

Eulerian CFD Modeling of Coupled Nozzle Flow and Spray with Validation Against X-Ray Radiography Data

Qingluan Xue

Argonne National Laboratory

Michele Battistoni

Universita degli Studi di Perugia

Sibendu Som

Argonne National Laboratory

Shaoping Quan, P. K. Senecal, and Eric Pomraning
Convergent Science Inc.

David Schmidt

Univ. of Massachusetts

Abstract

This paper implements a coupled approach to integrate the internal nozzle flow and the ensuing fuel spray using a Volume-of-Fluid (VOF) method in the CONVERGE CFD software. A VOF method was used to model the internal nozzle two-phase flow with a cavitation description closed by the homogeneous relaxation model of Bilicki and Kestin [1]. An Eulerian single velocity field approach by Vallet et al. [2] was implemented for near-nozzle spray modeling. This Eulerian approach considers the liquid and gas phases as a complex mixture with a highly variable density to describe near nozzle dense sprays. The mean density is obtained from the Favreaveraged liquid mass fraction. The liquid mass fraction is transported with a model for the turbulent liquid diffusion flux into the gas. Simulations were performed in three dimensions and the data for validation were obtained from the x-ray radiography measurements Kastengren et al. [3] at Argonne National Laboratory for a diesel fuel surrogate *n*-dodecane. The quantitative and time-resolved data consisting of fuel mass distribution and spray velocity in the near nozzle dense spray region are used to validate the coupled Eulerian approach. A standard k - ϵ Reynolds Averaged Navier Stokes based turbulence models is implemented in this study and the influence of model constants are evaluated. The effect of grid size is also evaluated by comparing the fuel distribution against experimental data. Finally, the fuel distribution predicted by the coupled Eulerian approach is compared against classical Lagrangian spray model results. The coupled Eulerian approach provides a unique way of coupling the nozzle flow and sprays so that the effects of in-nozzle flow can be directly realized on the fuel spray.

CITATION: Xue, Q., Battistoni, M., Som, S., Quan, S. et al., "Eulerian CFD Modeling of Coupled Nozzle Flow and Spray with Validation Against X-Ray Radiography Data," *SAE Int. J. Engines* 7(2):2014, doi:10.4271/2014-01-1425.

INTRODUCTION

High injection pressure and direct injection techniques are extensively implemented to achieve better air-fuel mixture formation for controlling combustion and pollutant formation processes. This has necessitated further understanding of the in-nozzle flow and near-nozzle spray phenomena both experimentally and numerically. For example, researchers

across the world have made many contributions in these areas in the Engine Combustion Network (ECN) [4] in the past few years.

The discrete droplet method (DDM) [5] has been widely used in the traditional Lagrangian-Eulerian approach for modeling fuel sprays in Internal Combustion Engines (ICEs). The Lagrangian-Eulerian approach treats the gas-phase in an Eulerian manner while the liquid phase is modeled in a

Lagrangian fashion with sub-models for many physical processes. This traditional approach together with some amount of model calibration has been a great success for modeling the spray, mixture formation, combustion, and engine-out emissions (NO_x, Particulates) [6][7][8][9][10][11][12]. The known challenges for this model are the mesh dependency and near-nozzle dense spray assumptions. The mesh dependency is attributed to the mass, momentum, and energy coupling between the discrete droplets and carrier gas phase, and the spray sub-models. The Adaptive Mesh Refinement (AMR) method has been implemented to numerically better resolve the interphase transfer with local high mesh resolution [13][14][15]. Grid convergence studies for fuel spray with a Reynolds Averaged Navier Stokes (RANS) turbulence model were conducted by Senecal et al. [16][17] on finest mesh resolutions of 0.03125mm by using AMR and fixed embedding techniques. Schmidt and Senecal [18] and Hou and Schmidt [19] developed a new collision algorithm with a secondary collision mesh. Schmidt and Rutland [20] and Are et al. [21] developed a collision sub model, a collision mesh approach, and second-order gas-to-liquid coupling to better predict the dense spray on a typical mesh size using the RANS approach within the Lagrangian-Eulerian framework. The other issue is the dense spray near nozzle region which may not be accurately described by the Lagrangian approach. Different models of injection are proposed to mimic the physics of the primary atomization in this dense region. For example, the 'blob' model of Reitz [22] is widely used.

The Eulerian-Eulerian approach for spray modeling has made significant progress in the past decade. Bekdemir et al. [23] predicted diesel combustion characteristics using a mesoscopic Eulerian formalism for the dispersed liquid phase in the in-house AVBP solver. An injector model was implemented [24] to deal with the dense spray region close to the injector. This model uses algebraic relations to bridge the dense region by imposing physical flow conditions at a distance approximately 10 nozzle diameters downstream of the injector outflow plane. An Eulerian model was originally proposed by Vallet et al. [2] for the atomization of a liquid jet which considered atomization as turbulent mixing process. Recently, variations of this model have been implemented by several groups to study its capability for near nozzle and farfield sprays [25, 26, 27, 28, 29]. The global parameters such as liquid penetration, Sauter Mean Diameter (SMD), and axial velocity are compared with measurements.

Another critical component for accurate spray modeling is that the boundary conditions for the spray should be linked with innozzle flow simulations. Schmidt et al. [30][31] developed a mixture-based model to calculate the cavitating nozzle flow considering thermodynamic equilibrium and non-equilibrium conditions. Zhao et al. [32] implemented and validated the above mixture-based model in a VOF method for in-nozzle flow simulations. Battistoni et al. [33] compared different modeling approaches for in-nozzle flows against x-ray measurements of cavitating flows. It is well known from literature that the turbulence, cavitation, and nozzle geometry can directly impact

the spray development. The incorporation of these findings into modeling the spray inlet conditions can facilitate spray models to be more predictive in nature. Som et al. [34] has developed the Kelvin Helmholtz - Aerodynamic Cavitation Turbulence (KH-ACT) primary breakup model to include the effects of cavitation, turbulence, and in-nozzle geometry by statically coupling the nozzle flow simulations with the Lagrangian spray. Since the nozzle flow features are incorporated in the model, the predicted spray dispersion, spray axial velocity, and spray cone angle showed improvement when compared with x-ray data. The effects of nozzle flow and geometry on the combustion and emissions were also shown in diesel engine conditions [11, 35].

Quantifying the nozzle geometry, needle transients (i.e., movement profile and off-axis motion), and near nozzle spray has been a great challenge for diagnostic techniques. Several optical techniques have been used to characterize spray parameters under both combusting and non-combusting conditions. The data-set from these studies include spray penetration, cone angle, liquid length, flame lift-off length, and the velocity field near nozzle region [36, 37, 38]. While these diagnostics have provided important insights regarding the farfield spray behavior, they can provide limited data regarding the internal structure of the fuel spray. Limited success has been achieved by the advanced optical diagnostics to overcome the optical density limitations in the dense spray regime. To overcome the limitations of optical diagnostics in the dense spray region, x-ray radiography technique has been developed as a spray diagnostics [39, 40, 41] tool. Since the main interaction between x-rays and fuel spray is absorption, this technique allows for quantitative measurements in the dense spray region thus providing unique insights into the internal spray structure. The x-ray technique has been used to characterize the near-nozzle distribution of fuel sprays under a wide variety of ambient and injection conditions.

It is clear from our literature review that Eulerian-Eulerian models existing in literature have not been extensively tested on their ability to capture near nozzle fuel distribution. The xray radiography technique provides quantitative information on the near nozzle internal fuel spray structure. The major objective of this study is to implement a turbulent-mixing based Eulerian model to resolve the near nozzle dense spray region by linking the nozzle flow simulations with downstream spray development. This is motivated by the need for predictive near nozzle spray models. The coupled nozzle flow and Eulerian spray simulations are extensively validated against x-ray radiography data. Following model validation, parametric studies are conducted to assess the influence of different turbulence model constants, Schmidt number effects, and mesh resolution on near nozzle fuel distribution. The coupled Eulerian spray model is also compared against state-of-the-art Lagrangian spray simulations.

The paper is arranged as following: first the model implementation and numerical algorithms are introduced. Then the computational domain and set-up is briefly described.

followed by the description of ECN experimental conditions for Spray A under non-evaporating conditions. Robust validation of the coupled Eulerian approach is presented next followed by parametric studies on the influence of model constants on near nozzle fuel distribution. Finally, the conclusion is drawn.

GOVERNING EQUATIONS AND NUMERICAL METHOD

In an Eulerian model [2], the gas and liquid fuel are described as a single fluid mixture. It is assumed that the large-scale flow features dominate rather than the smaller scale structures under the high Reynolds number and Weber number condition encountered in the near nozzle dense spray region. The governing equations are summarized here.

Fuel mass fraction ($\tilde{Y}$) transport equation:

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

where u' and Y' are the turbulent fluctuation in velocity and liquid fuel mass fraction. The last term of the right-hand-side is the source term due to evaporation which is zero in this case since the simulations are performed under non-evaporating conditions. Under the assumption of an immiscible two-phase mixture, the mass averaged density of the mixture is given by:

$$\frac{1}{\bar{\rho}} = \frac{\tilde{Y}}{\rho_l} + \frac{1-\tilde{Y}}{\bar{\rho}_g} \quad (2)$$

Here, the gas density is governed by an equation of state $\bar{\rho}_g = \bar{p} / (R_g \tilde{T})$ and liquid phase has a constant density. Here 'p' is the cell pressure, R_g is the gas constant calculated by $R_g = R/W_g$ with universal gas constant (R), gas molecular weight W_g , and 'T' is the cell temperature.

The closure for the liquid mass transport in Eqn. (1) is based on a standard turbulent gradient flux model:

$$\bar{\rho} \tilde{u}_i \tilde{Y}' = \frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}}{\partial x_i} \quad (3)$$

where Sc_t is the turbulent Schmidt number which is an input to the model.

Momentum equation is given as:

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = - \frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (4)$$

where σ_{ij} and τ_{ij} are the viscous and modeled Reynolds stress tensor respectively. τ_{ij} is calculated using the classical Boussinesq eddy viscosity concept:

$$\tau_{ij} = \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \bar{\rho} k \delta_{ij} \quad (5)$$

δ_{ij} is the Kronecker delta. The standard $k-\epsilon$ model is used to close the Eqn. (5):

$$\mu_t = \bar{\rho} C_\mu \frac{k}{\epsilon} \quad (6)$$

Turbulent kinetic energy (k) is given by,

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i k}{\partial x_i} = \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{\mu}{Pr_{tke}} \frac{\partial k}{\partial x_j} \right) - \bar{\rho} \epsilon \quad (7)$$

where the turbulent dissipation (ϵ) is transported by,

$$\begin{aligned} \frac{\partial \bar{\rho} \epsilon}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \epsilon}{\partial x_i} &= \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{Pr_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) - C_{\epsilon 3} \bar{\rho} \epsilon \frac{\partial \tilde{u}_i}{\partial x_i} \\ &+ \left(C_{\epsilon 1} \frac{\partial \tilde{u}_i}{\partial x_j} \tau_{ij} - C_{\epsilon 2} \bar{\rho} \epsilon \right) \frac{\epsilon}{k} - \bar{\rho} R \end{aligned} \quad (8)$$

where R is dependent on the turbulence model, $C_{\epsilon 1}$, $C_{\epsilon 2}$, and $C_{\epsilon 3}$ are model constants with values of 1.44, 1.92, and -1.0, respectively for standard $k-\epsilon$ model.

Energy equation ($\tilde{e}$):

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{e}}{\partial x_i} &= - \bar{P} \frac{\partial \tilde{u}_i}{\partial x_i} + \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial}{\partial x_i} \left(K \frac{\partial \tilde{T}}{\partial x_i} \right) \\ &+ \frac{\partial}{\partial x_i} \left(\bar{\rho} D_t \sum_m \tilde{h}_m \frac{\partial \tilde{Y}_m}{\partial x_i} \right) \end{aligned} \quad (9)$$

where K , $\tilde{T}$, D_t , and $\tilde{h}_m$ are conductivity, turbulent diffusion, gas temperature, and enthalpy of species m , respectively.

A VOF method is used to model the two-phase flow [32] in CONVERGE [42]. In the VOF method, a void fraction α is used to represent the volume fraction of liquid and gas, and is defined as follows:

$$\alpha = \begin{cases} = 0: \text{the cell is filled with pure liquid} \\ = 1: \text{the cell is filled with pure gas} \\ (0,1): \text{the cell is filled with both liquid and gas} \end{cases}$$

Typically, the void fraction can be solved with a conservation equation. In the present work, the void fraction is not solved directly from a transport equation. Instead, it is calculated with the transported mass fraction by:

$$\alpha = \frac{(1 - \tilde{Y})/\bar{\rho}_g}{(1 - \tilde{Y})/\bar{\rho}_g + \tilde{Y}/\rho_l} \quad (10)$$

where $\tilde{Y}$ is the mass fraction and the subscripts 'g', 'l' denote gas or liquid.

COMPUTATIONAL DOMAIN AND CONDITIONS OF SPRAY A

The single-hole Spray A injector and conditions from the ECN were used to validate the Eulerian model applied to coupled nozzle flow and spray. The x-ray radiography data for validation is obtained under non-evaporating conditions with ndodecane as the fuel. Since these experiments are performed in cold spray conditions the ambient pressure is changed to ensure the same ambient density as Spray A baseline condition. Further details about the experimental set-up are provided in Table 1 [3]. It should be noted that the x-ray data is ensemble-averaged over multiple shots. These ensemble-averaged data is compared against RANS based calculations. The number of shots used for average is from 32 at the near nozzle exit to 256 at farther downstream depending the noise. The uncertainties of measured projected mass density are 1% at the near nozzle region and 2% further downstream.

Table 1. The conditions for non-evaporating Spray A experiments at Argonne National Laboratory

Fuel	n-Dodecane
Ambient composition	0% O ₂
Ambient temperature (K)	303
Ambient density (kg/m ³)	22.8
Injection pressure (MPa)	150
Fuel injection temperature (K)	333
Nozzle diameter (mm)	0.09
Injection duration (ms)	1.5
Total mass injected (mg)	3.5

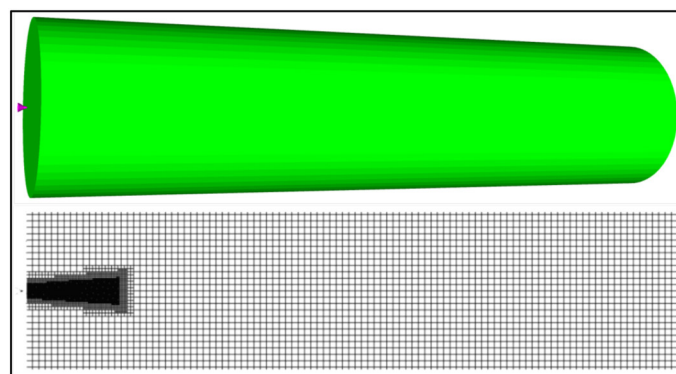


Figure 1. The three-dimensional computational domain (top) and mesh (bottom) for Spray A simulations.

Three-dimensional simulations were performed by coupling the nozzle calculation with the downstream spray. The 3-D computational domain and 2D cut-plane view of the mesh for the simulations are shown in Figure 1 along with the Spray A injector (the red small region on the top-left image). A close view of the fuel injector is also shown in Figure 2. It can be clearly seen from this image that the nozzle orifice is offset and is not centrally located on the sac. The spray chamber is cylindrical (Diameter × Length = 50 mm × 200 mm) and has similar dimensions as the one used in experiments. Fixed embedding (as shown in the Figure 1) was used in the near nozzle region with base line grid size of 2 mm. For the model validation purposes, three different minimum grid sizes i.e., 15 μm, 30 μm, and 60 μm, are simulated in this study. These fine resolutions are embedded inside the nozzle orifice and a few diameters downstream inside the spray chamber. The corresponding nozzle diameter to cell size ratios are: 6, 3, and 1.5 respectively. The transient inlet boundary condition was specified by imposing a needle movement profile measured in experiments [3]. The needle transients include both needle-lift and needle “off-axis” (wobble) motions, as shown in Figure 2.

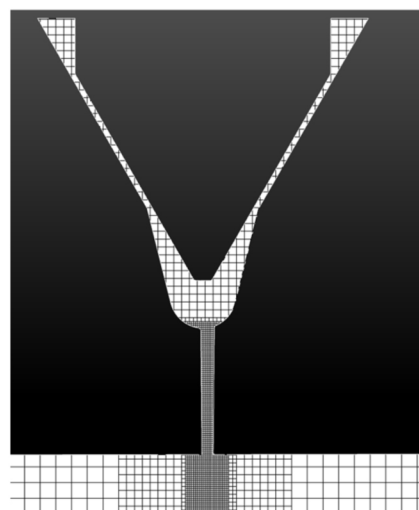


Figure 2. (Top) A zoomed view of the nozzle along a cut-plane showing the mesh generated in the seat, sac, orifice, and nozzle exit regions. (Bottom) The needle-lift and wobble profiles for the Spray A simulations are also shown