

Effects of Numerical Schemes on Large Eddy Simulation of Turbulent Planar Gas Jet and Diesel Spray

Chi-Wei Tsang and Christopher Rutland
Univ. of Wisconsin Madison

ABSTRACT

Three time integration schemes and four finite volume interpolation schemes for the convection term in momentum equation were tested under turbulent planar gas jet and Sandia non-reacting vaporizing Spray-H cases. The three time integration schemes are the first-order Euler implicit scheme, the second-order backward scheme, and the second-order Crank-Nicolson scheme. The four spatial interpolation schemes are cubic central, linear central, upwind, and vanLeer schemes. Velocity magnitude contour, centerline and radial mean velocity and Reynolds stress profiles for the planar turbulent gas jet case, and fuel vapor contour and liquid and vapor penetrations for the Diesel spray case predicted by the different numerical schemes were compared. The sensitivity of the numerical schemes to mesh resolution was also investigated. The non-viscosity based dynamic structure subgrid model was used. The numerical tool used in this study was OpenFOAM. Results showed that the first-order Euler implicit schemes predict wider range of length scales as seen in velocity and fuel vapor contour plots, while the second-order time integration schemes predict more small scale structures. The non-monotonic central schemes show less grid sensitivity than the monotonic schemes. Overall the cubic central scheme with the Euler implicit scheme gives the best performance. The first-order upwind scheme gave poor results, so it should be avoided to use in simulating high-pressure fuel injection process.

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INTRODUCTION

In recent years, large-eddy simulations (LES) have been used for simulating fuel injection process in internal combustion (IC) engines. As pointed out by Rutland [1], two of the expectations of LES are more flow structures and better predictive capability. Based on these two expectations, LES should be a better tool than Reynoldsaveraged Navier-Stokes (RANS) method to accurately predict spatial and temporal mixing of IC engine flows, and become a promising tool for improving engine efficiency and reducing emissions. In this study, we are particularly interested in fuel injection process in Diesel engines. This process is characterized by very high injection pressure (on the order of 100 MPa), two phases, and a wide range of length scales (two to three order of magnitude difference between injector hole diameter and cylinder diameter). These characteristics make LES of Diesel spray challenging. To meet the expectations of LES, good physical models and good numerical methods are equally important to overcome these challenges.

Physical models include liquid and gas phase sub-grid models, and spray sub-models such as atomization, drag, and vaporization. Researchers have been making substantial efforts on developing these models to capture complex physics involved in spray injection process. Review of spray and sub-grid models can be found in references [1] and [2].

Numerical methods and schemes for solving LES spray governing equations are also important. To capture more flow structures, eddies, and vortices, low-dissipative numerical schemes should be used. The choice of numerical schemes for LES spray may be more crucial than RANS spray simulations. However, compared to the literatures related to developments of physical models, literatures related to the effects of numerical schemes on LES spray are relatively few. Therefore, one of the purposes of this study is to investigate the numerical scheme effects. Hori et al. [3] studied the effects of numerical scheme for the convective term in momentum equation. They implemented a higher-order scheme named as Cubic-Interpolated Pseudo-Particle (CIP) into the KIVALES code. It was found that lower order monotonic scheme, QSOU (Quasi-Second Order Upwind) are too dissipative to capture development of vortex structures and unsteady behavior of sprays, while the third-order accurate CIP scheme is more capable of reproducing unsteady motion, and predicts vapor penetration well. Zhou et al. [4] compared the QSOU scheme and the third-order upwind MUSCL (Monotone Upstream-centered Schemes for Conservation Laws). They also found that the eddy structures of spray are suppressed using the QSOU scheme. In contrast, the MUSCL scheme shows better vapor penetration prediction even in coarser grid. These two studies are focused on the effects of numerical scheme for the convection term in the momentum equation. In addition to this, the time integration scheme for momentum equation is also important for predicting unsteady evolution of spray jet. It is known that the higher-order time

scheme can reduce phase error of numerical solutions. In this study, not only the effects of spatial discretization scheme but also time integration schemes are discussed.

The mesh resolution required to obtain reasonable predictions is of interest. Senecal et al. [5] did a grid convergence study for LES spray using the CONVERGE code [6,7]. It was found that the recommended grid size for simulating the Engine Combustion Network constant-volume spray bomb [8] is equal to or smaller than 0.125 mm. Although this paper did not describe what numerical scheme used for convection terms, only 1st order upwind and 2nd order central schemes are available. Also, if the flow becomes non-monotonic, the 2nd order central scheme is switched to the 1st order upwind scheme. This study was done using one numerical scheme. However, different numerical schemes may require different resolution levels to achieve grid convergence. Ideally, the required grid density to achieve grid convergence should be investigated in each numerical scheme, and grid-converged results predicted by different schemes are compared. But this would be computationally expensive particularly for lower-order schemes in full three-dimensional two-phase turbulent flow simulations. Thus, the aim of this study is to investigate how different numerical schemes behave in a number of selected mesh resolutions even if grid convergence has not achieved. The open-source CFD toolbox, OpenFOAM version 2.1.1 [9] is used in this study.

LES MOMENTUM EQUATION AND SUB-GRID MODELS

The compressible LES momentum equation is written as

$$\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \bar{p} + \nabla \cdot (\bar{\rho} \nu \nabla \tilde{\mathbf{u}}) + \nabla \cdot \bar{\rho} \nu \left((\nabla \tilde{\mathbf{u}})^T - \frac{2}{3} \nabla \cdot \tilde{\mathbf{u}} \mathbf{I} \right) - \nabla \cdot \boldsymbol{\tau} + \bar{\mathbf{S}}_{mom} \quad (1)$$

where $\bar{\rho}$ is the filtered density, $\tilde{\mathbf{u}}$ is the Favre-averaged filtered velocity, $\bar{p}$ is the filtered pressure, ν is the kinematic viscosity, and $\bar{\mathbf{S}}_{mom}$ is the spray momentum source term. The sub-grid stress tensor $\boldsymbol{\tau}$ is defined as

$$\tau_{ij} = \bar{\rho} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j). \quad (2)$$

The dynamic structure model with additional artificial viscosity [10] is applied to close this term,

$$\tau_{ij} \approx \frac{2L_{ij}}{L_{kk}} \bar{\rho} k_{sgs} - 2\bar{\rho} \nu_{noz} \left(\tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) \quad (3)$$

where L_{ij} is the Leonard stress tensor $\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j$ and $\tilde{S}_{ij}$ is the filtered strain rate tensor $\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$. The artificial viscosity term is modeled as

$$\nu_{noz} = \begin{cases} C_{noz,1} \Delta k_{sgs}^{1/2}, & \frac{|\tilde{S}| \Delta^2}{\nu_{\mathcal{L}}} \geq C_{noz,2} \\ 0.0, & \text{otherwise} \end{cases} \quad (4)$$

where $|\tilde{S}| = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}$ is the characteristic velocity which is averaged injection velocity for Diesel spray, and L is the characteristic length which is nozzle hole diameter for Diesel spray, Δ is the cell size defined as $(\Delta x \Delta y \Delta z)^{1/3}$. The two constants $C_{noz,1}$ and $C_{noz,2}$ are chosen to be 5.0 and 0.42 respectively. The artificial viscosity is only added in the near-nozzle region where strain rate is high. The purpose of adding this term is to enhance sub-grid mixing in the near-nozzle region. The sub-grid kinetic energy k_{sgs} is obtained from solving the transport equation,

$$\begin{aligned} \frac{\partial \bar{\rho} k_{sgs}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} k_{sgs}) \\ = -\boldsymbol{\tau} : \tilde{\mathbf{S}}_{ij} - C_e \bar{\rho} \frac{k_{sgs}^{3/2}}{\Delta} + \nabla \cdot (\bar{\rho} C_k \Delta k_{sgs}^{1/2} \nabla k_{sgs}) + \bar{W}_{s,sgs} \end{aligned} \quad (5)$$

where the two constants C_e and C_k are 0.3 and 0.05 respectively. The term $\bar{W}_{s,sgs}$ accounts for the spray-subgrid interactions [11]. Species and energy equation are also solved. Detailed formulation and subgrid models for these two equations can be found in [10].

The planar gas jet case considered in this study is incompressible, isothermal and single-phase, so Eq. (1) can be reduced to

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}} \bar{\mathbf{u}}) = -\frac{1}{\bar{\rho}} \nabla \bar{p} + \nu \nabla^2 \bar{\mathbf{u}} - \frac{1}{\bar{\rho}} \nabla \cdot \boldsymbol{\tau}. \quad (6)$$

For the plane jet, since the velocity gradients are not as strong as the diesel spray, ν_{noz} is zero in the whole domain.

NUMERICAL SCHEMES FOR SOLVING THE MOMENTUM EQUATION

In this study, the pressure-implicit with splitting of operators (PISO) method [12] was used for solving Navier-Stokes equations. One predictor and two corrector steps are utilized. In this study, we are focused on the effects of time integration scheme and discretization scheme for the convection term in the predictor step. Three different time integration schemes are studied: **Euler implicit (EI)**, **backward differencing (BD)**, and **Crank-Nicolson (CN)** schemes. The finite-volume formulation of Eq. (1) with the EI method for solving the momentum equation can be written as

$$\frac{\bar{\rho}_p \tilde{\mathbf{u}}_p^* - \bar{\rho}_p \tilde{\mathbf{u}}_p^n}{\Delta t} V_p + \sum_f F \tilde{\mathbf{u}}_f^* - \sum_f (\bar{\rho} \nu)_f \mathbf{S} \cdot (\nabla \tilde{\mathbf{u}})_f^* = R V_p. \quad (7)$$

A variable name with the subscript p , with the subscript f , with the superscript n , and with the superscript $*$, mean the value of that variable at the centroid of the cell p , at the face f of cell p , at the previous time-level n , and at the intermediate step during the splitting process, respectively. Note that the new time-level is denoted as $n + 1$. The term, F , is the mass flux, $\mathbf{S} \cdot (\bar{\rho} \tilde{\mathbf{u}}^n)_f$ where $\mathbf{S}$ is the face area vector. To get $\bar{\rho}^n$ and $\tilde{\mathbf{u}}^n$ at cell face belonging to two adjacent cells, the linear interpolation using the two values stored at those two cell centroids is utilized. The term, $\mathbf{R}$, is the discretization form of the sum of the terms other than $\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t}$, $\nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}})$, and $\nabla \cdot (\bar{\rho} v \nabla \tilde{\mathbf{u}})$ in Eq. (1). All variables in $\mathbf{R}$ are at the previous time-level n . Since the focus on this study is the discretization of the convection term, detailed formulation of the spatial discretization of the diffusion term and the source term $\mathbf{R}$ is not described here. Detailed finite-volume formulation of these terms can be found in [13]. The EI method is first-order accurate in time.

The BD method is written as

$$\frac{3\bar{\rho}_p \tilde{\mathbf{u}}_p^* - 4\bar{\rho}_p \tilde{\mathbf{u}}_p^n + \bar{\rho}_p \tilde{\mathbf{u}}_p^{n-1}}{2\Delta t} V_p + \sum_f F \tilde{\mathbf{u}}_f^* - \sum_f (\bar{\rho} v)_f \mathbf{S} \cdot (\nabla \tilde{\mathbf{u}})_f^* = \mathbf{R} V_p. \quad (8)$$

The only difference between the EI and the BD methods is the discretization of the $\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t}$ term. Note that the BD method uses velocity at time-level $n - 1$. This method is second-order accurate in time.

The CN method is written as

$$\frac{\bar{\rho}_p \tilde{\mathbf{u}}_p^* - \bar{\rho}_p \tilde{\mathbf{u}}_p^n}{\Delta t} V_p + \frac{1}{2} \left[\sum_f F \tilde{\mathbf{u}}_f^* + \sum_f F \tilde{\mathbf{u}}_f^n \right] - \frac{1}{2} \left[\sum_f (\bar{\rho} v)_f \mathbf{S} \cdot (\nabla \tilde{\mathbf{u}})_f^* + \sum_f (\bar{\rho} v)_f \mathbf{S} \cdot (\nabla \tilde{\mathbf{u}})_f^n \right] = \mathbf{R} V_p. \quad (9)$$

The CN method is also second-order accurate in time.

To obtain the value at cell face, $\tilde{\mathbf{u}}_f^*$ or $\tilde{\mathbf{u}}_f^n$, interpolation using the values stored at cell centroids must be performed. In this study, four different interpolation schemes are studied. They are: **first-order upwind**, **linear central**, **cubic central**, and **vanLeer** schemes. To illustrate the differences of these schemes, one-dimensional Cartesian grid with uniform grid size as shown in Figure 1 is considered. The first-order upwind scheme for a scalar variable ϕ_f at the cell face, which can be a vector component of $\tilde{\mathbf{u}}_f^*$ or $\tilde{\mathbf{u}}_f^n$ is of the form

$$\phi_f = \begin{cases} \phi_{p_2} & \text{for } F \geq 0 \\ \phi_{p_3} & \text{for } F < 0 \end{cases} \quad (10)$$

The linear central scheme is of the form,

$$\phi_f = \frac{1}{2} (\phi_{p_2} + \phi_{p_3}). \quad (11)$$

The cubic central scheme is written as

$$\phi_f = \frac{-3\phi_{p_1} + 27\phi_{p_2} + 27\phi_{p_3} - 3\phi_{p_4}}{48}. \quad (12)$$

The vanLeer scheme is of the form,

$$\phi_f = \phi_{p_2} + \Psi \left[\frac{1}{2} (\phi_{p_2} + \phi_{p_3}) - \phi_{p_2} \right] \text{ if } F \geq 0 \quad (13)$$

where Ψ is the flux limiter. For the vanLeer scheme,

$$\Psi = \Psi(r) = \frac{|r| + r}{1 + |r|} \quad (14)$$

where the consecutive gradient r is defined as

$$r = \frac{\phi_{p_2} - \phi_{p_1}}{\phi_{p_3} - \phi_{p_2}} \text{ if } F \geq 0. \quad (15)$$

Note that ϕ_{p_1} , ϕ_{p_2} , ϕ_{p_3} , ϕ_{p_4} , and ϕ_f are all at the same time-level. That is, they are all at the intermediate step of the splitting process denoted as $*$, or the previous time-level denoted as n .

It can be seen that the vanLeer scheme is a blend of the second-order central and the first-order upwind schemes with the flux limiter. The first-order upwind scheme and the vanLeer schemes belong to a class of the total variation diminishing (TVD) schemes, which prevent spurious oscillations arising from non-TVD schemes. The linear central and the cubic central schemes are non-TVD schemes. Note that the linear central and the cubic central are both second-order accurate in space, but it can be shown that the truncation error of the cubic scheme is six times smaller than the linear scheme if uniform grid is used. The orders of accuracy of these four interpolation schemes were verified by numerically solving the one-dimensional wave equation using OpenFOAM. Results can be found in Appendix II.

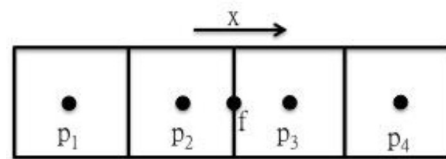


Figure 1. One-dimensional Cartesian grid with uniform grid size.

In this study, we tested six different combinations of the time integration and the interpolation schemes for the convection term in the momentum equation, as listed in [Table 1](#).

Table 1. Six combinations of numerical schemes for momentum equation to be tested.

	Time integration scheme	Interpolation scheme for the convection term in the momentum equation
Case 1	Euler implicit (EI)	Cubic central
Case 2	Euler implicit (EI)	Linear central
Case 3	Euler implicit (EI)	First-order upwind
Case 4	Euler implicit (EI)	vanLeer
Case 5	Backward differencing (BD)	Cubic central
Case 6	Crank-Nicolson (CN)	Cubic central

Numerical schemes for species, energy, and sub-grid kinetic energy equations do not change in this study. The Numerical schemes for these equations are listed in [Table 2](#).

Table 2. Numerical schemes for species, energy and sub-grid kinetic energy equations.

Time integration scheme for k_{sgs} , enthalpy, and species transport equations	Euler implicit (convection and diffusion terms are implicit, and other terms are explicit)
Convection term for k_{sgs}	TVD second order central with the Sweby limiter [14]
Convection term for enthalpy and species	First order upwind

SPRAY MODELS

The traditional Lagrangian-Eulerian approach is employed [15,16] where the spray is characterized in terms of computational parcels, with each parcel representing a statistical sample of droplets having the same size, temperature, velocity, physical position, and chemical composition. The droplet atomization, breakup, vaporization, and drag force are described by a number of spray sub-models listed in [Table 3](#). The difference between the traditional and the stochastic breakup model is that the KH breakup time model constant is determined dynamically and stochastically according to local flow conditions in the stochastic model. The stochastic KH-RT model has improved the prediction of liquid and vapor penetrations. Detailed formulation of the model and validation are in [Appendix I](#).

Table 3. Spray sub-models.

Breakup and atomization	Stochastic Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) model [17]
Dispersion	Stochastic Gaussian distribution [11]
Drag	Amsden <i>et al.</i> [18]
Vaporization	Amsden <i>et al.</i> [18]
Collision and coalescence	none

TEST CASES SETUP

Two test cases were selected in this study to test numerical schemes effect. The first case is a turbulent planar gas jet, and the second case is Engine Combustion Network (ECN) Spray-H [8].

Turbulent Planar Gas Jet

The planar gas jet is a statistically two-dimensional flow. It develops mainly in the streamwise x-direction and spreads in the lateral y-direction. It is statistically homogeneous in the spanwise z-direction. The Reynolds number of this flow is defined as $Re = U_j d / \nu$. The injection velocity is denoted as U_j and d is the slot height of the nozzle. The Reynolds number is 30,000 in this simulation. We chose three sets of data from experiments ([19], [20], and [21]) and two sets of data from direct numerical simulation (DNS) ([22] and [23]) to compare against our LES results. It should be noted that the Reynolds numbers from these five sets of data range from 3,000 to 30,000. In other words, inflow conditions such as turbulence levels and momentum thicknesses are different in these five cases. These discrepancies have major impacts on the position of the virtual origin, the core length, the position where self-similarity is achieved, but have minor effects on the self-similar profiles. The Reynolds number of the experiment done by Gutmark and Wignanski [21] is 30000, which is identical to the current LES study.

The mesh used in the plane gas jet simulations is shown in [Figure 2](#). The domain dimensions are $L_x/d = 225$, $L_y/d = 150$, and $L_z/d = 20$. Note that the domain size in the y direction is about the same as the experiments done by Gutmark and Wignanski [21]. This diminishes the effects of the upper and the lower boundaries on the development of the jet. The mesh has three levels of grid resolution as noted in the different regions displayed in [Figure 2](#). The jet develops mainly in the inner region where the finest mesh is used. Two different mesh resolutions of the inner region are studied. The resolution is $\Delta x/d = \Delta y/d = \Delta z/d = 0.5$ or 0.25 . In the intermediate region, the resolution is $\Delta x/d = \Delta y/d = \Delta z/d = 1.0$. The outer region allows a substantial extension of the physical domain and is instrumental in the assignment of boundary conditions far from the jet inlet. We do not collect any flow statistics in this region. The corresponding resolution is $\Delta x/d = \Delta y/d = \Delta z/d = 2.0$. The number of total cells for the $\Delta x/d = 0.5$ case is around one million and 4.28 million for the $\Delta x/d = 0.25$ case.

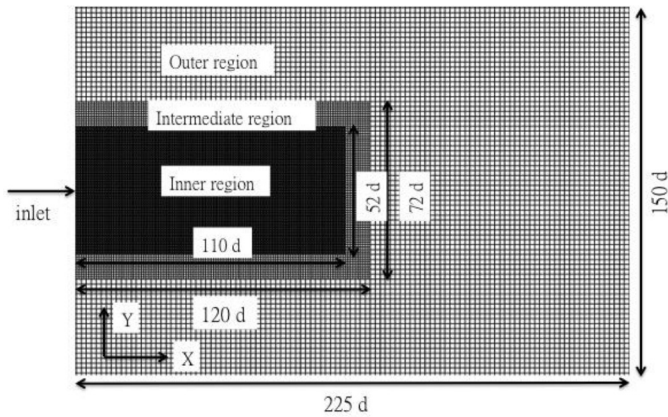


Figure 2. 2-D cut-plane of the plane jet mesh.

The top-hat-like velocity profile is used for the velocity boundary condition at inlet,

$$u = \frac{U_j}{2} + \frac{U_j}{2} \tanh\left(\frac{-|y| + 0.5d}{2\theta_m}\right), v = w = 0.0, \quad (16)$$

where θ_m is the momentum thickness. We set it equal to $d/20$. The injection velocity U_j is 9 [m/s] and the diameter d is 5×10^{-2} [m]. Neumann boundary conditions are used for k_{sgs} and v_{sgs} at the inlet. Neumann boundary conditions and slip boundary conditions for the velocity field are used at the outlet and the upper/lower wall, respectively. For the pressure field, all boundaries use the Neumann boundary condition except for the outlet where the pressure is set to be zero. Periodic boundary conditions are used in the homogeneous z-direction. The initial k_{sgs} is chosen to be $0.4 \text{ m}^2/\text{s}^2$, where it is assumed that the sub-grid velocity u' is ten percent of the injection velocity U_j . The computational time step is determined dynamically based on the maximum Courant number criterion. In this simulation, the max Courant number is limited to 0.3.

ECN Spray-H

Fuel is injected from a round single-hole injector into a constant volume chamber with high pressure (4.4 MPa), high temperature (1000 K), and 0% oxygen. The temperature and pressure reflect conditions in a combustion chamber in a typical diesel engine, but no chemical reactions occur. Experimental conditions of Spray-H are listed in Table 4. The injection profile used in the simulation follows the ECN recommended injection rate as shown in Figure 3. The injection duration is 6.8 ms, but due to computational resource we only simulated the injection until 1.5 ms.

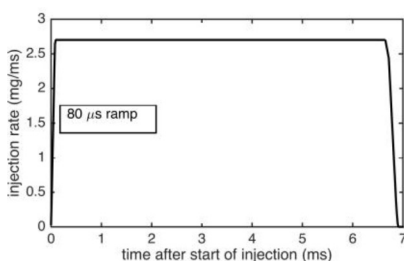


Figure 3. Spray-H injection profile used in the simulation.

Table 4. Spray-H experimental conditions.

Fuel	100 % n-heptane
Oxygen concentration	0 %
Ambient temperature [K]	1000
Ambient density (kg/m³)	14.8
Nozzle hole diameter [mm] (single hole)	0.1
Fuel injection pressure [MPa]	154
Total injection mass [mg]	17.8
Injection duration [ms]	6.8

Figure 4 shows the 2-D cut plane of the computational mesh. The injection position is at the cell node instead of the cell center in order to distribute momentum to more than one cell, and parcels come out at a fixed point rather than within a disc. No internal nozzle flow simulations were performed in this study. Three levels of grid resolutions were tested, 0.5 mm, 0.25 mm, and 0.125 mm as shown in Figure 4. Note that the size of the cells at the spray axis is larger than the injector hole diameter even the smallest grid size 0.125 mm is used, so the length scales near the nozzle may not be adequately resolved. However, this size is typical, or even finer, for engineering applications. The number of cells for the 0.5 mm, 0.25 mm, and 0.125 mm are 0.48 million, 1.93 million, and 12 million.

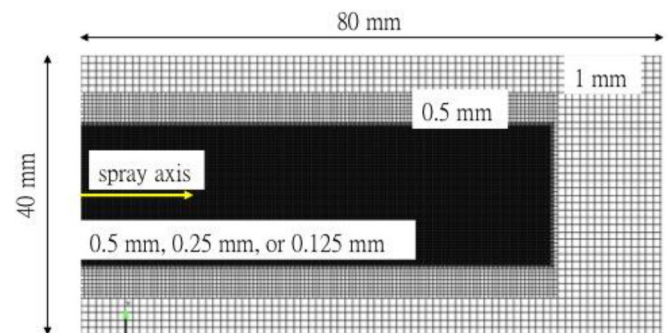


Figure 4. 2-D cut plane of the Spray-H mesh.

Table 5 shows the time step size and total parcel number used in the three different mesh resolutions. Note that the fixed time step size is used. Time step size is reduced by a factor of 2 and parcel number is increased by a factor of 4 when mesh size is reduced by a factor of 2. The reason for increasing the parcel number in finer mesh is to ensure sufficient number of parcels in each cell. The maximum Courant number is smaller than 0.6 for all mesh resolutions and all numerical schemes.