Modeling Primary Atomization

Vivek Kumar\(^1\), Shitalkumar Joshi\(^1\), Jochen Schuetze\(^2\), Markus Braun\(^2\) and Muhammad Sami\(^3\)

ANSYS Software Pvt. Ltd., 32/2 Rajiv Gandhi Infotech Park, Pune, 411057, India \(^1\)
ANSYS Germany GmbH, Birkenweg 14a, 64293 Darmstadt, Germany \(^2\)
ANSYS Inc, 15915 Katy Freeway, Houston, TX 77084, USA. \(^3\)

Abstract
The physical processes involved in spray formations are complex. In order to understand these processes, researchers have measured various quantities characterizing different sprays. Based on these studies, numerical models have been proposed that cover various aspects of these processes. One such aspect is the primary atomization or initiation of droplets from a liquid jet. Among the models proposed, \(\Sigma-Y\) model has gained popularity for its simplicity and robustness. In the present study, we validate this model using the Computational Fluid Dynamics Code, ANSYS FLUENT. This model is implemented via a user defined function which makes it flexible for adding any other physical aspects to the model. A 3D test case is setup based on experimental work by Hiroyasu et al \([3]\) and CFD work by Mandloi et.al \([4]\). The computed data is then compared with available experimental data. Liquid penetration length matches well with the available measurements.

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 \([7]\)

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 other hand, Eulerian description may be found appropriate for modeling flow inside the spray and near nozzle zone \([1]\). One such model, \(\Sigma-Y\) model \([1]\), 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 nozzle \([6]\). In this paper, we have studied the \(\Sigma-Y\) approach.

The next section describes the model details and model equation. This is followed by problem set up for simulation to compare to experimental data given in Hiroyasu et al. \([3]\). The results section discusses the performance of \(\Sigma-Y\) model. Conclusions and future works will be explained in the last section.

The \(\Sigma-Y\) Model

The \(\Sigma-Y\) model, originally proposed by Borghi and Vallet \([1]\), 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 \([5, 6, 7, 8, 9]\) since its first introduction. This model is intended for application involving turbulent spray with both high Re and We 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 per unit volume 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 then be used as an input for Lagrangian secondary breakup models which can be used to predict fuel vaporization.

The key assumptions in \(\Sigma-Y\) 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 $\bar{Y} = \frac{\bar{\rho}Y}{\rho}$. The transport equation for $\bar{Y}$ then takes the form:

$$\frac{\partial (\bar{\rho} \bar{Y})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{Y}) - \frac{\partial (\bar{\rho} u' Y')}{\partial x_i} = 0$$

(1)

Where $u'$ denotes the turbulent fluctuations in velocity and $Y'$ denotes turbulent fluctuations in volume fraction.

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

$$\frac{1}{\bar{\rho}} = \frac{\bar{Y}}{\rho_{tiq}} + \frac{1 - \bar{Y}}{\rho_{gas}}$$

(2)

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

$$\bar{\rho} = \frac{\bar{\rho} \rho_{tiq} T_g}{\rho_{tiq}}$$

(2a)

The turbulent diffusion of liquid $u'Y'$ 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.[5] proposed the following term capturing the enhancement of liquid mixing caused by accelerated large density gradients via a Rayleigh-Taylor type mechanism.

$$\bar{\rho} u' Y' = \bar{\rho} \left[ \frac{\rho}{\rho_{tiq}} + \frac{k}{\epsilon} \left( \frac{1}{\rho_g} + \frac{1}{\rho_{di}} \right) \bar{Y}(1 - \bar{Y}) \right] \frac{d\bar{Y}}{dx_i}$$

(3)

With the large scale flow features described, a transport equation for the evolution of the interfacial surface area ($\Sigma$) 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 generalized derivation, having terms capturing the effects of convection, diffusion, surface stretching and coalescence.

$$\frac{\partial (\Sigma)}{\partial t} + \nabla \cdot (D_a \nabla \Sigma) + \frac{1}{\tau_{prod}} \Sigma - \frac{1}{\tau_{destr}} \Sigma^2 = 0$$

(4)

where, $D_a$ is an appropriate diffusion coefficient. Here $\tau_{prod}$ a time scale representing the rate at which turbulence creates surface area, and $\tau_{destr}$ 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

$$\frac{d_{S2}}{\rho_{tiq} \Sigma} = 6$$

(5)

$$n = \frac{\rho_{tiq} \Sigma^3}{36\pi \bar{\rho}^2 \bar{Y}^2}$$

(6)

Model verification

The model was tested on experimental conditions described in [3] and [4]. Nozzle diameter is 0.3mm. The domain chosen here is a 6 degree slice with radius 30mm and extended to 100mm in axial direction. Computational domain is shown in figure 1. Mesh is shown in figure 2. Only one layer of cell is created in azimuthal direction. The nozzle exit section is resolved with 6 elements as shown in figure 3 and subsequently refined to do a grid independence study. A typical element size near the nozzle is 25 microns in axial direction and 30 micron in radial direction. The mesh size is grown in axial and radial direction at a fixed growth rate of 1.006 for all three meshes.

The boundary condition is shown in Figure 2. Chamber pressure is initialized with 5Mpa which corre-
sponds to test case-3 of [4]. Mass flow at the nozzle exit is 5.13g/s.

As suggested by Pope [10] and verified in [7], round jet correction for turbulence is used in this study.

Results and Discussions

The effect of mesh size on penetration length is shown in Figure 4. Here Penetration length is defined as the axial distance up to which 97% of mass of liquid injected is found. The results are close to identical for medium and fine grids which suggest that a grid-independent solution is achieved. The experimental measurements are also plotted in the same plot and the result from current $\Sigma$-Y model implementation seems to marginally overpredict the experimental measurements. For remainder of this section, the results will be shown for medium grid.

Figure 5 shows the effect of including source terms in turbulent kinetic energy equation and turbulent dissipation energy equation in the new formulation ($\Sigma$-Y model) on penetration length. Clearly, turbulent dispersion of liquid in gas is affected by the inclusion of these source terms which is over predicted without these modifications. Liquid penetration prediction is vastly improved in the new formulation.

Currently the transition of $\Sigma$-Y Eulerian model to Lagrangian particles is not implemented as a part of the code. For the time being, Sauter mean diameter of the particle is computed as a part of the post-processing using Equation 5. The same has been plotted in Figure 6. Here only those cells are selected where liquid fraction is within a certain range which gives SMD in the range 0.1 $\mu$m to 20 $\mu$m. The shape of the spray at 4ms is shown in Figure 7 using contours of liquid fraction.

Conclusion

An Eulerian model commonly referred to as $\Sigma$-Y model is implemented in Ansys FLUENT using user-defined function and has been successfully tested against experimental measurements of Hiroyasu et. al. [3]. The correction in the source terms for turbulence equations results in a better prediction of penetration length. This work needs to be further extended to make switch to Lagrangian particles in dilute regions of the spray as Lagrangian model are ideally suited in this region and offer less computational efforts.

References


Acknowledgement: The authors would like to acknowledge Shitanshu Gohel, Rajarao P.L and Ankit Adhiya for their contribution during the implementation of the code and subsequent testing.
Figure 1. 3-D 6 degree slice domain showing symmetry planes

Figure 1. Meshed domain with boundary condition

Figure 3. Mesh close to the nozzle exit. (Nozzle is slightly extended to account for uniform profiles at inlet

Figure 4. Liquid penetration for three different meshes.

Figure 5. Comparison of new Σ-Y model formulation with default model for Liquid penetration length

Figure 6. Sauter Mean Diameter based on equation.5 is shown (clipped between 0.1 µm to 20µm)
Figure 7. Spray shape characterized by liquid fraction at 4ms.