The effect of momentum flux ratio and turbulence model on the numerical prediction of atomization characteristics of air assisted liquid jets

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Abstract

The physical processes involved in a liquid jet breaking up are complex. Accurate prediction of such flows is computationally very expensive, as it involves transient LES modeling and VOF method to track liquid-gas interfaces. A relatively novel and easier approach to predict jet penetration was proposed by Vallet et. al \cite{Vallet1}, called Sigma-Y model. Lebas et.al\cite{Lebas2} later modified it into what is known as Omega-Y model. This modified form is implemented in this study using ANSYS FLUENT's user defined function approach. Steady state solver is used along with a user defined scalar to compute the interfacial area density transport equation. The liquid fraction is tracked via a species transport equation. A grid independence study is carried out for a fixed momentum flux ratio and results are compared with experimental data. Effect of momentum flux ratio and turbulence model on breakup length and droplet Sauter mean diameter is also investigated.

Keywords: CFD, Sprays, Modeling, Atomization

Introduction

Atomization involving complex gas-liquid flow near nozzle region and subsequent evaporation and mixing of fuel-air is of utmost importance in determining the combustion efficiency and emission production in internal combustion engine. In addition, primary atomization is also analyzed in studies of propulsion, power and many other process applications. Computational Fluid Dynamics (CFD) has become one of the most important tools for both understanding and improving diesel spray development. The complex interaction still makes it a challenge to be modeled.

The main difficulty in analyzing primary atomization is that the complex break up phenomenon involves different length scales. Droplets formed are very small and can be appropriately tracked using Lagrangian approaches; however the same may not be able to accurately predict the near nozzle dense zone where no droplets are formed. On the other hand, an Eulerian description may be found appropriate for modeling flow inside the spray and near the nozzle zone\cite{Vallet1}. One such model, the \checkmark-Y model \cite{Vallet1}, attempts to capture the near nozzle flow features of practical interest. This model can also be extended to include transition from Eulerian description of fluid to Lagrangian description of particles in the dilute zone away from the nozzle. In this paper, we have studied the \checkmark-Y approach and its variant the \checkmark\cdot Y model.

The next section describes the model details and model equation. This is followed by the problem set up for a simulation to compare to experimental data. The results section discusses the performance of \checkmark\cdot Y model. Conclusions and future works will be explained in the last section.

The \checkmark\cdot Y Model

The \checkmark\cdot Y model, originally proposed by Borghi and Vallet \cite{Vallet1}, attempts to capture the features of the flow of practical interest to the design engineer while simplifying the complexities of the flow via simple closures within an Eulerian framework. The approach has been under development \cite{Lebas2, Lebas3, Lebas4, Lebas5, Lebas6} since its first introduction. This model is intended for application involving turbulent spray with both high Reynolds and Weber Numbers. By solving the governing equations of motion in a Reynolds averaged paradigm, the bulk liquid movement is predicted. Instead of attempting to resolve individual atomization events, a transport equation of the interfacial area density is solved to characterize the rate at which surface area is created. From local interfacial surface area and liquid volume fraction, the Sauter mean diameter can then be extracted. This can further be used as an input for Lagrangian secondary breakup models.

The key assumptions in \checkmark\cdot Y model are:
1. At large length scales, flow will be independent of surface tension and viscosity and depending only on density variation and bulk momentum transport. Surface tension and viscosity act only at the small length scales which correspond to limit of infinite Reynolds number.

2. Dispersion of liquid in the gas phase can be modeled by turbulence dispersion.

3. The average shape of the liquid structures can be characterized by mean surface area per unit volume, which can be tracked like any other transport quantity.

To track the dispersion of the liquid phase an indicator function $Y$ is introduced with value 1 in the liquid phase and 0 in the gas phase. The mean liquid volume fraction of the fluid is then defined as $\bar{Y}$, and the mean mass averaged fraction is defined as $\bar{\rho} Y = \bar{\rho} \bar{Y}$. The transport equation for $\bar{Y}$ then takes the form:

$$\frac{\partial(\bar{\rho} \bar{Y})}{\partial t} + \frac{\partial(\bar{\rho} \bar{u}_i \bar{Y})}{\partial x_i} = -\frac{\partial(\bar{\rho} \bar{u}_i \bar{Y}')}{\partial x_i} \quad (1)$$

Where $\bar{u}'$ denotes the turbulent fluctuations in velocity and $\bar{Y}'$ denotes turbulent fluctuations in volume fraction.

If the liquid density and gas density are both constants, the relation between $\bar{Y}$ and $\bar{\rho}$ is given as,

$$\frac{1}{\bar{\rho}} = \frac{\bar{Y}}{\bar{\rho}_{\text{liq}}} + \frac{1 - \bar{Y}}{\bar{\rho}_{\text{gas}}} \quad (2)$$

However if the gas phase is a compressible ideal gas, relation between $\bar{Y}$ and $\bar{\rho}$ is given as,

$$\bar{\rho} = \frac{\bar{\rho}(1 - \bar{Y})R_g T_g}{1 - \bar{\rho} \bar{Y}} \frac{1}{\bar{\rho}_{\text{liq}}} \quad (2a)$$

The turbulent diffusion of liquid $u_i \bar{Y}'$ needs to be modeled. To close the turbulent diffusion liquid flux term, a simple turbulent diffusion hypothesis has been shown to yield good results far from the primary atomization zone. For primary atomization processes, Demoulin et al. [3] proposed the following term capturing the enhancement of liquid mixing caused by accelerated large density gradients via a Rayleigh-Taylor type mechanism.

$$\bar{\rho}u_i \bar{Y}' = \rho \left[ \frac{\theta_1}{Sc} + C_p \frac{k^2}{\bar{\rho} \bar{u}_i \bar{Y} (1 - \bar{Y})} \right] \frac{d \bar{Y}}{dx_i} \quad (3)$$

With the large scale flow features described, a transport equation for the evolution of the interfacial surface area density, $\Sigma$ (with units m$^{-1}$) determines the small scale behavior of the flow. The transport equation of $\Sigma$ as proposed by Vallet [1] takes the same form as Morel’s [8] generalized derivation, having terms capturing the effects of convection, diffusion, surface stretching and coalescence.

$$\frac{\partial(\Sigma)}{\partial t} + \frac{\partial(u_i \Sigma)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( D_a \frac{\partial \Sigma}{\partial x_i} \right) + \frac{1}{\tau_{\text{prod}}} \Sigma - \frac{1}{\tau_{\text{destr}}} \Sigma^2 \quad (4)$$

where, $D_a$ is an appropriate diffusion coefficient. Here $\tau_{\text{prod}}$ a time scale representing the rate at which turbulence creates surface area, and $\tau_{\text{destr}}$ is a velocity scale corresponding to the rate at which collision and coalescence destroy surface area. A detailed derivation of these terms can be found in Vallet’s original description of the model [1]. Since the model was initially published, several alternative forms of this equation have been proposed to better resolve differences in primary and secondary atomization. The knowledge of $\Sigma$ allows the prediction of the Sauter mean diameter and the droplet number density via

$$d_{32} = \frac{6 \bar{\rho} \bar{Y}}{\rho_{\Sigma} \bar{\Sigma}} \quad (5)$$

$$n = \frac{\rho_{\Sigma} \Sigma^3}{36 \pi \bar{\rho}^2 \bar{\Sigma}^2} \quad (6)$$

The $\Sigma-Y$ model is primarily based on the spherical droplet interface density (m$^{-1}$) calculations and as such cannot represent the liquid surface of the jet in the near-nozzle region (around 20 diameters downstream of injection). To address this deficiency, Lebas [2] proposed a new formulation for the transport equation of liquid/gas interface per unit mass (m$^{-1}$/kg). The equation takes the following form:

$$\frac{\partial \bar{\rho} \bar{\Omega}}{\partial t} + \frac{\partial \bar{u}_i \bar{\rho} \bar{\Omega}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu_i \frac{\partial \bar{\Omega}}{\partial x_i} \right)$$

$$+$$

$$\frac{\partial}{\partial x_i} \left( \frac{1}{Sc} \frac{\partial \bar{\Omega}}{\partial x_i} \right)$$
\[ \Psi(S_{\text{init}} + S_{\text{turb}}) + (1 - \Psi)(S_{\text{coll}} + S_{\text{solid}}) + S_{\text{vapor}} \]

(7)

Where, \( \Omega = \sum \rho \) and \( \Psi \) is an indicator function for liquid that ranges from 0 (no liquid) to 1 (liquid-only). This indicator function is applied based on the determination of the dense and dilute regions. The function used in current work is taken from Lebas [2] as shown in the sketch below.

The values used for \( \phi_{\text{dense}} \) is 0.5 and for \( \phi_{\text{dilute}} \) is 0.1. The source terms are switched based on the value of the indicator function in the regime at hand.

Other terms are sources for vaporization, collision and breakup, turbulence interaction and surface area at the injector.

Model verification

The \( \Omega \)- Y model was tested on experimental conditions described in [5]. Liquid enters at 12.7 gm/s through a 1.8 mm diameter nozzle while 1.03 gm/s of gas comes through an annular face with internal diameter of 2.3 mm and external diameter of 3.4 mm with a gap of 0.25 mm between the liquid and gas entrance. The axisymmetric computational domain is shown in Figure 1. The mesh is refined to do a grid independence study. The default mesh has cells that are 0.1 mm in size in axial and radial direction in the mixing layer. This mesh is further refined such that the final cell size is 1/15th of the original cell size.

The density of liquid is 1000 kg/m³ and the density ratio varies from about 90 (Case D) to 830 (Cases A, B and C). These cases are defined in Table 1. The momentum flux ratio is defined as:

\[ J = \frac{\rho_g u_g^2}{\rho_l u_l^2} \]

(8)

The model is tested on Cases A and C since experimental data is not available for cases B and D. Case C has the least momentum flux ratio while Case A has the highest.

Results and Discussions

Figure 2 shows the effect of near nozzle mesh size on the liquid fraction along the nozzle axis for Case C. Three mesh sizes were used. The medium and fine mesh results are almost identical and hence medium mesh results were used as the grid independent solution.

The effect of turbulence model on the penetration length was studied by running two cases: one with standard k-ε (SKE) and the other with RNG k-ε model (RNG). The mesh size for this testing was 260K. Figure 3 plots the liquid fraction along the axis of the nozzle for both turbulence models along with experimental data. The RNG model predicts no dispersion of the liquid on the axis until about 20 mm downstream. This is in sharp contrast to the SKE which predicts a liquid fraction of about 0.6; the experimental data at this location shows liquid fraction of around 0.3. Another interesting feature with RNG result is a rather steep drop in the liquid fraction. Apparently, the liquid disperses very quickly and is fully disintegrated within a distance of 10 mm. It is clear that the RNG model under predicts the penetration length. The Standard k-ε predictions are in a better agreement with the experimental data.

Figure 4 and 5 shows the grid independent solution for Case A and D and how it compares with the experimental data. Based on the turbulence model comparison, SKE model was used here. Overall, the agreement is pretty good both quantitatively and qualitatively. However, we did observe a deviation from the experimental data for the lower momentum case (Case D) a few diameters downstream. The liquid core diffuses faster than the measured behavior. This needs to be further investigated by testing the Demoulin’s correction for mixture diffusivity.

Figure 6 shows the SMD plot as obtained from \( \Omega \)-Y implementation for Case A. The SMD is obtained from equation (5). This shows that the surface area density is higher near the nozzle which produces large sizes at the interface of around 55 micron. At 20 mm downstream, on the axis, the calculation predicts an SMD of less than 10 micron.

Figure 7 shows the effect of momentum flux ratio as defined in equation (8) on penetration length. As expected, a shorter liquid penetration length is observed as the momentum flux ratio increases (from Case C to Case A).

Conclusion
The implementation of Ω-Y model in Ansys FLUENT via user-defined function is validated using data provided in [2]. Grid independent studies are carried out and appropriate mesh sizes are chosen for best results. The effects of momentum flux ratio and turbulence model are analyzed and compared to experimental data. Standard k-ε model performs better than the RNG. The momentum flux ratio effect is also in line with expected behavior i.e. a higher gas velocity reduced the liquid penetration length.

More investigations can be carried out to validate the effect of the gap between the liquid and gas inlets on the penetration length. Moreover, the work can be extended by switching to Lagrangian particles in dilute regions of the spray and make it more efficient computationally.

References


Table 1. Four different test conditions (all SI units)

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<td>0.16(J_0)</td>
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Figure 1. Meshed domain with boundary condition

Figure 2. Liquid fraction along normalized nozzle axis for three different meshes (Case C).

Figure 3. Effect of turbulence models on liquid fraction, Case C, medium mesh 260K
Figure 4: Case A: SKE, Near Nozzle liquid fraction

Figure 5: Case D: SKE, Near Nozzle liquid fraction

Figure 7. Effect of increasing momentum flux ratio on the liquid fraction along the axis: Case C shows largest liquid penetration.

Figure 6. SMD, Case A.