Simulation of 3-D Disinfectant Spray to Study Optimal Spray Cone Angle and Discharge Rate

Submitted by

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ABSTRACT

Despite the controversies surrounding the use of disinfectant tunnel, they are still used in many partsof the world as an augment to the fight against SARS-CoV-2. Since 99 percent [10] of such disinfectant spray is water, it is necessary to use it efficiently to conserve water. So,one of the ways to conserve the water is to increase the coverage area of the spray for the given disinfectant fluid. This project aims to present 3-dimensional simulation of spray and to obtain the optimum discharge and spray cone angle to have the maximum coverage area using OpenFOAM -v7. In this project, I have used sprayFoam solver; RAS (k-epsilon) turbulence model; the discrete medium is water. The discrete medium is treated as water because 99% of disinfectant is water.

1. INTRODUCTION

Sprays are utilized in a wide variety of applications consisting of cooling combustion, agriculture, disinfection and medicine. Disinfecting the public areas, public, medical appliances etc has become the most fundamental step to control the spread of COVID-19. Generally, Chlorine is used as disinfectant because it is cheaper and easily available. The disinfectant consists of 99% of water and 1% of Chlorine. Since, the usage of disinfectant spray of disinfectant has been increased. So, the wastage of water. This requires to optimize different parameters associated with the spray flow to conserve water. The spray of water in air is studied using Eulerian-Lagrangian model. Here, air is the continuous medium and is modelled using Eulerian approach and Water droplets are the dispersed medium and studied using Lagrangian approach. The solver uses two way coupling process to link the two phases in a computational domain so they will affect each other. In two way coupling process, the flow characteristics of water droplets will be affected by air like the aerodynamic drag etc and the governing equations of air will be modified due to the presence of water droplet in the cell. To control the wastage of water it is important to have the maximum coverage area and the penetration length (Figure 01). In the simulation, I have used full cone spray nozzle. Full-cone spray nozzle covers the complete circular region. I have considered parameters like discharge rate and the angle of spray for having maximum spray coverage area.

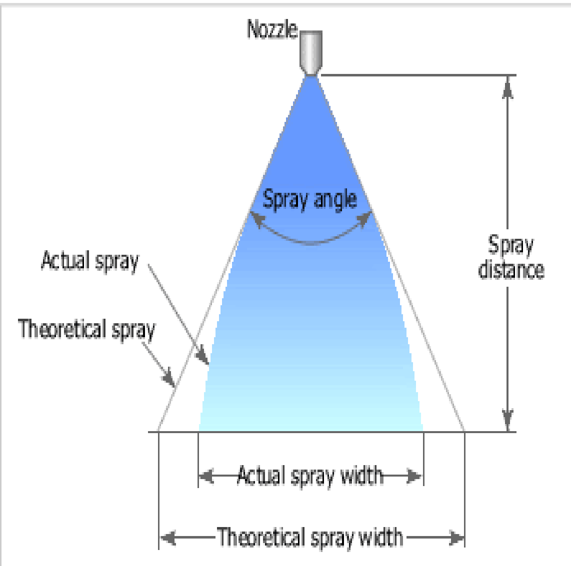

Fig. 01: specification of nozzle spray (wikipedia[6])

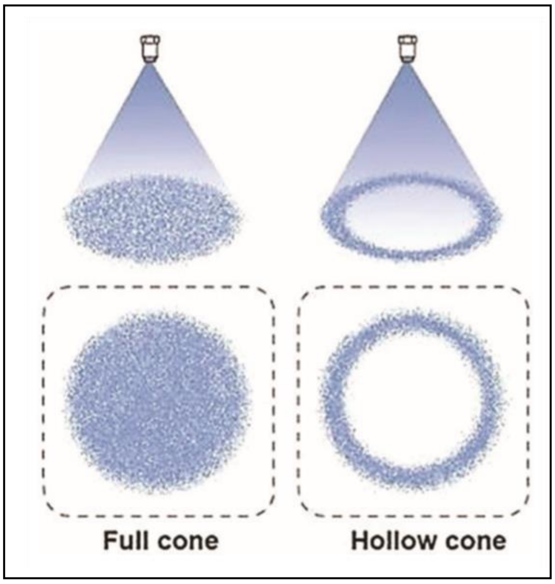

Fig. 02: Schematic diagram of full-cone and hollow-cone pressure-swirl atomizers. (Mohammad Amin Hassan et al.,2018[1]).

Injected water undergoes many complicated processes like primary breakup (Atomization), secondary breakup, dispersion, evaporation, droplet size distribution etc. It is important to consider each process for correct simulation. When water is injected into air it starts forming the ligaments due to the Kelvin Helmholtz instabilities. This is called primary breakup or atomization. The interaction between liquid and gas phase creates turbulence and aerodynamic forces which act on the liquid droplets and it leads to the disintegration of ligament into even smaller droplets which is known as secondary Breakup (Figure 04). It is important to notice that the reason of disintegration of water in the primary and secondary break up is different. Break up of water into smaller droplets is the very important process because water/disinfectant is sprayed as mist so that the it will not wet the body. The droplet size becomes so small that it will evaporate quickly from the body/object which has been disinfected. It is also equally important to have lower limit of diameter of droplets. Otherwise, it may be affected by the turbulence in air, may evaporate so quickly from the object/body that it will unable to disinfect them. There is a wide range of diameter present in the spray. The droplet size can be defined using different types of diameter e.g. SMD (Sauter Mean Diameter), MMD (Mass Mean Diameter), Volume Mean Diameter (VMD). There are 3 different regimes in spray: 1. Dense (In this regimes, Primary and secondary breakup happen and liquid sheet breakup and collision happens),2. Dilute (Interaction between the droplet phase and the gaseous phase is of higher importance) and 3. Very dilute regime (2-phase interaction is less significant) (Fig. 05).

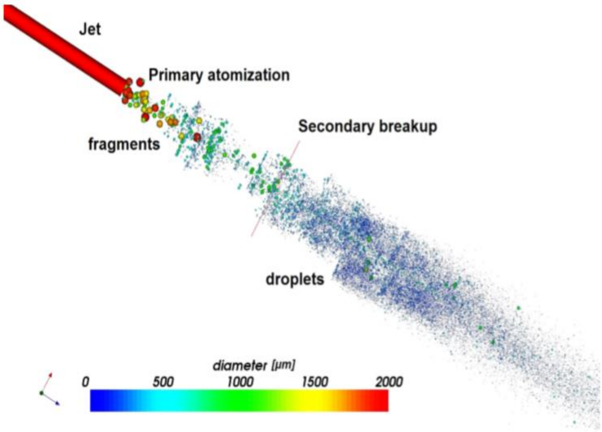

Fig. 04: Different regions in the Lagrangian phase model, coloured by liquid diameter. (Rasmus Gjesing et.al, 2009[4])

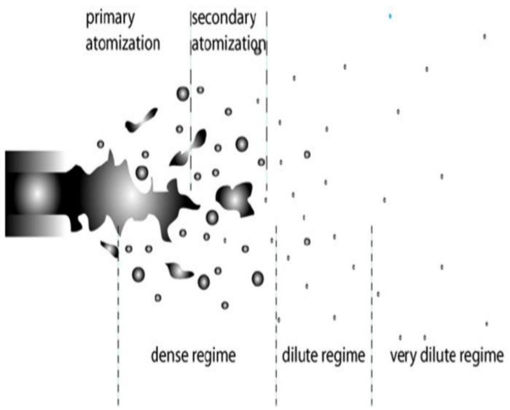

Fig. 05: Different flow regimes during spray injection process (Tariq Ahmed Adul Kalam, 2015[12]).

Evaporation is the natural process which has to be included here because the change of phase (either from liquid to vapour or vapour to liquid) will affect the governing equation of both the phases. Since evaporation will lead to reduce the mass of water and increase the mass of vapour in the computational domain. Similarly, Condensation will lead to increase mass of liquid and decrease the mass of vapour. Both the cases have to be incorporated into the governing equations of both the phases. Turbulence occurs in the computational domain due to gaseous phase, dispersion of water droplets. Turbulence also occurs at the interface of water droplet and gaseous phase but it is very complex process to perform so usually it is avoided. Collisions occur between the water droplets and it results in momentum transfer between them. There are many properties have to be studied for spray to have a good result. For that purpose, I have provided my whole case setup along with my report.

The governing equations for the Eulerian Phase (gas)

1. Conservation of Mass

$$\frac{\partial \rho_g u_j^g}{\partial x_j} = 0$$

2. Conservation of Momentum

$$\rho_g \frac{\partial u_j^g}{\partial t} + \rho_g u_j^g \frac{\partial u_j^g}{\partial x_j} = -\frac{\partial P_g}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu_j \frac{\partial u_i^g}{\partial x_i}\right) - \frac{M_p}{\rho_g} + F$$

The governing equations for the Lagrangian phase (droplets)

The governing equations are solved on each particle (here droplets). So, I am providing the most trivial form of the governing equations for lagrangian approach. It can be modified further as per the extra terms required depending upon the cases. M is mass of particle, (x, y, z) is the particle position, (u, v, w) is the particle velocity. F is the total force on the particle. In this case only gravity and drag force have been considered. $\dot{Q}$ is the net heat exchange and $\dot{W}$ is the net work done. E is the total energy transfer.

1. Continuity Equation

$$M = \text{Constant}$$

2. Equation of Motion

$$\frac{\partial x}{\partial t} = u; \quad \frac{\partial y}{\partial t} = v; \quad \frac{\partial z}{\partial t} = w$$

$$\frac{\partial (Mx)}{\partial t} = \sum F_x; \quad \frac{\partial (My)}{\partial t} = \sum F_y; \quad \frac{\partial (Mz)}{\partial t} = \sum F_z \quad \text{(Conservation of Momentum)}$$

$$\sum F = \sum F_x + \sum F_y + \sum F_z$$

$$\sum F = F_D + F_G$$

$$F_D\,\text{(Drag Force)} = m_p \frac{18\mu}{\rho_p d_p^2} \frac{C_d R_e}{24} (\vec{u} - \overrightarrow{u_p})$$

$$F_G = M * g$$

3. Energy Equation

$$\frac{\partial E}{\partial t} = \dot{Q} - \dot{W}$$

2. CASE SETUP

The computation domain used for the setup is 20cm *30cm*20cm (figure 06). The diameter of the nozzle is 1.54mm. The pressure injection is 5 atm. The sprayed liquid is water and it is sprayed in air. The grid size is 2mm in all the three directions. This grid size gives grid independent results (Mohammad Amin Hassan et al.,2018[1]).

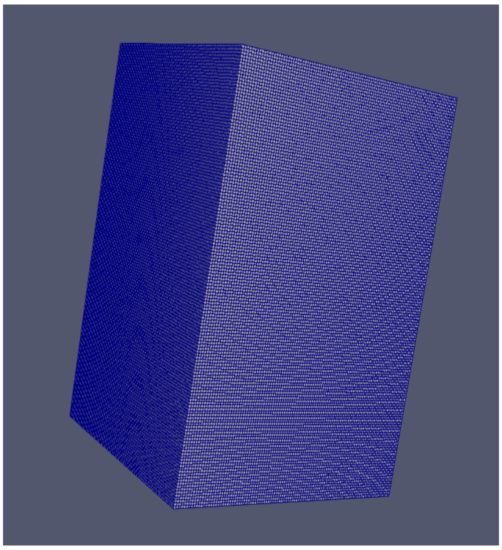

Fig. 06: Computational Domain

The boundary conditions and Initial Conditions are provided in table 01. The constant folder consists of gravity (g) file, sprayCloudProperties file, turbulence property and thermophysicalProperty file. Gravity file contains the value of acceleration due to gravity (9.8 m/s^2). The sprayCloudProperties file contains the properties of spray and nozzle. The turbulence property file consists of the turbulence model used in the case setup. I have used RAS (K-epsilon model). The other properties of turbulence are kept as default (like in the 0 file). Thermophysical file consists of the values of thermophysical properties, Nature of mixture, names and properties of different species present in the domain for complete simulation. I have kept as the default setup of aachenBomb tutorial. I have only replaced ethanol with water. Within the thermophysicalProperty file, there is a reference folder called chemkin. Chemkin consists of chemical, transport and thermo properties of sprayed water and air constituents. Some spray constant properties are provided in table number 2. For rest properties my case setup file can be referred.

This project presents two cases

1. Case 01: Validation case setup
2. Case 02: Optimization Case setup

The difference between both the cases is the setting of 2 parameters i.e. flow discharge rate and cone angle. The optimization case setup has been taken from Ghasem Ghavami Nasr et al., 2012[11].

For Case 01: Cone Angle is 56^0 and flow rate 0.05 Kg /s.

For Case 02: Cone Angle is 45^0 and flow rate is 9.2 Kg/s.

S. No.	Parameters	Conditions
1.	Velocity	Internal Field Condition: - 0m/s
		Wall Condition: Fixed Value (0m/s) at each wall
2.	Pressure	Internal Field Condition: 1 atmosphere
		Wall Condition: zeroGradient at each wall.
3.	Temperature	Internal Field Condition: - 298.15 K
		Wall Condition: zeroGradient at each wall.
4.	N2	Internal Condition: 0.766
		Wall Condition: zeroGradient at each wall
5.	O2	Internal Condition: 0.234
		Wall Condition: zeroGradient at each wall

Table: 01 (Initial and Boundary Conditions)

S. No.	Parameters	Values
1.	Type of spray	Cone Injection
2.	Mass Total	0.1288 Kg
3.	Injection Method	Disc
4.	Injection Pressure	5e5 Pa
5.	Inner diameter of cone	0
6.	Half outer diameter of cone	22.5
7.	Duration	14e-3 s
8.	Position of nozzle	(0.10 m, 0.29 m ,0.10 m)
9.	Parcel/second	2e7
10.	C_d	0.9
11.	Flow rate	9.2 Kg/S

Table: 02 (Some spray properties for case 2)

3. RESULTS

3.1 Validation

My case setup is same as that of the validation paper except for some parameters due to the unavailability of those data in the paper. I have provided the graph 01 which compares the penetration length of my case set up and case setup in Mohammad Amin Hassan et al.,2018[1]. There is some deviation between both the results due to the differences in some parameters like range of droplet diameter, some properties of spray, air etc; I was able to capture the physics of the spray agreed to the Mohammad Amin Hassan et al.,2018[1] and trend of the penetration graphs are same for both the results (Fig. 06).

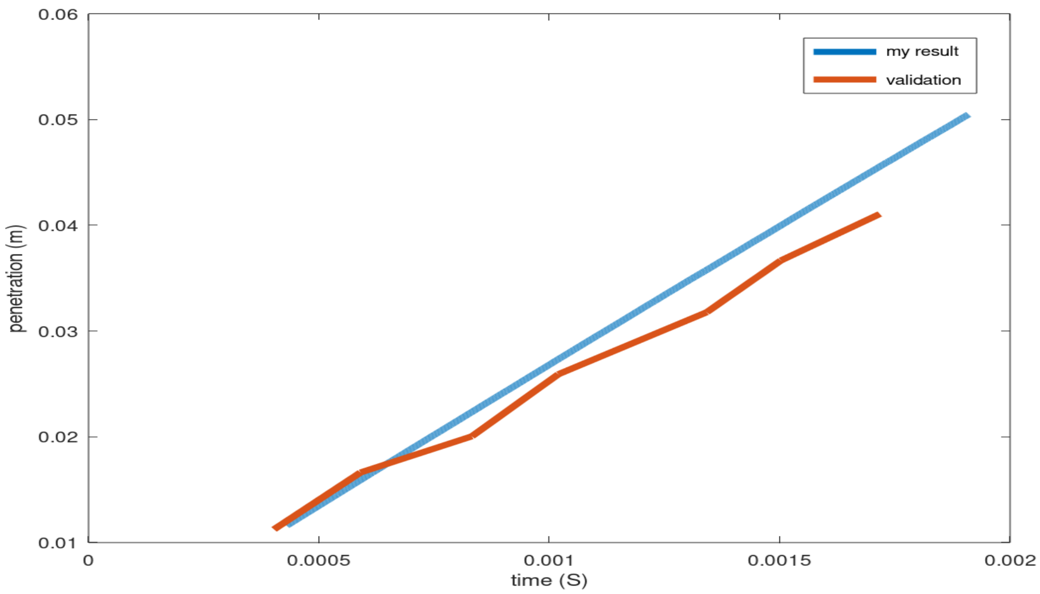

Fig 06: Validation Graph

3.2 Results obtained after optimization

Figure 07 and figure 08 represent the side view and the cross section of coverage area at 0.16 m below the nozzle at 7 ms. The highest water fraction can be seen in the middle portion as it was expected from experiments. Figure 09 and figure 10 show the comparison between the coverage area of both the case setup. For case 01, at 9 ms, the spray has reached 0.07 m below the nozzle, the diameter of maximum coverage area is 0.01 m, and water fraction at the centre of the coverage area is 92 % larger than that on the circumference. For Case 02, at 7 ms, the spray has covered 0.16 m below the nozzle, the diameter of the maximum coverage area is 0.15 m, and water fraction at the centre of the coverage area is 91% larger that on the circumference.

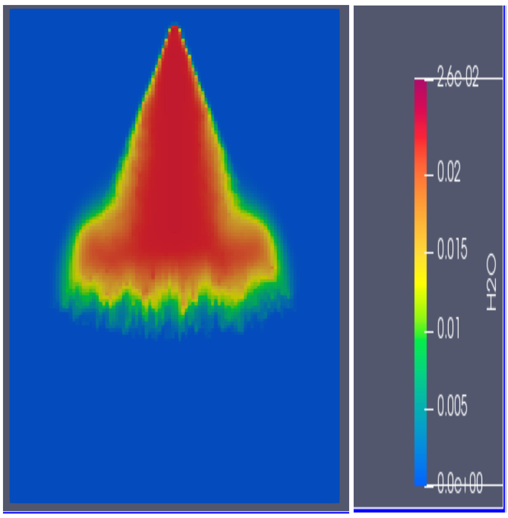

Fig. 07: Side view of spray

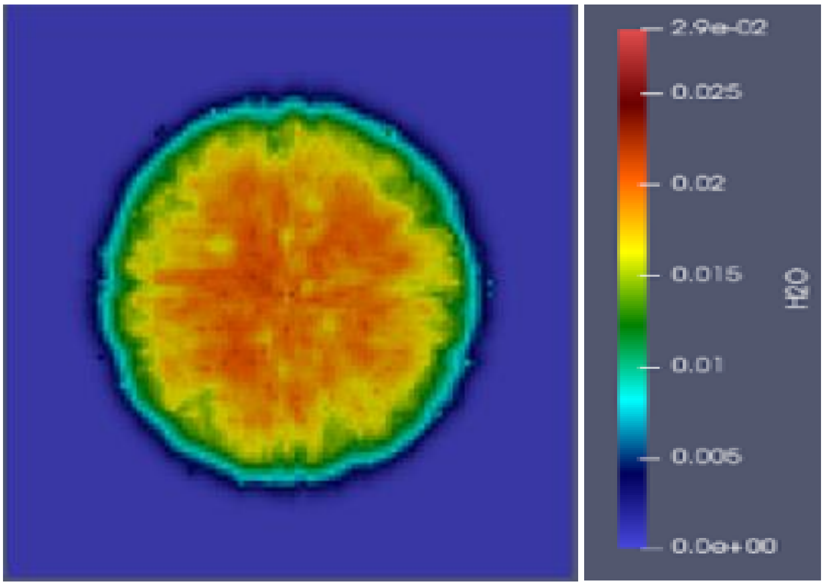

Fig. 08: Coverage Area

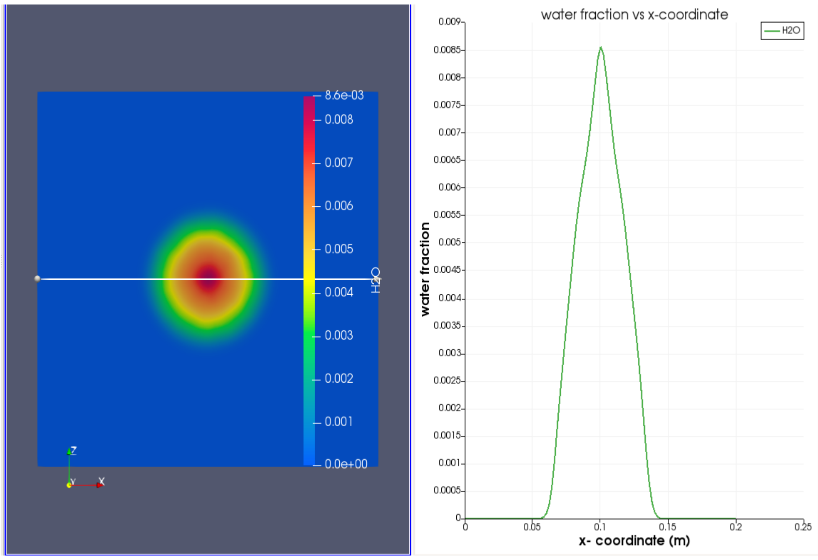

Fig. 09: Case 1 (Before Optimization) at 9ms and 0.07m below nozzle

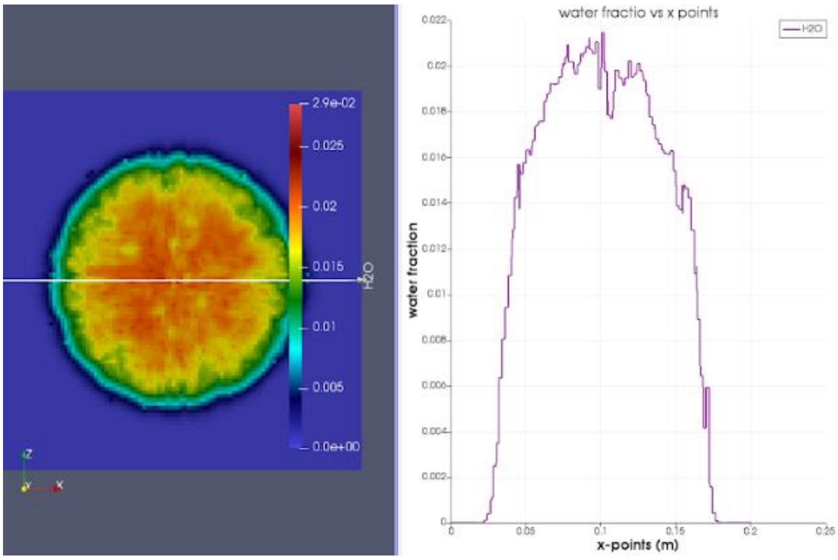

Fig. 10: Case 2 (After Optimization) at 7ms and 0.16m below the nozzle

4. CONCLUSIONS

The obtained results agree with the results of Mohammad Amin Hassan et al.,2018[1]. So, I can conclude that using sprayFoam solver and OpenFOAM software correct results for spray modelling can be expected. The results for case 02 clearly show that spray has covered more distance below the nozzle in smaller time than that of the case 01. The lesser time taken by the spray to reach the destination point helps in conserving water; coverage area is increased by 75%. So, it can be concluded from this project that by varying discharge rate and cone angle larger coverage area can be obtained.

5. FUTURE SCOPE

I have changed only 2 parameters and much better results for having maximum coverage area is expected by increasing the injection pressure. More factors influencing water spray have to be considered to make it more feasible and practical.

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