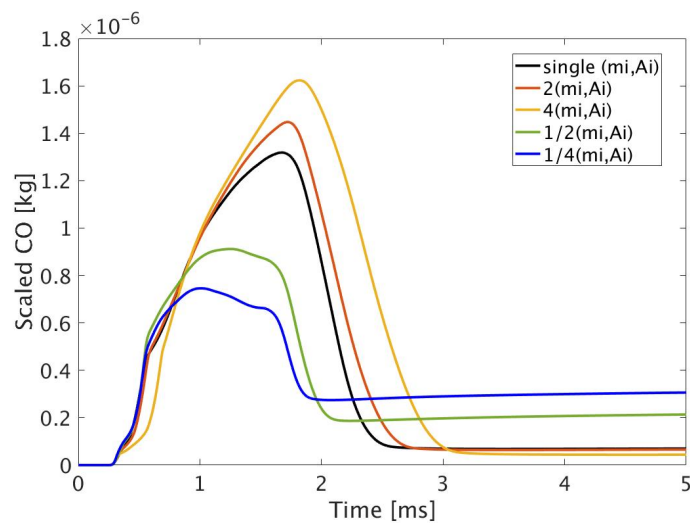
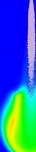
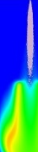
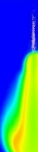
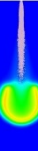
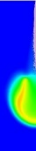
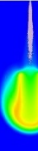
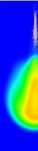
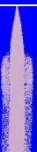
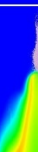


Figure 9- Inversely scaled CO mass concentration for scaled sprays.

Spray evolution for the spray-A and two scaled cases is shown by temperature contours in Table 3. Note that the initial steps of the liquid jet penetration have been enlarged to make the spray droplets more visible. Right after the start of injection (less than 0.5 ms after SOI), the spray penetration reaches the local maximum, that is approximately 18, 13 and 26 mm, for spray-A, half size orifice and double size orifice, respectively. The ignition starts afterward, mainly at the tip of the liquid jet and grows both axially and radially. Spray penetration and plume growth rate do not correspond linearly to the spray size and injected mass ratio, however, they are increased with the increase of injector size and injected mass, as expected.

Table 3- Evolution of the scaled sprays, shown by temperature contours.

Time (ms)	0.05	0.2	0.45	0.7	1.0	1.5	2.0
Spray-A (m_i, A_i)							
1/2 (m_i, A_i)							
2 (m_i, A_i)							

Colliding Sprays

Above-mentioned results proved the feasibility of burn rate improvement with smaller sprays. To find the optimum configuration for these smaller sprays, three scenarios are investigated here, locating the two half size sprays in parallel, colliding (with an inclined angle) and coaxial colliding configurations, respectively. See figure 1. In the parallel configuration, the distance between the two sprays are varying from 0.254 mm to 30 mm. The smallest distance is inspired by the investigation of Gao et. al [22] on group-hole nozzle, that is an approach to facilitate atomization and evaporation for direct injection diesel engines. Their results showed the potential of better fuel atomization and reducing particulate emission formed in D.I. diesel engines [22-25], while it adversely affected the spray spatial distribution. In Figure 10, HRR for parallel configuration sprays are compared with original spray-A case.

As is shown in Figure 10, when the two half size sprays are located very close (0.254 mm apart), such as the group-hole nozzle concept, no burn rate or HRR improvement is achieved while it has a longer delay in pre combustion peak (see the first peak in HRR plots). In parallel configuration, comparing the cases with 3 to 30 mm in distance between the sprays, the simulation case with 3 mm distance has longer burn rate compared to spray-A, hence, the sprays interaction is not beneficial. The longer combustion duration could be due to the less available fresh charge, and lower air entrainment between the two sprays. However, when the distance between the two sprays is optimal, (i.e. 12 mm), the air entrainment between the sprays is sufficient and each spray has adequate radial space to propagate individually. As a result, when

the plumes are grown, (approximately after the lift-off length), they interact and enhance one another. Despite the closely located parallel sprays in which the liquid spray interaction is dominant, the plume interaction is the reason of HRR improvement.

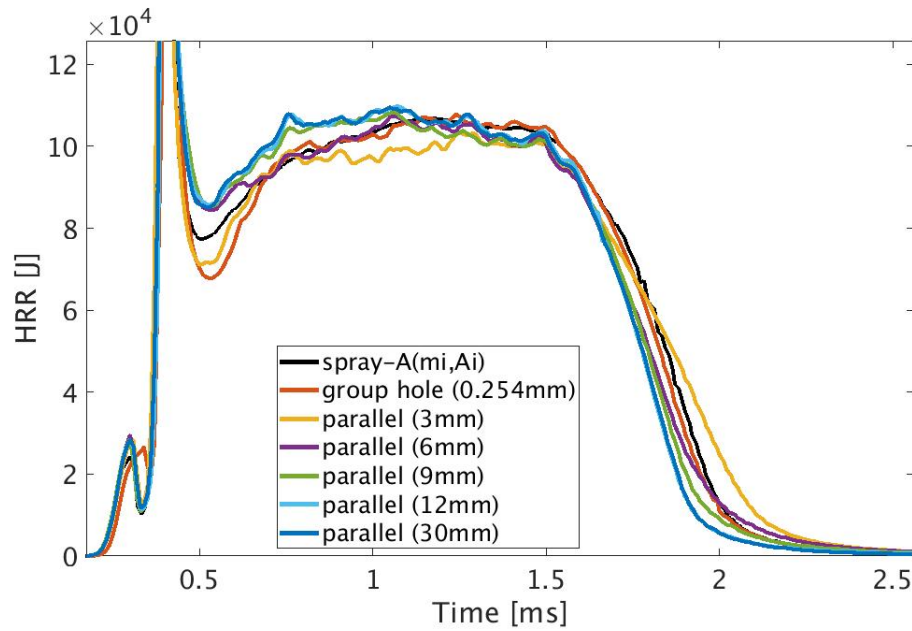


Figure 10- Heat release rate comparison for parallel sprays.

In Figure 11, accumulated heat release (HR), plots for group-hole case (0.254 mm) and parallel cases of 3 and 12 mm are compared to the spray-A. To make the differences clearly visible, the other parallel cases are not shown here. The apparent heat release is zero before the start of ignition and reaches a constant value, close to the fuel energy [30, 45] at the end of combustion. As is shown in Figure 11, and expected from the literature [22], the group-hole orifices have higher accumulated heat release, which is an indication of a complete combustion. This leads to lower exhaust emission and unburned hydrocarbons as well as particulate matters. On the other hand, when the sprays are well apart and act as two individual sprays, accumulated heat release reaches a lower value, indicating an incomplete combustion. It is worth mentioning that although the heat release errors exist (compared to the heating value of n-dodecane), they are negligible (0.42% for spray-A, 0.23% for group-hole orifices and 0.75% for the sprays that are 12 mm apart).

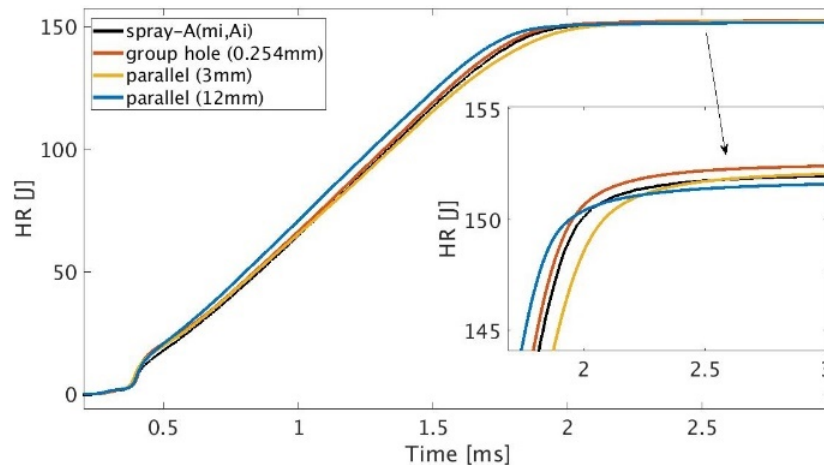


Figure 11- Accumulated heat release comparison for parallel sprays.

The next configuration that is investigated in the present study is the non-coaxial colliding sprays, for which an inclined angle is considered while the spray distance is maintained constant at 12 mm. As summarized in Table 2, 6 simulations are performed, and HRR results are compared to the spray-A and the parallel configuration sprays (12 mm distance). As is shown in Figure 12, ignition delay is shorter than the original spray-A and ignition starts quicker for cases with the inclined angle below 60. The burn duration is longer for these cases as well. To make it more clearly visible, only few cases are enlarged in the span of 1.5-3 msec. A faster combustion and shorter heat release duration is achieved with colliding sprays of the inclination of 60. Results for this configuration is in good agreement with the parallel sprays of 12 mm distance.

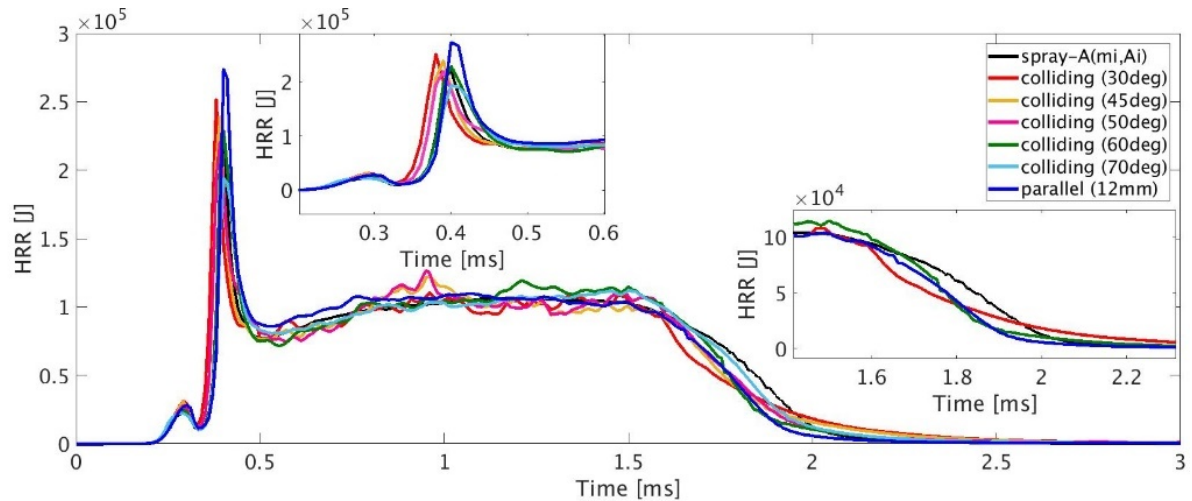


Figure 12- Heat release rate comparison for non-coaxial colliding sprays.

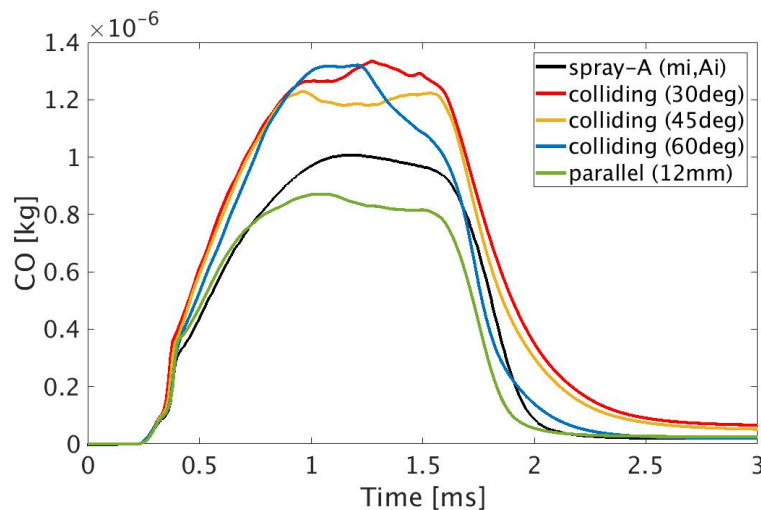


Figure 13- Carbon monoxide mass concentration comparison for non-coaxial colliding sprays.

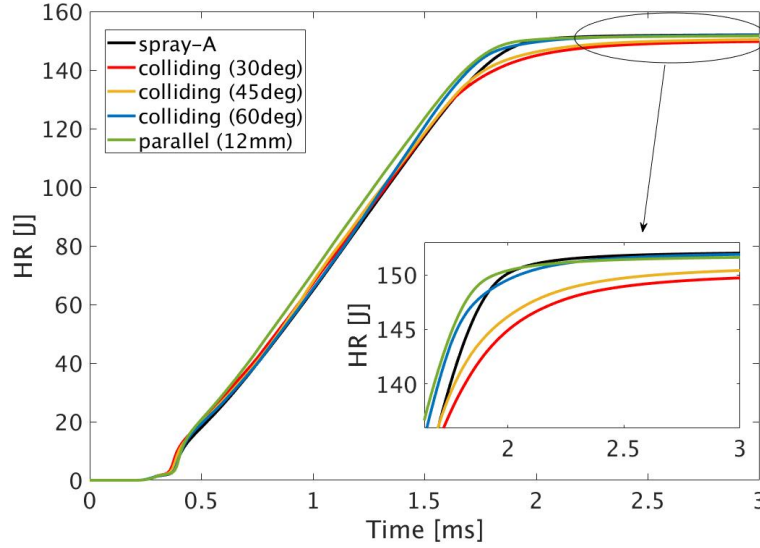


Figure 14- Accumulated heat release comparison for non-coaxial colliding sprays.

Figures 13 and 14 shows that when the inclined angle is below 60, more unburned carbon monoxides remain in the domain (not all of the fuel energy is released), while in the case with inclined angle equal to 60, the spray and plume interactions enhance the combustion. The burn duration enhancement can also be shown with T90, as is shown in Figure 15. T10 and T90 are defined as the needed time span to obtain 10% and 90% of the total released energy of the fuel, respectively. It is clear that the 60 deg configuration is beneficial in both the pre combustion stage (T10) and later stage of combustion (T90) while the smaller inclinations are only beneficial in earlier stages of combustion. Considering the advantages of a more complete combustion, it is reasonable to use two smaller orifices, in either the parallel configuration (12 mm apart) or colliding (with the inclination angle of 60 deg.).

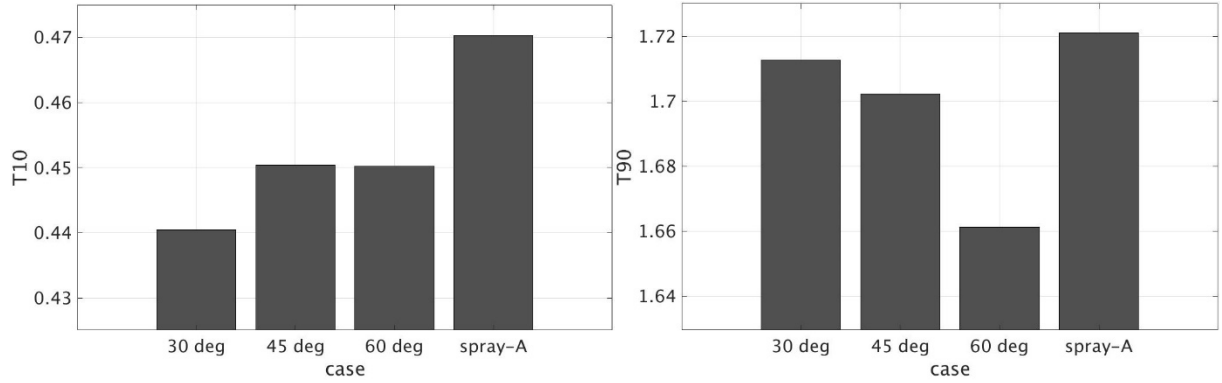
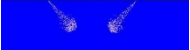
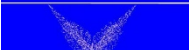
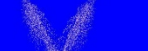


Figure 15- T10 and T90 results for colliding sprays.

Table 4 summarizes the spray formation, liquid droplet interaction, start of ignition and flame propagation for the two cases with 30 and 60 inclinations, respectively. Due to the later collision between the two sprays, the case with 60 degrees inclination has longer vapor penetration length and higher turbulent kinetic energy (TKE) especially at the end of injection event. This leads to a higher air entrainment in each spray, hence, stronger and more effective ignition and heat release resulting in lower unburned hydrocarbons. Table 4 shows that there is an asymmetry in the flame formation after the spray collision. One main reason for this asymmetric behavior could be the random movement of parcels and since the temperature is favorable, the ignition

spots and flame propagation are asymmetric. Needless to say that numerical uncertainties and errors can play a role specially when reacting flows are simulated.

Table 4- Evolution of sprays, shown by temperature contours.

Time (ms)	Incline (degree)	
	30	60
0.05		
0.1		
0.15		
0.35		
0.4		
0.7		
1.5		

The second configuration for colliding sprays is the coaxial collision for which two simulations are performed with the distance of 12 and 18 *mm* between the sprays. Similar to the previous simulation cases, all the numerical settings are preserved and only the spray configuration is changed. Besides, the focus is on the heat release and burn rate enhancement. As is shown in Figures 16 and 17, a comparison is made between the two coaxial colliding sprays, the results for non-coaxial spray with 60 degrees inclination and spray-A.

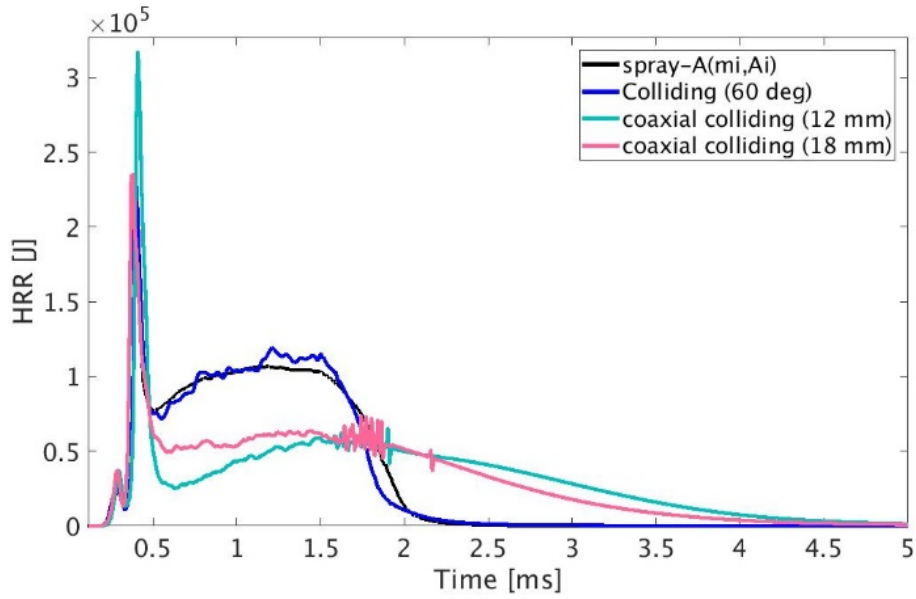


Figure 16- Heat release rate comparison for coaxial colliding sprays.

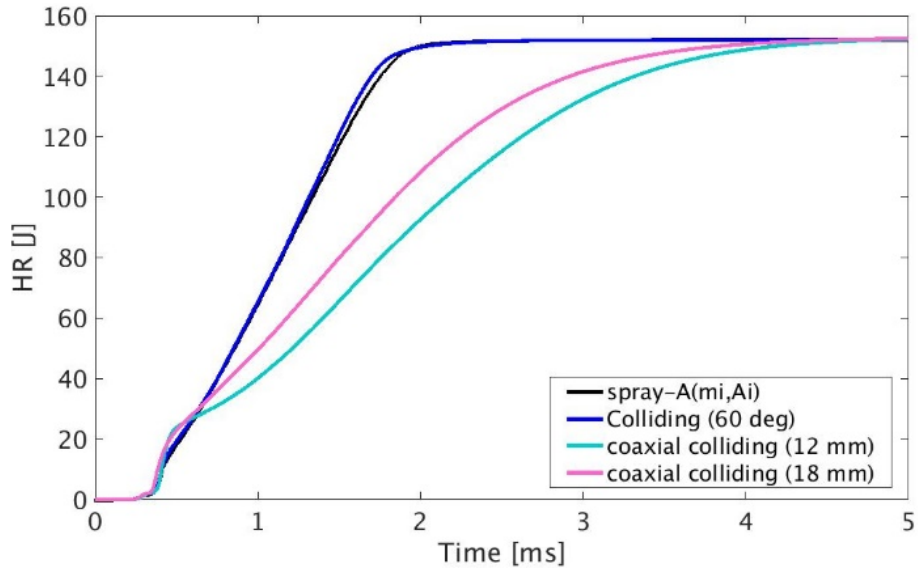
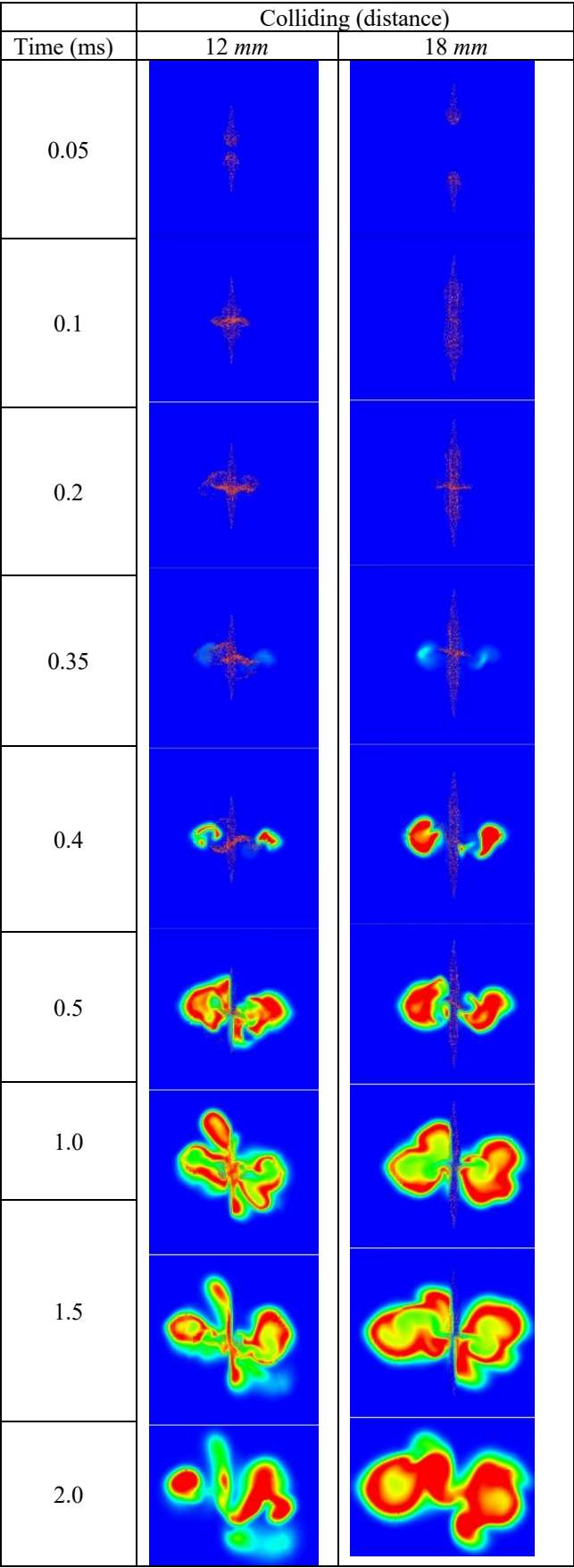


Figure 17- Heat release comparison for coaxial colliding sprays.

The pre combustion peak is higher for the two coaxial cases as they have higher air entrainment rate as a reason of being imposed to more available air from radial direction. The two sprays act as two separate sprays and do not enhance one another's ignition even after collision. The complete combustion process is prolonged, although a more complete combustion is achieved. The spray collision and ignition processes are shown through temperature contours in Table 5.

The collision starts right after the start of injection and forces the droplets to spread radially, hence the ignition starts in a radial ring at the collision plane, outside of the collision zone. It should be noted that the cut planes in Table 5 can only be the representative of a section of this ring-shape plume.

Table 5- Evolution of the coaxial colliding sprays, shown by temperature contours.



Conclusions

A set of numerical simulations is performed in order to find a proper configuration by which the heat release and burn rates can be optimized for a diesel spray. The spray-A which is a diesel spray from ECN [15] data base, has been used as the reference case for validation of current simulations. The numerical models, constant parameters and grid resolution is adjusted in a way to achieve similar pressure rise as for the experimental data from ECN and ifpn [15]. Initially, the idea of scaling the diesel jet is investigated in which the injected mass and cross-sectional area of the injector is scaled with similar scaling factor while the injection pressure is remained constant. It was found that using a larger injector (scaling factor > 1.0) leads to a longer spray penetration and ignition delay, longer burn duration but a more complete combustion. On the other hand, using a smaller orifice improves the burn duration and reduces the heat release, while it results in a slightly higher unburned hydrocarbons and hence, incomplete combustion. Using this information, it is reasonable to take multiple smaller orifices (i.e. two half size ($1/2 (m_i, A_i)$) or four quarter size ($1/4 (m_i, A_i)$) injectors) in place of one single injector, in order to improve the burn rate and tune the configuration to possibly achieve a complete combustion. In order to reduce the amount of unburned hydrocarbons, the configuration of these multiple injectors can be optimized. In the current investigation, three configurations are considered, parallel, non-coaxial colliding and co-axial colliding sprays for which the distance between the sprays and the inclination of the sprays are optimized.

In the first scenario in which the two sprays are parallel, if the distance in between is very small, similar to the group-hole sprays [22] the burn and heat release rates are not improved, however, a more complete combustion is achieved and the unburned hydrocarbons are less than the original spray-A case. For the cases that was numerically investigated here, the distance of 12 *mm* between the two sprays are found to be the best performing case in terms of HRR with negligible increase in unburned hydrocarbons. It was found that if the two sprays are very close, air entrainment in between the sprays is limited. In addition, the initial liquid spray momentum is reduced due to the spray interaction and transfer to the entrained air. This leads to a longer combustion duration. On the other hand, if the distance is adequate, the momentum of the two sprays is preserved and each individual spray will be formed with atomization and initial break-up without the interfere of another spray. Once the plumes are grown, they interact, and enhance the heat release rate.

In the second scenario, in which the sprays are colliding along the streamwise direction with an inclination angle, the distance between the two sprays is kept constant at 12 *mm*. Here, the inclination angle is varying between 30 to 70. It is found that the best performing angle to reach shorter HRR is 60 degrees. Once the angle is below 60, the two sprays interact at their earlier stage of penetration, larger parcels collide, and the spray momentum is exhausted. On the other hand, when the smaller parcels are colliding at a later stage of spray formation, they break into yet smaller parcels and facilitates evaporation and combustion. If the inclination is below 60 degrees, the pre combustion peak is advanced and ignition delay is shorter.

The last configuration considered in the present study is the coaxial collision of two small sprays ($1/2(m_i, A_i)$) with the distance of 12 and 18 *mm* in between. After the spray tip collision, the parcels are spreading radially where they evaporate and ignition starts on a radial region around the center line (similar to a ring). With this configuration, if the two sprays are close, they interfere one another's formation and confine the spray momentum, however, if the

distance is enough, the spray formation and secondary-breakup take place with no external interfere, and the spray interaction appears between the smaller parcels, resulting in a shorter burn duration. In any case, the coaxial collision prolongs the combustion process and does not improve the HRR. It should be noted that the underlying results may not hold for other sprays from ECN [15] data base and to be able to pain a complete picture of the influence of orifice size, similar simulations and hence analysis for other sprays are required.

Acknowledgement

This research is performed at Scania CV AB. The authors greatly appreciate the High Performance Computing Center (HPCC) at Scania for providing the computational resources of this research.

References

1. Liu, K. and D.C. Haworth, *Development and Assessment of POD for Analysis of Turbulent Flow in Piston Engines*. 2011, SAE International.
2. Kastengren, A.L., et al., *Engine combustion network (ECN): measurements of nozzle geometry and hydraulic behavior*. Atomization and Sprays, 2012. **22**(12): p. 1011-1052.
3. Bardi, M., et al., *Engine combustion network: comparison of spray development, vaporization, and combustion in different combustion vessels*. Atomization and Sprays, 2012. **22**(10).
4. Gong, C., M. Jangi, and X.-S. Bai, *Large eddy simulation of n-dodecane spray combustion in a high pressure combustion vessel*. Applied energy, 2014. **136**: p. 373-381.
5. Lucchini, T., G. D'Errico, and D. Ettorre, *Numerical investigation of the spray-mesh-turbulence interactions for high-pressure, evaporating sprays at engine conditions*. International Journal of Heat and Fluid Flow, 2011. **32**(1): p. 285-297.
6. Meijer, M., et al., *Engine Combustion Network (ECN): Characterization and comparison of boundary conditions for different combustion vessels*. Atomization and Sprays, 2012. **22**(9).
7. Pei, Y., et al., *Engine Combustion Network (ECN): Global sensitivity analysis of Spray A for different combustion vessels*. Combustion and Flame, 2015. **162**(6): p. 2337-2347.
8. Pickett, L.M., S. Kook, and T.C. Williams, *Visualization of Diesel Spray Penetration, Cool-Flame, Ignition, High-Temperature Combustion, and Soot Formation Using High-Speed Imaging*. 2009.
9. Senecal, P.K., et al., *Multi-Dimensional Modeling of Direct-Injection Diesel Spray Liquid Length and Flame Lift-off Length using CFD and Parallel Detailed Chemistry*. 2003, SAE International.
10. Duva, B.C., L. Chance, and E. Toulson, *Laminar Flame Speeds of Premixed Iso-Octane/Air Flames at High Temperatures with CO₂ Dilution*. 2019, SAE International.
11. Allen, C., *Advanced rapid compression machine test methods and surrogate fuel modeling for bio-derived jet and diesel fuel autoignition*. 2012.
12. Gentz, G., M. Gholamisheeri, and E. Toulson, *A study of a turbulent jet ignition system fueled with iso-octane: Pressure trace analysis and combustion visualization*. Applied Energy, 2017. **189**: p. 385-394.
13. Gentz, G., et al., *A study of the influence of orifice diameter on a turbulent jet ignition system through combustion visualization and performance characterization in a rapid compression machine*. Applied Thermal Engineering, 2015. **81**: p. 399-411.
14. Mittal, G. and C.-J. Sung, *Aerodynamics inside a rapid compression machine*. Combustion and Flame, 2006. **145**(1-2): p. 160-180.

15. *Engine Combustion Network*. 2019 [cited 2019 07/29/2019]; Available from: <https://ecn.sandia.gov/>.
16. Pickett, L.M., et al., *Relationship Between Diesel Fuel Spray Vapor Penetration/Dispersion and Local Fuel Mixture Fraction*. SAE International Journal of Engines, 2011. **4**(1): p. 764-799.
17. Payri, R., et al., *Fuel temperature influence on diesel sprays in inert and reacting conditions*. Applied Thermal Engineering, 2012. **35**: p. 185-195.
18. Benajes, J., et al., *Instantaneous pressure measurement in pulsating high temperature internal flow in ducts*. Applied Thermal Engineering, 2013. **61**(2): p. 48-54.
19. Luo, Z., et al., *Development and validation of an n-dodecane skeletal mechanism for spray combustion applications*. Combustion theory and modelling, 2014. **18**(2): p. 187-203.
20. D'Errico, G., et al., *Combustion Modeling in Heavy Duty Diesel Engines Using Detailed Chemistry and Turbulence-Chemistry Interaction*. 2015, SAE International.
21. Bhattacharjee, S. and D.C. Haworth, *Simulations of transient n-heptane and n-dodecane spray flames under engine-relevant conditions using a transported PDF method*. Combustion and Flame, 2013. **160**(10): p. 2083-2102.
22. Jian, G., Y. MATSUMOTO, and K. Nishida, *Effects of group-hole nozzle specifications on fuel atomization and evaporation of direct injection diesel sprays*. 2007, SAE Technical Paper.
23. Heywood, J.B., *Internal combustion engine fundamentals*. 1988, New York, N.Y.: McGraw-Hill.
24. Hiroyasu, H. and M. Arai, *Structures of Fuel Sprays in Diesel Engines*. 1990, SAE International.
25. Smallwood, G.J. and O.L. Gulder, *VIEWS ON THE STRUCTURE OF TRANSIENT DIESEL SPRAYS*. 2000. **10**(3-5): p. 355-386.
26. Novella, R., et al., *The role of detailed chemical kinetics on CFD diesel spray ignition and combustion modelling*. Mathematical and Computer Modelling, 2011. **54**(7): p. 1706-1719.
27. Desantes, J.M., et al., *Influence of cavitation phenomenon on primary break-up and spray behavior at stationary conditions*. Fuel, 2010. **89**(10): p. 3033-3041.
28. Pickett, L.M. and J.P. Abraham, *COMPUTED AND MEASURED FUEL VAPOR DISTRIBUTION IN A DIESEL SPRAY*. 2010. **20**(3): p. 241-250.
29. Richards, K., P. Senecal, and E. Pomraning, *CONVERGE (Version 2.2)*. Converge Science Inc.: Middleton, WI., 2014.
30. Gholamisheeri, M., S. Givler, and E. Toulson, *RANS and LES of a Turbulent Jet Ignition System Fueled with Iso-Octane*. Flow, Turbulence and Combustion, 2019.
31. Deardorff, J.W., *A numerical study of three-dimensional turbulent channel flow at large Reynolds numbers*. Journal of Fluid Mechanics, 1970. **41**(02): p. 453-480.
32. Senecal, P.K., et al., *A New Parallel Cut-Cell Cartesian CFD Code for Rapid Grid Generation Applied to In-Cylinder Diesel Engine Simulations*. 2007, SAE International.
33. Mahesh, K., et al., *Progress toward large-eddy simulation of turbulent reacting and non-reacting flows in complex geometries*.
34. Pomraning, E., K. Richards, and P.K. Senecal, *Modeling Turbulent Combustion Using a RANS Model, Detailed Chemistry, and Adaptive Mesh Refinement*. 2014, SAE International.
35. *DieselNet*. [cited 2019; Available from: <https://www.dieselnet.com/>].
36. Gorokhovski, M. and M. Herrmann, *Modeling primary atomization*. Annu. Rev. Fluid Mech., 2008. **40**: p. 343-366.

37. Bracco, R.D.R.a.F.V., *Mechanisms of Breakup of Round Liquid Jets*, " *Encyclopedia of Fluid Mechanics*. 1986, Gulf Publishing Company. p. 223-249.
38. Amsden, *KIVA-3V: A block-structured KIVA program for engines with vertical or canted valves*, r. 1997.
39. Amsden, A.A., T.D. Butler, and P.J. O'Rourke, *The KIVA-II computer program for transient multidimensional chemically reactive flows with sprays*. SAE transactions, 1987: p. 373-383.
40. Schmidt, D.P. and C. Rutland, *A new droplet collision algorithm*. Journal of Computational Physics, 2000. **164**(1): p. 62-80.
41. Naber, J. and R.D. Reitz, *Modeling engine spray/wall impingement*. SAE transactions, 1988: p. 118-140.
42. Manuel, A., et al., *A Study of Diesel Cold Starting using both Cycle Analysis and Multidimensional Calculations*. 1991, SAE International.
43. Peters, N., *Turbulent Combustion*. Measurement Science and Technology, 2001. **12**(11): p. 2022-2022.
44. *Open foam CFD*. [cited 2016; Available from: <https://www.openfoam.com/>].
45. Nguyen, H., et al., *Performance and efficiency evaluation and heat release study of a direct-injection stratified-charge rotary engine*. 1987, SAE Technical Paper.