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NUMERICAL SIMULATION OF PRIMARY ATOMIZATION WITH LARGE EDDY SIMULATION METHOD

Ming P. J.* and Zhang X.Y.
*Author for correspondence
College of Power and Energy Engineering,
Harbin Engineering University,
Harbin 150001,
China,
E-mail: pingjianming@hrbeu.edu.cn

ABSTRACT

As the awareness of the environmental protection and energy conservation, a more restricted rule is proposed on engine performance, e.g. high power output, fuel economy and low pollution. It is very important to understand the spray atomization mechanism and the factors which have effects on the characteristics spray and its regulation. The combination of LES (Large eddy simulation) and the VOF method by using open source CFD software OpenFoam in Linux system is used to imitate umbrella morphology on the oil spray and fracture mechanism in the primary atomization stage. The radial and axial velocity, pressure and droplet distribution are obtained by present method and some meaningful results are concluded. Finally, the influence of the air dynamics on the fuel primary breakup and the effects of grid sizes for LES are analyzed.

INTRODUCTION

Atomization and spray process is a typical gas-liquid two-phase flow of great practical relevance in applications such as the fuel injection in gas-turbine combustors of aircraft engines and in internal combustion engines [1]. The combustion performance and emissions are mainly influenced by the atomization of the liquid fuel, the motion and evaporation of the fuel droplets and mixing of fuel with air. Fuel atomization is a very complicate process and is influenced by liquid surface tension forces, viscous forces, inertial and aerodynamic forces and so on. Liquid fuel injects into the combustion chamber with high velocity to generate continuous liquid column and becomes into tiny droplets by secondary atomization. There are many factors effect on fuel spray atomization, and some of them are still uncertainties. It is essential that the effects of these important factors are identified and understand, and to do so, both extensive experimental and computational fluid dynamics (CFD) tests have been carried out. Fuel atomization process is usually divided into primary and secondary atomization by crushing breakup and droplet atomization. The final droplet production is greatly dependent on primary breakup, but it has been difficult to know what is actually occurring in the primary breakup region.

Therefore, further study of the mechanism of atomization helps to develop atomization theory and improve fuel atomization quality. Many researchers conducted a lot of research on fuel atomization process, but due to its complexity, so far still a perfectly reasonable explanation is not made for the fuel injector atomization mechanism. A lot of hypotheses are used depending on different experiments and analysis according to researchers, but most of the atomization process is not comprehensive consideration of various factors and subjective guess work is not universal [2,3].

There are several hypothesis on atomization theories which includes turbulent disturbances, air flow disturbances, sudden changes on boundary conditions， cavity disturbance and pressure oscillations. Aerodynamic interference first proposed by Castleman in 1932. He believes that an unstable surface is due to the fluctuations in the jet interference with ambient air.

With the velocity and the difference between air and liquid surface increases, the wavelength of unstable waves becomes shorter, even short to the order of microns, so atomized jet surface quickly spreads. There are different technical methods of achieving atomization. Carburetors, airbrushes, and spray bottles are only a few examples of atomizers used ubiquitously. Essentially, all that is needed is a force such as a high pressure or a large shear force from the high relative velocity between the liquid to be atomized and the surrounding air or gas to overcome the surface tension of the liquid. Most practical atomizers are of the pressure, rotary or twin-fluid type. In a pressure type of atomizer used frequently in fuel injection in combustion engines, the pressure force overcomes the liquid surface tension. In a rotary or twin-fluid type atomizer (all nozzle types in which atomization is achieved using high-velocity air, gas or steam), the shear force or the centrifugal force overcomes the liquid surface tension. Many other forms of atomizers have also been developed that are useful in special

applications, including electrostatic atomizer where electrical force is used to overcome surface tension forces and achieve atomization, impinging jet atomizer where liquid jets collide outside the nozzle to achieve atomization, ultrasonic atomizer in which high frequency (20-50 kHz) vibration is utilized to produce narrow drop size distribution and low velocity spray from a liquid, whistle atomizer in which sound waves are used to shatter a liquid jet into droplets, and windmill atomizer which is a rotary atomizer used for aerial application of pesticides with a unique feature of using wind forces to provide rotary motion.

So far, the mostly accepted reasons leading to the atomization of the fuel injection fuel injection are disturbed turbulent flow, shear force and cavity air flow in nozzle hole [4]. Atomization and spray process remains a significant challenge to CFD practitioners. In most of the atomization and spray processes, the breakup of liquid jets and sheets results in chaotic generation of drop sizes and velocities. In current spray systems, the variation in drop size and speed can be vastly different.

Ishimoto used a combination method of VOF and large eddy simulation to study round nozzle spray and got some important parameters, but these parameters were not obtained a good description of the initial crushing mechanism and fuel atomization process. Shinjo used direct numerical simulation methods combined with level set for primary spray and he studied aerodynamic effects on crushing process in details, but he mainly focused on the dynamics and did not dealing with statistic characteristics [5].

NOMENCLATURE

a_{ZY}	[-]	*y-z* view aspect ratio of rectangular region between two adjacent cooling layers
C_{GTP}	[m^3K/W]	Coefficient dependent on geometric, thermal and material property values
$E_{\%}$	[%]	Allowable volumetric heat generation density increase
k	[W/mK]	Thermal conductivity
n	[-]	Normal direction
p	[N/m^2]	Pressure
u	[m/s]	Velocity
T	[K]	Temperature
x	[m]	Cartesian axis direction
y	[m]	Cartesian axis direction
z	[m]	Cartesian axis direction

Special characters

ρ	[kg/m^3]	Density
κ	[-]	Liquid interface curvature
μ	[Pa.s]	Viscosity
Φ	[-]	Volume fraction
τ	[-]	Shear stress
σ	[-]	Surface tension coefficient
δ	[-]	Delta function

Subscripts

sv	Volume source
g	Gas
l	Liquid
i,j	Direction

CONTROL EQUATION FOR TWO PHASE FLOW

In this research the two phases are treated as immiscible and incompressible Newtonian fluids, each of which has constant fluid density and viscosity. In the calculation, permeability and surface tension of the gas and liquid phases are taken into account, and the flow is assumed isothermal and non evaporation, so it is not necessary to solve the energy equation. In accordance with the ideal VOF model, the control equations for two-phase flow can be described by mass and momentum conservation as the following:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \int_{s(t)} \sigma \kappa' n' \delta(x - x') dS \tag{2}$$

wherein, u_i 、 u_j are velocity components;

ρ is density;

ν is kinetic viscosity;

σ is surface tension coefficient;

κ' is curvature of gas liquid interface;

n' is normal direction outward to interface;

$\delta(x)$ is Diracfunction.

In a gas-liquid two-phase flow there is a source of momentum due to the presence of surface tension. This requires the addition of a source term in the Navier-Stokes momentum equations. This is shown in eq. (2) as the integral term on the right side. The problem of directly solving the momentum integral due to surface tension can be alleviated by the use of a continuum surface force (CSF) model. The surface tension effect is similar to volume force term in a continuous gas-liquid mixing zone. The force is expressed as following:

$$F_{s\upsilon} = \int_{s(t)} \sigma \kappa' n' \delta(x - x') dS \approx \sigma \kappa \Delta \phi \tag{3}$$

In which, Φ is the liquid volume fraction which can be obtained by solving the transport equation VOF method to get, κ is liquid interface curvature which is defined by the liquid volume fraction as follows:

$$\kappa = \nabla . \left(\frac{\nabla \phi}{|\nabla \phi|} \right) \tag{4}$$

FRONT TRACKING METHOD WITH VOF

Since the fuel injection atomization process is a typical gas-liquid two-phase flow and it is important to track the gas-liquid interface, discontinuity of material properties such as viscosity and density is the primary problem for the calculation. In this paper, VOF (Volume of Fluid) method is used to track the gas-liquid interface of the two phases.

VOF method was first proposed by Hirt et al, and its basic principle is a function of the fluid and the volume ratio of the grid is determined by the free surface grid cell research, tracking fluid interface changes, rather than tracking the

movement of the free surface of the particle, and the fluid transport function satisfies the eq. (5).

We define the liquid volume fraction as ϕ in each cell, which is the ratio of the volume taken by the liquid in the cell and the volume of the cell itself. Thus ϕ is 1 for a cell full of water and 0 for a cell full of air. For a cell containing both liquid and air $0<\phi<1$. The evolution of ϕ in each cell is based on the following equation:

$$\frac{\partial \phi}{\partial t}+\nabla\cdot(\phi \boldsymbol{U})=0 \tag{5}$$

Within each cell the density and viscosity used in Eq. (2) are obtained using the following weighting:

$$\rho=\phi\rho_l+(1-\phi)\rho_g, \tag{6}$$

$$\mu=\phi\mu_l+(1-\phi)\mu_g, \tag{7}$$

The subscripts l and g indicate liquid and gas.

LARGE EDDY SIMULATION CONTROL EQUATION

As we all know, the LES method requires the use of a filter function for filtering equations used herein. For example, we have instantaneous variables Φ: □

$$\overline{\phi}=\int_D \phi G(x,x')dx' \tag{8}$$

Wherein the filtered variable $\overline{\phi}$, that is, the analog portion of the LES calculated directly, D is the fluid domain.

x' is the actual flow of the spatial coordinates;

x is the coordinate large-scale space filtered on;

$G(x,x')$ is the filter function that determines the scale of the resolved scale.

That is only retained $\overline{\phi}$ on the filter function is greater than the width dimension variability $G(x,x')$. Here we employ the finite volume method (FVM) to approximate the differential equations. The finite-volume discretization itself implicitly provides the filtering operation, namely a control volume averaged quantities, so here is the use of the following expression.

$$G(x,x')=\begin{cases}1/V, x'\in V\\ 0, x'\notin V\end{cases} \square \tag{9}$$

The size of the space occupied by the liquid in the grid cell, the formula can be written as:

$$\overline{\phi}=\frac{1}{V}\int_D \phi dx' \tag{10}$$

The filtered governing equations for LES of the incompressible, two-phase flow can be given as follows:

$$\frac{\partial \overline{u_i}}{\partial x_i}=0 \tag{11}$$

$$\frac{\partial \overline{u_i}}{\partial t}+\frac{\partial(\overline{u_i}\,\overline{u_j})}{\partial x_j}=-\frac{1}{\rho}\frac{\partial \overline{\rho}}{\partial x_i}+\nu\frac{\partial^2 \overline{u_i}}{\partial x_j\partial x_j}+\frac{\partial \tau_{ij}}{\partial x_j}+\overline{F_{sv}} \tag{12}$$

In this paper, the above two equations constitute a large eddy simulation obtained using two-phase flow. For the subgrid-scale stress, which reflects the contribution of small scales to the large-scale transport equation, can be written as follows:

$$\tau_{ij}=\overline{\overline{u_i}\,\overline{u_j}}-\overline{u_i u_j} \tag{13}$$

A comparison of eq. (2) and eq. (12) shows that the filtered Navier-Stokes equations do not retain the same form, the differences appear in subgrid-scale stress term on the right side, which can not be solved directly and has to be modelled. In the present work, the spaced filtered equations are closed using a turbulent eddy viscosity hypothesis. The subgrid-scale stress τ_{ij} is linked to the eddy viscosity ν_τ by the following expression:

$$\tau_{ij}-\frac{\delta_{ij}}{3}\tau_{kk}=-2\nu_\tau\overline{S_{ij}} \text{ with } \nu_\tau=C\overline{\Delta}^2|\overline{S}| \text{ and } |\overline{S}|=\sqrt{2\overline{S_{ij}}\,\overline{S_{ij}}} \tag{14}$$

where C is the dimensionless model coefficient, $\overline{\Delta}=(\Delta_x\Delta_y\Delta_z)^{1/3}$ the grid filter width and S_{ij} the strain rate tensor.

In summary, this paper is a mathematical model for the numerical simulation of jet fuel atomization process.

SIMULATION MODEL AND GRIDS

In the CFD simulation, the physical model is a simplification of reality and the research is studied to achieve outstanding principal factors by ignoring secondary factors. To achieve a desirable result, the physical model whether correct or not is very important.

GRID GENERATION

To solve the equations numerically, the primary problem is discretization. Mesh generation is a discrete area of the premise that the space is divided into a number of discrete areas subdomains, and to determine the relevant geometric parameters of each sub-domain. General requirements for grid generation systems are as follows: grid should be consistent with solving boundary; grid should be able to depict the dramatic changes in the relevant region; grid lines intersected with the boundary and the boundary should be as orthogonal as possible; grid lines should coincide with the direction of flow as much as possible.

According to the above ideas, and combined with jet-hole injector nozzles commonly used in internal combustion engines, a three-dimensional simplified model is established by PRO/E as shown in Figure 1. The injection hole type fuel injector nozzle diameters are now generally 0.15mm~0.8mm, therefore, the selection of the injection hole is 0.2mm. The front portion of the injection hole is the pressure chamber and behind the hole is the combustion chamber near the nozzle area; the axial length of the model is 3.6mm. Figure 2 is the pressure chamber nozzle area and mesh.

Fig.1 Simplified model

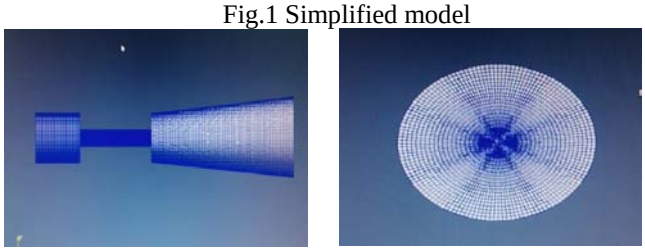

Fig.2 Computation grids of nozzle with a pressurized chamber

Through analysis of the mesh used in the relevant literature, we can see that the refine mesh method with a scale about 5 to 10 microns is used near the liquid breakup to balance between the accuracy for using large eddy simulation theory in atomized fuel injection process simulation and the amount of computation to save computing time. The first example is a three-dimensional model constructed by Pro/E and using Gambit for mesh generation. And then it is transformed into OpenForm format through Fluent3D to Foam command. According to this idea, computational model selected for this paper, combining the characteristics of Gambit meshing tools, are shown in Figure 2, the computational domain is divided into three zones, the pressure chamber, the combustion chamber near the nozzle area, and the middle area of the jet fragmentation. In order to reduce computation cost without affecting the calculation results, non-uniform grid system is employed in the mesh generation. Grid is highly concentrated near the area of the intermediate jet may be broken. And we divide the computational domain into multi zone and refine the mesh so as to get better fuel droplet breakup near the nozzle, and take the diffusion of fuel atomization into account. In this way, it is not only realizes the local refinement of liquid phase region, but also ensures the orthogonality between grids near the boundary and the boundary.

Four grids with different number meshes are used to study the grid independency for large eddy simulation turbulence model. The mesh size is uniform in radial direction and the mesh size is between 1 micron and 10 micron. In axial direction, the mesh size gradually decreases from 40 micron to 5 micron (40 micron, 20 micron, 10 micron, 5 micron). The number of cells used in each example is shown in Table 1.

Table 1 grid numbers

Case	1	2	3	4
Grids	512033	997330	1333840	2101202

INITIAL AND BOUNDARY CONDITIONS

Due to the use of modern advanced high pressure common rail injection system in internal combustion engines, the injection pressure is up to 120MPa ~ 200MPa, and jet speed up to hundreds of meters. Thus, in present work, the following boundary conditions are used; we set the average inlet velocity v = 50m/s, which is equivalent to the outlet nozzle hole 450m/s ejection speed, the no-slip condition is specified on the wall, and the exit boundary condition is specified by using constant pressure outlet condition. The liquid phase is assumed to be diesel, gas pressure is assumed to be air at 5.2MPa and a temperature of 900K. Gas-liquid density ratio is 42. Other required material parameters and initial conditions are shown in Table 2.

It can be seen that the fuel injection state is turbulent, subsonic and in the so called atomization zone where surface tension and viscous force have significant effect in a small scale from the dimensionless number .e.g. Reynolds number, Weber number, and Mach number. These characteristics mentioned above are commonly appears in diesel injection systems of modern large-scale transport. Due to limitations of the algorithm, the performance of compressibility can be ignored with Mach number 0.76.

Table 2 material parameters and initial conditions

	dimension	value
Liquid density	$\rho_f, kg/m^3$	840
Gas density	$\rho_g, kg/m^3$	20
Density ratio	ρ_f/ρ_g	42
Liquid viscosity	$\upsilon_f, m^2/s$	$5.952\text{x}10^{-6}$
Gas viscosity	$\upsilon_g, m^2/s$	$8.5\text{x}10^{-7}$
Surface tension	$\sigma, N/m$	0.0261
Hole diameter	d, mm	0.2
Liquid velocity	$U_b, m/s$	450
Reynolds number	$\mathrm{Re}_{fd}, U_b d/\upsilon_f$	15500
Weber number	$We_{fd}, \rho_f U_b^2 d/\sigma$	$1.36\text{x}10^6$
Mach number	$Ma, u/u_s$	0.76

Core calculation formulas used herein is the open source CFD software OpenFoam, finite volume method for discretised equations, Euler method for the time discretization, spatial discretised form are second order accuracy, and time step is determined by Courant number. The PISO method is selected to solve the pressure-velocity coupling, combined with the conjugate gradient method for solving linear algebraic equations.

NUMERICAL RESULTS AND DISCUSSION

As shown in Figure 3, the head of the umbrella liquid column occurs, where red represents high volume fraction and blue represents low volume fraction of liquid fuel. The digital images are arranged by the picture ID, and the time between two pictures of each adjacent interval is 0.5 microseconds.

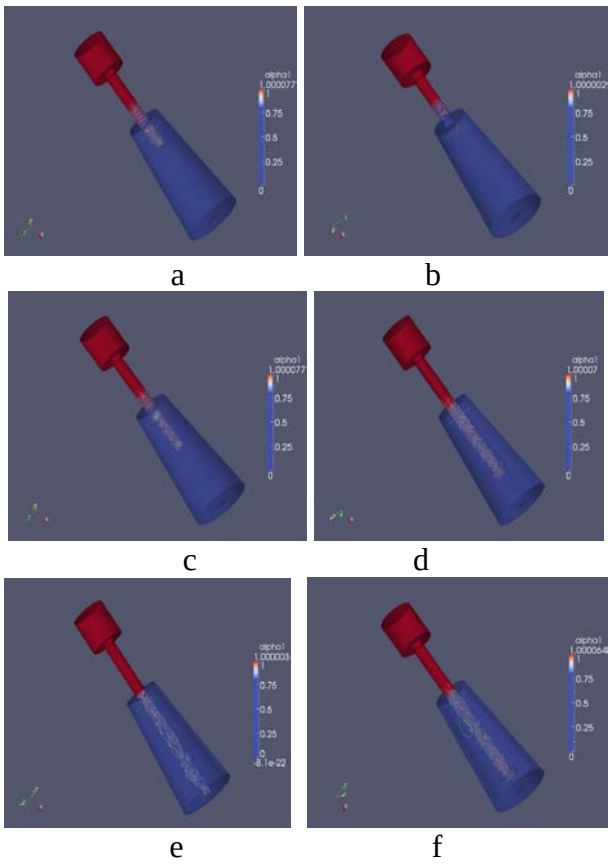

Fig.3 Development of jet flow

Figure 3 shows the formation and development process of the umbrella head when fuel injects from the nozzle. In Figure 3a we can see that the liquid column is intermediate projections in the nozzle, due to the velocity near the wall is smaller than the center of the nozzle. The liquid column gradually turns up from the center to the surrounding due to strong shearing action of the air in the combustion chamber, and reveals the so-called umbrella head, which is similar to the phenomenon of the fountain sprayed into the air. As the injection continues, the head of the umbrella begins to extend to the surrounding, and forms a lot of ligament-like liquid film. Then, the liquid film slowly breaks up to a large amount of small droplets. As can be seen, a lot of “potholes” and “wrinkle” appear on the surface of the liquid column. This is mainly because there is a big velocity difference between the injected fuel and adjacent air, which causes the formation of numerous small air vortices near the liquid surface. Under the interaction and mutual influence of internal turbulent fluid motion and external gas flow disturbances, the liquid surface becomes unstable and appears distortion and shedding process. In order to get a close observation of the process, enlarged scale pictures are shown in Fig.4 which record the shedding process of the liquid from the liquid column, and the interval between the adjacent maps is 0.1 microseconds.

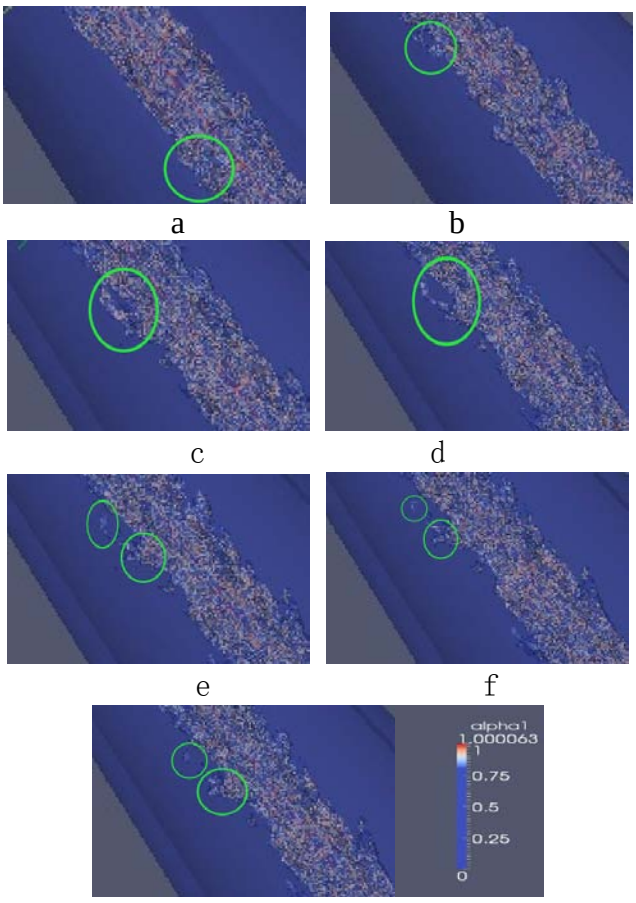

Fig.4 Surface breakup of liquid column

Fig. 4a and 4b are the liquid film formed on the surface of the liquid due to interaction between liquid turbulence and air shear force. Fig. 4c and 4d show the process that the liquid film further breaks up under aerodynamic effect, and is gradually peeled off from the surface of liquid column, which is called primary breakup. From Fig. 4d, 4e, 4f and 4g we can see that the initial fuel droplets get into the gas-fuel mixing area, and deformation occurs on the surface under the non-uniform pressure and aerodynamic effect due to the high relative velocity between the droplets and the air. When the force is greater than the liquid surface tension, droplets will break up into smaller droplets which are called secondary atomization. What can be seen from this simulation is the interaction and mutual influence of turbulent fluid motion and internal aerodynamics cause the fuel breakup.

CONCLUSION

The combination of LES (Large eddy simulation) and the VOF method by using open source CFD software OpenFoam in Linux system is used to imitate umbrella morphology on the oil spray and fracture mechanism in the primary atomization stage. The radial and axial velocity, pressure and droplet distribution are obtained by present method and some meaningful results are concluded. Finally, the influence of the air dynamics on the fuel primary breakup and the effects of grid sizes for LES are analyzed.

The initial breakup of fuel which affected by the aerodynamic is the result of the disturbance of the air and the shear stress. Initial breakup mainly occurs in the tip and the surface of the liquid column. Numerical simulation can obtain the desirable data which is difficult to get by experiment. It is shown that the numerical simulation has a lot of advantages on the research of fuel atomization mechanism.

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