Effect of Different Parameters on Spray Tip Penetration in a Constant Volume Combustion Chamber

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Abstract: *A comprehensive work has been carried out by performing simulations on a constant volume combustion chamber (CVCC) where a spray of liquid n-heptane is injected in a volume of compressed air maintained at a given pressure and temperature, thereby initiating combustion. The computation time is set to 2.5 ms, time step is 1 micro second and 12000 parcels are injected for each computational cycle. The geometry consists of a block filled with air with a 0.02x0.02 meter base and a length of 0.1 meter. An injector which is a single hole unit injector (hollow cone) with diameter 140 micrometer and outer cone angle of 15^o, modeled for a common rail injection system with a given fuel mass flow rate is centrally placed on the top boundary where n-heptane (C_7H_{16}) fuel spray is injected. Unit injector is also used in certain simulations. Standard k-ϵ model is used for turbulence. Open FOAM is used for simulating spray combustion behaviour. The solver used for implementation is diesel Foam. Finite volume method is used to numerically solve the Navier-Stokes equations for any 3D grid of unstructured polyhedral cells. It is observed that Reitz KHRT Break up model together with Standard evaporation model and Trajectory collision model provides the best result for spray tip penetration length (STPL). This combination is used with subsequent simulations. Also, an increase in ambient temperature from 800K to 1500K leads to a higher flame temperature, and enhancement in STPL (for an optimum value of 1000K), further increase in ambient temperature decreases STPL. Higher values for STPL are obtained for an outer cone angle of 20^o. As ambient pressure is increased, the flame temperature increases, however STPL decreases. An increase in injection pressure leads to an enhanced STPL.*

Keywords: Constant Volume Combustion; Numerical Simulation; diesel Foam; Spray Tip Penetration Length

1. INTRODUCTION

Engine combustion simulation has always been a challenging area due to its complexity and computational cost [1-3]. Due to the complex nature of spray combustion, some new experimental techniques such as shock tubes, rapid compression machines, flow reactors, and constant volume combustion chamber (CVCC) have been developed recently for experimentally measuring important parameters related to engine performance. Out of these, constant volume method has several advantages to offer over other methods such as pressure and temperature can be controlled (unlike in actual engines) and are uniform at time of injection, thermodynamic analysis is simplified due to constant volume configuration and fuel injection pressures can be varied through a high pressure injection system similar to that of typical petrol/diesel engine.

However, these set ups are expensive and sometimes dangerous due the high pressure and temperature involved. Also, it is difficult to understand the underlying physics and chemistry of the spray combustion processes from experimental results.

1.1. Spray Combustion Modelling

Spray combustion has vast industrial, automotive and aircraft applications. Once liquid fuel is injected into a combustion chamber, it undergoes atomization which causes the liquid to break up into a large number of droplets of various sizes and velocities. Depending upon the spray density and ambient conditions, some of the droplets may continue to shatter, and some may recombine in droplet collisions. Vaporization takes place during this time and the fuel vapour produced mixes with the surrounding gas and combustion of air-fuel mixture occurs. To follow the process through vaporization region, a model is needed for air motion including turbulence and the interaction of air and droplet momentum. To follow droplet motion, droplet drag coefficients and droplet vaporization models are needed. If emissions are to be predicted, models for reaction kinetics are required.

The submillimeter scales associated with spray problem have made detailed experimental measurements very difficult and hence theory and computation have led experiments in analysing complex spray systems [4].

Spray behavior, including atomization and breakup of droplets during injection process has close relationship with the performance and efficiency of the engine [5-6]. A homogenous mixture causes reduction in emission of particulate matter and improves combustion efficiency of the engine [7]. Predicting the abrupt behavior of a droplet after collision, measuring range of droplet diameter and defining the satellite droplets properties, makes experimental methods difficult to implement and hence may produce unreliable results [8].

That is why great deal of attention is currently dedicated to computer models. However, investigating the spray behavior through numerical models is itself challenging because of limited computational sources and complex underlying physics. A comprehensive overview of work done in this area is presented by Moreira et al. [6].

1.2. Spray tip penetration

The speed and extent to which fuel spray penetrates across the combustion chamber has an important influence on air utilization and fuel-air mixing rates. In some engine designs, where the walls are hot and air swirl is present, the fuel impingement on the walls is desired. However, in DI diesel combustion systems, over penetration gives impingement of liquid fuel on cool surfaces which especially with little or no air swirl lowers mixing rates and increases emissions of unburned and partially burned species while under penetration results in poor air utilization, since air on the periphery of chamber does not comes into contact with the fuel [3]. Hence in engine applications, spray tip penetration is an important piece of information that can be useful to engine designers. It may provide insight regarding drop sizes, spray angle and the physics of the spray close to the orifice and be indicative of the presence of a liquid core and the importance of collisions and coalescence.

Huang, Chen et al. [9] performed experiments using a high pressure/high temperature spray rig in terms of gas pressure (30-70 bar), gas temperature (603-770 K) and injection pressure (600-1200 bar). The main focus was on the prediction of spray tip penetration length (STPL) of fuel. Kösters and Karlsson [10] did a comprehensive numerical study of diesel fuel spray formation with OpenFOAM for different conditions of ambient pressure, temperature and injection pressures for predicting STPL using different turbulence models.

The goal of researchers in this area has been to investigate the role of effective parameters on penetration length of a spray, optimizing combustion conditions to reach the optimum penetration length and deriving theoretical and empirical governing correlations.

2. Problem formulation

Our problem constitutes a constant volume combustion chamber CVCC which contains ambient air compressed at a given pressure and temperature (which can be varied). A liquid hydrocarbon fuel is injected at some injection pressure (also variable), thereby initiating combustion leading to the formation of a diffusion flame.

For present case the liquid fuel chosen is n-Heptane. The geometry of the combustion chamber is cuboidal having dimensions 0.1mx0.02mx0.02m. The injector is single hole unit injector (hollow cone) with diameter 140 micrometer and outer cone angle of 15 degree, modeled for a common rail injection system with a given fuel mass flow rate. The computation time is set to 1 micro second and 12000 parcels are injected for each computational cycle.

We are analyzing the effect of different sub models, in addition to the effects of ambient temperature, ambient pressure and cone angle on STPL. The obtained result is then validated with the existing experimental data for the same conditions. OpenFOAM is used for simulating spray combustion behaviour. The solver used for implementation is dieselFoam. Finite volume method is used to numerically solve the Navier-Stokes equations for any 3D grid of unstructured polyhedral cells.

2.1. Implementation of Code

Open FOAM is an open source code which is object oriented written in C++, which makes it reasonably straight forward to implement new models and fit them into the whole code structure. The code includes polyhedral mesh support, making it possible to create meshes using any form of cells, as long as the quality of the resulting mesh is high. All solvers written in OpenFOAM can be easily run in parallel, since the code is parallelized at such a fundamental level, removing the need for the user to consider multiple processor simulations. OpenFOAM code was chosen both because of the high scope it offers for developing new models, and the demands it places on the user. It is not difficult to know in OpenFOAM what you are doing than in other simulation codes which appear to be more or less as a black box.

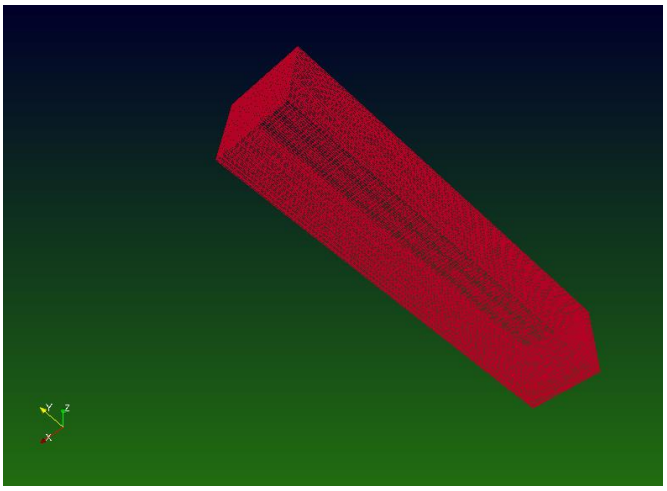

Figure 1. Geometry of the problem.

The geometry consists of a block filled with air, with a 0.02x0.02 meter base and a length of 0.1 meter (Figure.1). An injector is centrally placed on the top boundary where n-Heptane (C_7H_{16}) fuel spray is injected. When the discrete droplets enter the domain they evaporate and combustion takes place in the gas phase. There are several gas phase reaction schemes supplied with the case ranging from a reaction scheme with 5 species and one reaction up to a reaction scheme involving 300 reactions and 56 species.

Results of the present work indicate that out of the given submodels which simultaneously govern the spray combustion process. Three important models which are most important and seem responsible for correct prediction of spray tip penetration are: (i) standard evaporation model which is the d^2-law model, (ii) breakup model (including secondary break up) which is ReitzKHRT break up model and (iii) trajectory collision model.

3. Important Governing Equations Used in the Present Numerical Simulation

3.1. Standard Evaporation or the d^2-law Model

While models like droplet breakup model/ droplet collision model etc are primarily governed by fluid dynamics, droplet evaporation model is evolved from thermodynamics considerations. Inclusion of oversimplified models may give approximate results whereas complex models are generally overlooked to avoid costly computations. Hence, droplet evaporation model has to be simple, but realistic [4,11].

The model which has been extensively used in spray combustion modelling is the d^2-law model. It is a simple approach meaning that the spherically symmetric, discrete liquid droplets in the spray are evaporating at a steady rate. When modeling the evaporation of a droplet, the key parameter is the droplet lifetime or evaporation relaxation time of the droplet. The derivation of this time starts by evaluating the time derivative of the mass of the spherical droplet and the expression for evaporation relaxation time of droplet is given as:

$$\tau_e = \frac{\rho_v D^2}{6 D_V Sh \rho_v \ln\left(1+\frac{X_{v,s}-X_{v,\infty}}{1-X_{v,s}}\right)} \quad (2.1)$$

Where: D is the instantaneous droplet diameter, ρ_v is the fuel vapour density, D_v is the mass diffusivity, Sh is Sherwood number, $x_{v,s}$ and $x_{v,\infty}$ are respectively the mole fractions at the droplet surface and far away from droplet center.Expression for droplet lifetime can also be derived from various other sources available in the literature [11-12].

3.2 ReitzKHRT Break up Model

It is known that liquid droplets in sprays have very high initial velocities and decelerate rapidly due to drag forces. In this case, Rayleigh–Taylor instability may also play an important role on droplet breakup mechanisms in addition to the Kelvin–Helmholtz instability. The droplet breakup model due to Rayleigh–Taylor instability is described by Su, T. F et al. [13]. Neglecting liquid viscosity and considering surface tension only, the analytical fastest growing frequency and the corresponding wave length are provided by Bellman and Pennington [14].

In the KHRT model, the aerodynamic force on the drop flattens it into the shape of a liquid sheet, and the decelerating sheet breaks into large-scale fragments by means of RT instability. KH waves with a much shorter wavelength originate at the edges of the fragments and then these waves breakup into micrometer-size drops.

3.3. Collision Model

OpenFOAM offers three collision models: O'Rourke [15], referred to as O'Rourke collision model which further serves as a basis for other collision models, namely Schmidt and Nordin (Trajectory model). In the O'Rourke collision model, both the number and the nature (collision or coalescence) is governed by a probability density function, hence it is rather a statistical than a deterministic approach.

Nordin collision model: This model is also similar to the O'Rourke collision model, but since it considers the entire droplet population when calculating the probability of droplet collisions, it overcomes the grid dependency of O'Rourke and Schmidt collision models. The pre-condition of droplet collision is that the droplets considered travel toward each other. This is obtained from the trajectories of the parcels containing the droplets. If there is an intersection point of the two trajectories, it is determined whether the two droplets reach the intersection point approximately at the same time.

This method provides more realistic modeling of droplet collision, but is very time consuming. The simulation time required when this model is used is approximately three times as much as those of the other methods.

Another important aspect of spray combustion apart from STPL is the ignition delay.A detailed numerical investigation into constant volume combustion [16] was carried out by Varshney et. al and validated with sensor based experimental analysis.

An interesting fact of in variance inignition delay characteristics at high injection pressures, high cylinder air pressure and elevated hot surface temperature was observed.

4. Results and Discussion

Results for Spray evolution in the CVCC and Spray Tip Penetration Length (STPL) are presented for the conditions given below with different break up models.
Initial Pressure inside Combustion Chamber (P_∞ in bar: Variable)

Initial Temperature inside Combustion Chamber (T_∞ in K: Variable)

Injector Type → Common Rail Injector

Atomization Model → LISA

Drag Model→ Standard Drag Model

Evaporation Model→ Standard Evaporation Model

Collision Model→ Trajectory

Heat Transfer Model→ Ranz Marshall Model

Wall Model→ Reflect Model

Injector Model→ Hollow Cone Injector Model

Distribution Model→ Rosin Rammler Model

Injection pressure→ (in bar : Variable)

Diameter of Injector: 140 μm, (Outer Cone Angle: Variable)

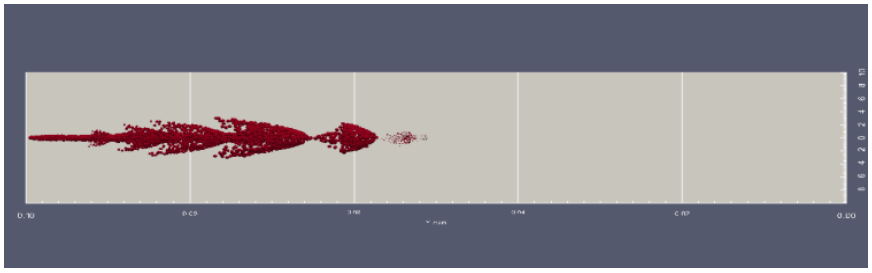

Figure 2. Comparison of spray penetration at different burning times

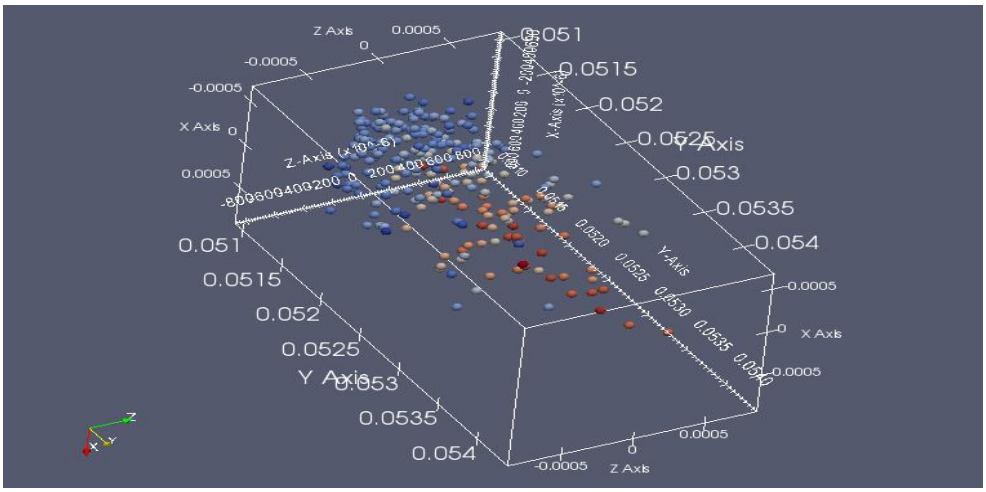

Figure 3.3D distribution of droplets in the combustion chamber.

Figures 2 captures the image of spray penetration at different burning times. Figure 3 shows the 3D distribution of droplets in the given domain.

As observed from Figure 4, the best comparison for spray tip penetration length (STPL) of present study with results of Kosters and Karlsson [10] is shown by ReitzKHRT break up model followed by ReitzDiwaker (WAVE) and ETAB models. Here, Trajectory collision model and Standard evaporation model are used in the simulation together with different break up models as mentioned above.

Figure 5 suggests that incorporation of collision model is mandatory to obtain realistic STPL variation, other conditions remaining same.

Figure 6 shows that the maximum STPL is obtained for T_∞=1000K, for this condition, the kinetic energy of liquid droplets (in the spray) is maximum, therefore maximum penetration is achieved. As the ambient temperature is increased beyond 1000K, the evaporation rate of liquid spray is enhanced, leading to a shorter STPL.

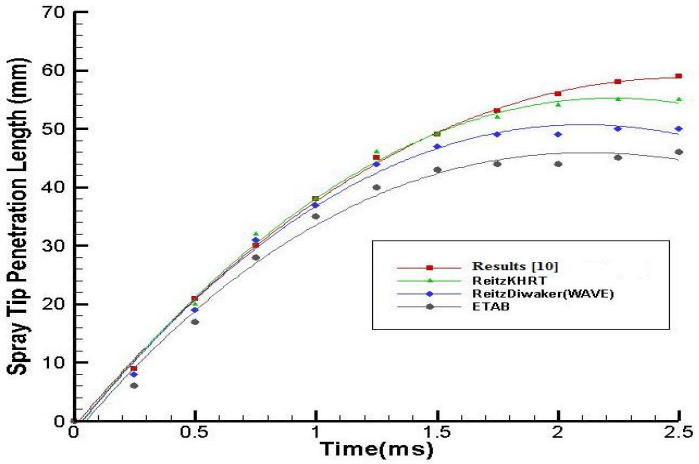

Figure 4. Comparison of spray tip penetration length for different breakup models (Fuel: n-heptane, P_∞ = 50 bar, T_∞ = 683K, $P_{injection}$ = 600 bar, outer cone angle = 15^o).

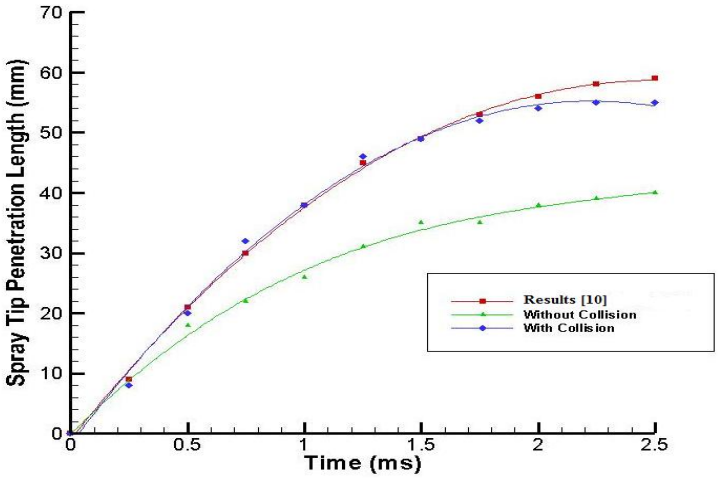

Figure 5. Comparison of STPL with and without collision model

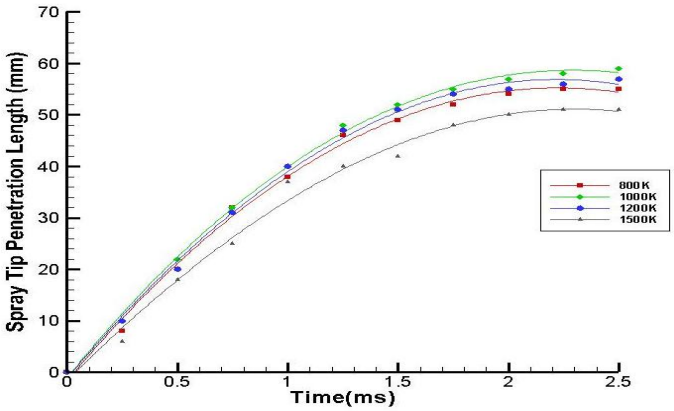

Figure 6. Comparison of STPL for different ambient temperatures (P_∞ = 50 bar, outer cone angle = 20^o).

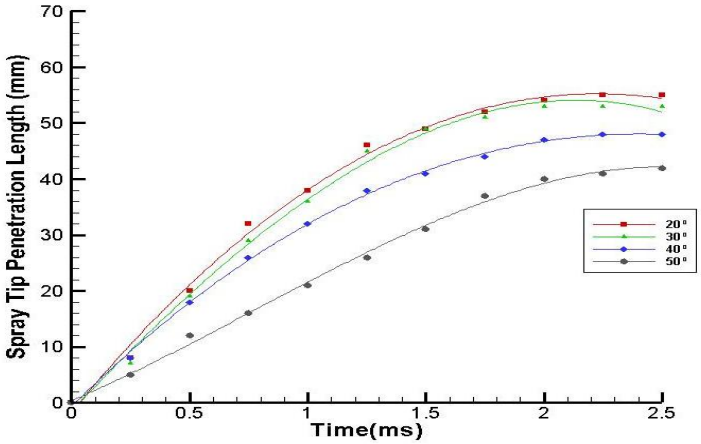

Figure 7. Comparison of STPL for different outer cone angles(P_∞ = 50 bar, T_∞ = 800K).

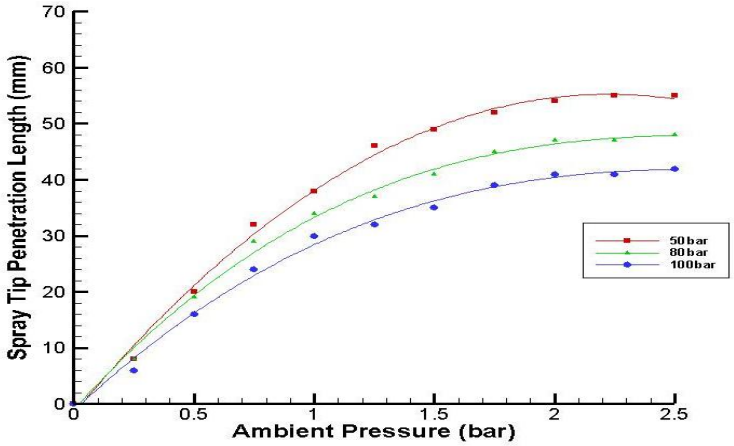

Figure 8. Comparison of STPL for different ambient pressures (T_∞ = 800K, outer cone angle = 20^o).

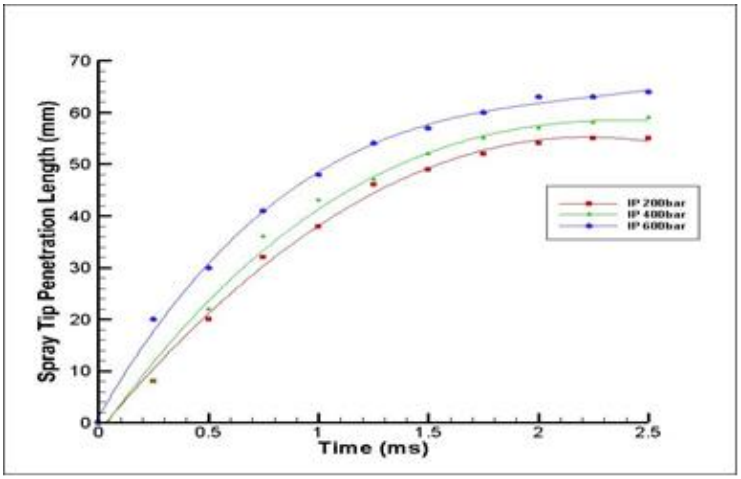

Figure 9. Comparison of STPL for different injection pressures (P_∞ = 50 bar, T_∞ = 800K, outer cone angle = 20^o).

Variation of STPL with different outer cone angles for a fixed value of P_∞ = 50 bar, T_∞ = 800K is depicted in Figure 7. It is observed that best values for STPL are obtained for an outer cone angle of 20^o. This may be due to better mixing of fuel and air, hence maximum flame temperature and velocity at the flame leading to higher STPL values.

Figure 8 shows that as ambient pressure $P_\infty$is increased for a fixed ambient temperature and cone angle, value of STPL decreases. This behaviour is justifiable since at higher ambient pressure, the surrounding air density increases thus reducing liquid penetration.

As suggested by Figure 9, an increase in injection pressure leads to an enhanced STPL, which is understandable, also, higher injection pressure means more turbulence and better mixing leading to better combustion and heat release.

5. Conclusions

- ReitzKHRT Break up model together with Standard Evaporation model and Trajectory collision model provide the best result for STPL. This combination is used with subsequent simulations.
- It is observed that an increase in ambient temperature from 800K to 1500K leads to a higher flame temperature and enhancement in STPL (for an optimum value of 1000K), further increase in temperature decreases STPL.
- Optimum values for STPL are obtained for an outer cone angle of 20^{o}.
- As ambient pressure is increased, the flame temperature is increased, but STPL decreases.
- An increase in injection pressure leads to an enhanced STPL

6. Future Work

- Effects of different variables can be quantified on other important parameters like ignition delay, rate of heat release, NOx formation and soot.
- The results of the present work obtained using OpenFOAM can be compared with other commercial software like Ansys Fluentfor the same fuel and operating parameters.

Conflict of Interest

The authors declare no conflict of interest.

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