

# **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.

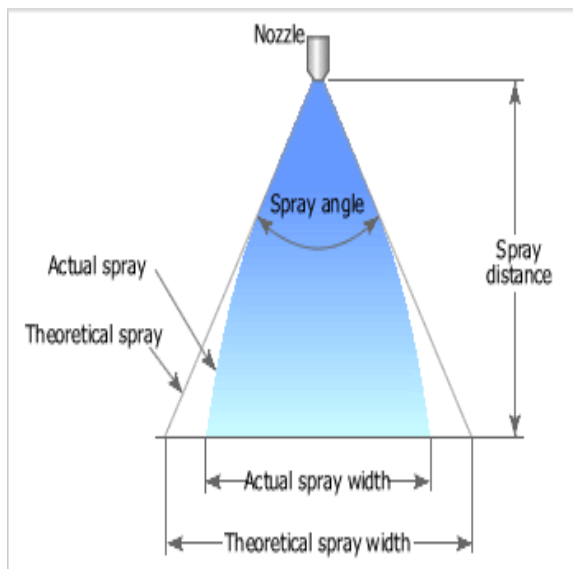


Fig. 01: specification of nozzle spray (wikipedia<sup>6</sup>)

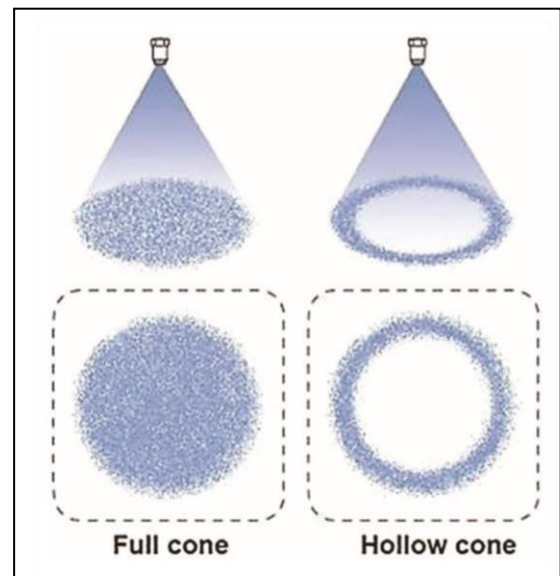


Fig. 02: Schematic diagram of full-cone and hollow-cone pressure-swirl atomizers. (Mohammad Amin Hassan et al.,2018<sup>1</sup>).

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).

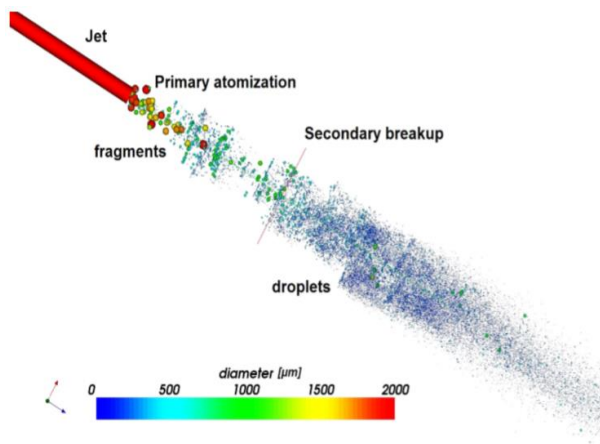


Fig. 04: Different regions in the Lagrangian phase model, coloured by liquid diameter. (Rasmus Gjesing et.al, 2009<sup>4</sup>)

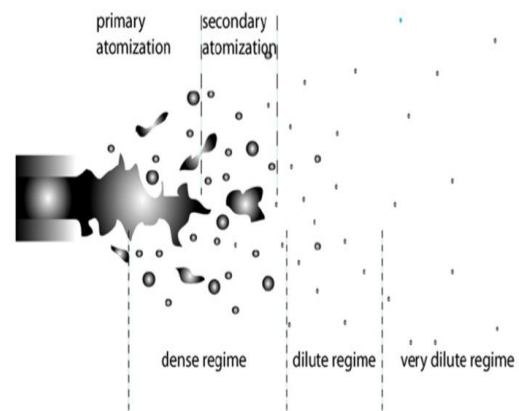


Fig. 05: Different flow regimes during spray injection process (Tariq Ahmed Abdul Kalam, 2015<sup>12</sup>).

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

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

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

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

$$\sum F = F_D + F_G$$

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

$$F_G = M * g$$

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<sup>1</sup>).

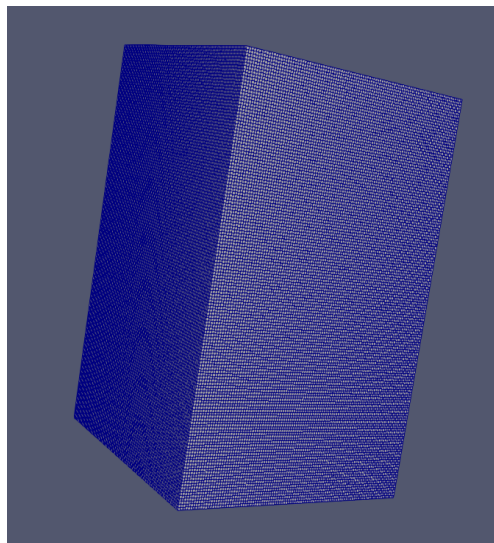


Fig. 06: Computational Domain

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 ( $9.8 \text{ m/s}^2$ ). 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<sup>11</sup>.

For Case 01: Cone Angle is  $56^\circ$  and flow rate  $0.05 \text{ Kg/s}$ .

For Case 02: Cone Angle is  $45^\circ$  and flow rate is  $9.2 \text{ Kg/s}$ .

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<sup>1</sup>. 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<sup>1</sup> and trend of the penetration graphs are same for both the results (Fig. 06).

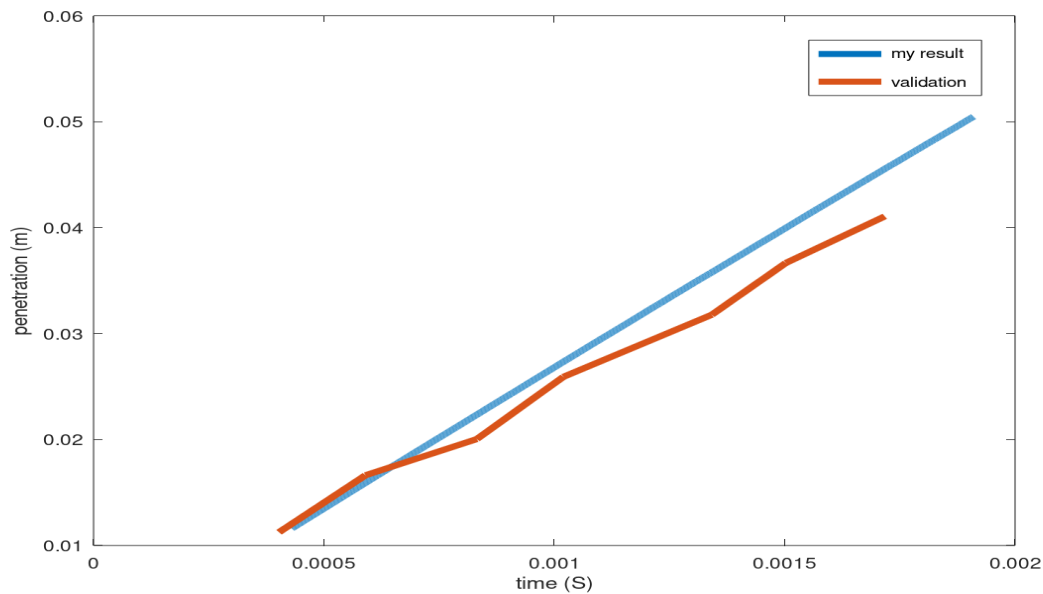


Fig 06: Validation Graph

#### 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 than that on the circumference.

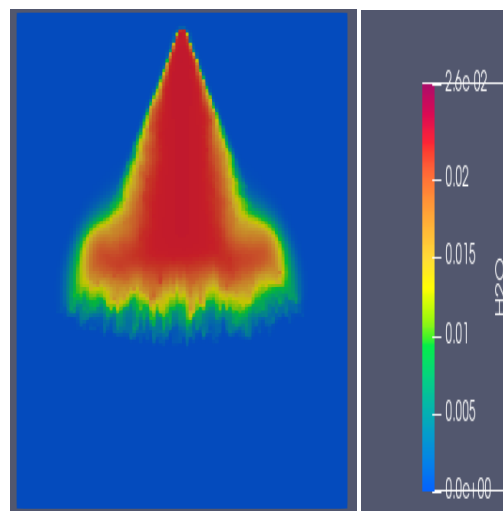


Fig. 07: Side view of spray

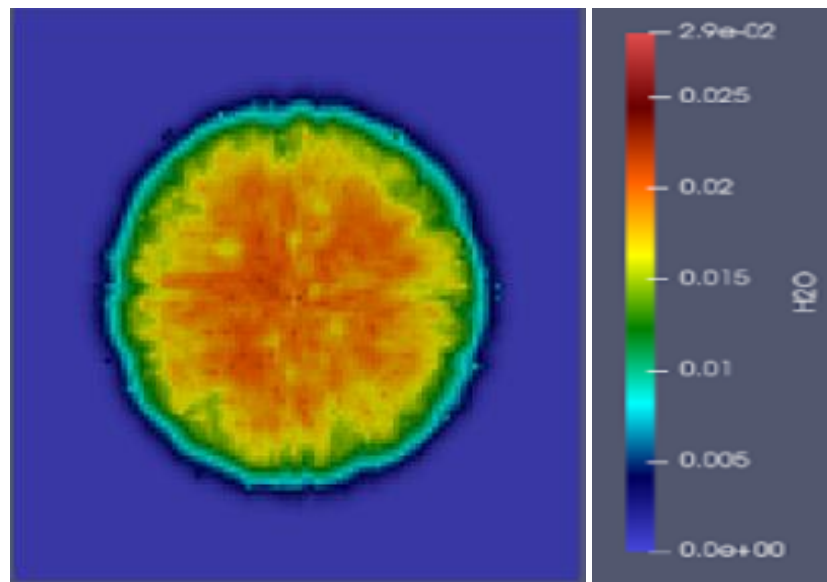


Fig. 08: Coverage Area

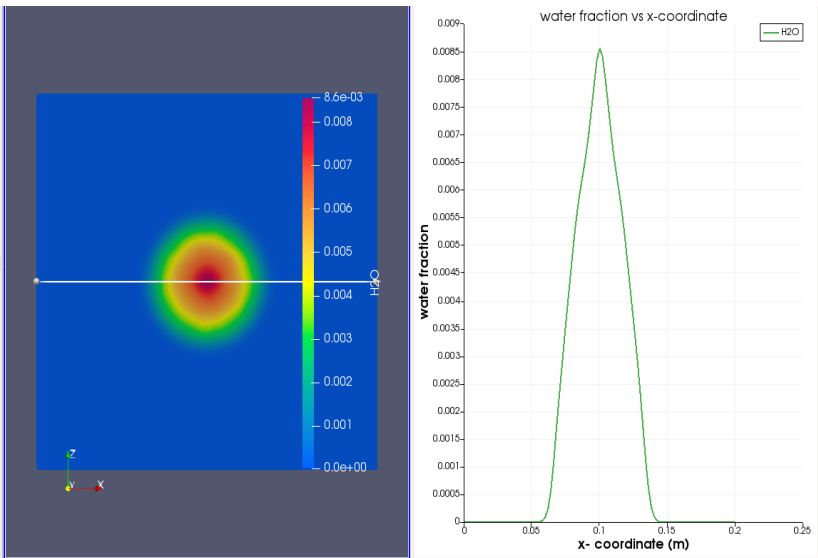


Fig. 09: Case 1 (Before Optimization) at 9ms and 0.07m below nozzle

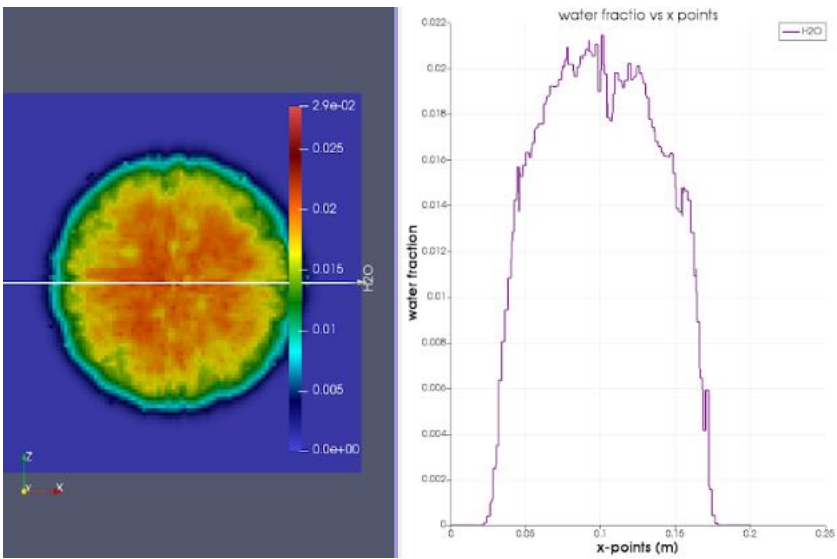


Fig. 10: Case 2 (After Optimization) at 7ms and 0.16m below the nozzle

#### 4. CONCLUSIONS

The obtained results agree with the results of Mohammad Amin Hassan et al.,2018<sup>1</sup>. 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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12. Tariq Ahmed Adul Kalam Azad,"Computational Modeling of Turbulent Ethanol Spray Flames in a Hot Diluted Coflow using OpenFOAM", (2015).



# **Reduction of Pressure Fluctuation on Hydrofoil NACA 0015 Using Cavitation- Bubble Generator**

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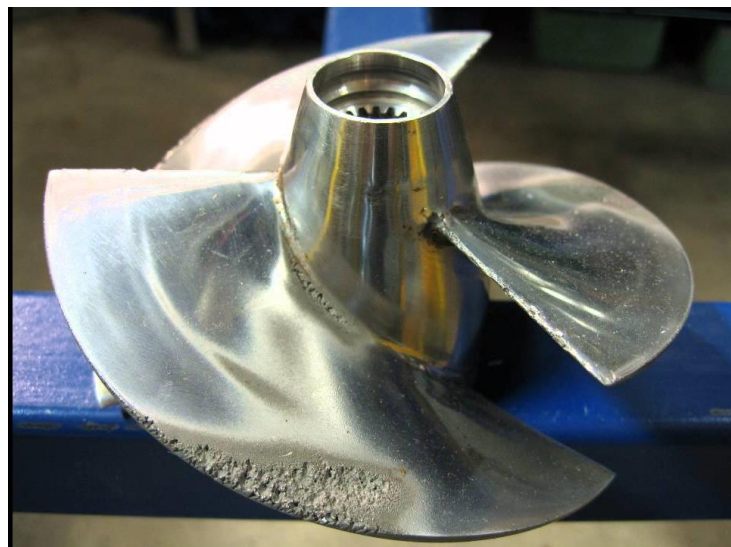
## ABSTRACT

Cavitation is the formation, increment and rupture of bubble in liquid. Cavitation occurs in the region in which local pressure decreases below the vapour pressure of the liquid. The sudden rupture of bubble causes the release of high energy and the narrow water jet. This process causes cavities on the surface of hydrofoil. Hydrofoil is used in many instruments like turbine, Propeller etc. Cavitation reduces the efficiency and the working range of the hydrofoils and so the instrument. The aim of the project is to reduce cavitation on the hydrofoil NACA0015 using a passive cavitation controller. I have also presented the effect of the position and size of the passive cavitation controller on the cavitation on the suction side of the hydrofoil. I have used OpenFoam-v7 for the simulation of the case. I have used “interPhaseChangeFoam” solver.

## 1. INTRODUCTION

Cavitation is the very common, destructive problems associated with fluid flow. This problem occurs when there is chance of pressure drop below vapour pressure of liquid. when cavitation occurs on the solid surface, it creates dentations on the surface, sound, shocks etc. Cavitation can be seen on the surface of pipe, turbine, propeller etc. The dentations on the surface reduces the efficiency of machines. Consequently, maintenance expenses and efforts are increased. Bubbles are formed in the zone which pressure is lesser than the saturate pressure. The bubbles move toward high pressure zone. On reaching the high-pressure zone the bubbles bursts. The sudden collapse on the bubbles generate large pressure on the surface which further creates dentations on the surface. It also creates noise and the collapse is so sudden that shock is formed. Hence, it has become important to control cavitation by different methods like adding passive appendage, active methods etc.

In this project, I have used Hydrofoil NACA 0015 as the solid body on which cavitation will be studied. I have used hydrofoil because this shape is commonly found in propeller, turbine and these are highly affected by cavitation. I have focused only on the suction side of the hydrofoil. Cavitation becomes more devastating due to its periodic nature. Cavitation repeats its nature again and again. Due to this periodicity, the pressure on the suction side changes and this periodicity has to be controlled to reduce the cavitation problem on the suction side. In this project, I have used the concept of artificial cavitation generator to reduce the periodicity of pressure variation on the suction side. This process can be used to reduce the periodicity of cavitation within certain range or at a certain point on the suction side by using one passive appendage. The location and the size of the appendage plays an important role in controlling cavitation. I have also shown the effect of the location and size of the appendage on the cavitation.



Submarine propeller Cavitation (source: Wikipedia)

To obtain the correct physics, it is important to have correct combination of cavitation and turbulence model. I have used Sauer and schnerr cavitation model with k-omega turbulence model. This combination gives good results (M. Lopez et al., 2017<sup>1</sup>). There are two major challenges for capturing the correct physics of the cavitation. Firstly, there should be the correct combination of the number of bubbles/nuclei and number of nodes in the computational domain. This plays crucial role in capturing the cavitation on the surface of the hydrofoil.

## 2. CASE SETUP

I have simulated 4 cases to locate the best position of the appendage to control cavitation at  $0.3c$ , where  $c$  is the chord length; I have also the effect of size of the appendage on cavitation. I have simulated the following cases:

Case 1: Without appendage.

Case 2: With appendage at  $0.295c$  of height  $0.0015$  m.

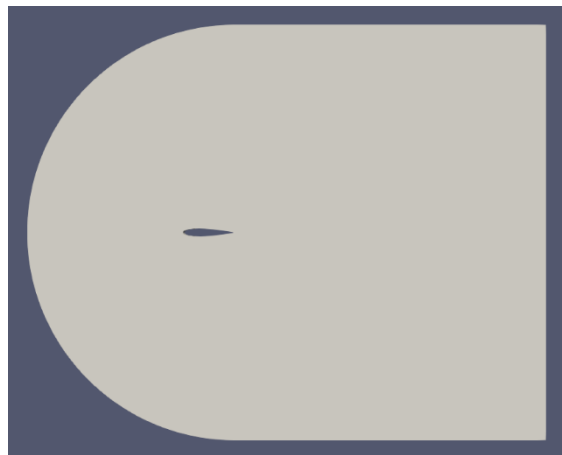
Case 3: With appendage at  $0.295c$  of height  $0.0025$  m.

Case 4: With appendage at  $0.181c$  of height  $0.0015$  m.

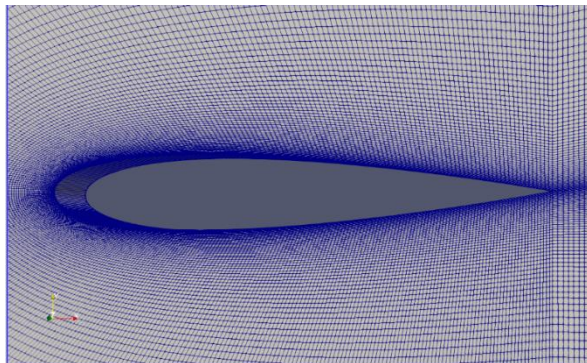
The initial and boundary conditions are same for all the four cases, only there is a difference in the blockmeshDict file, i.e. location and size of appendage on the suction side.

### 2.1 Meshing

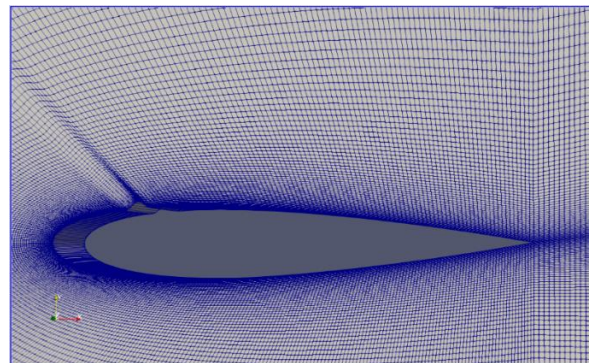
The total length of the computational domain is  $10c$  and breadth is  $8c$ . The radius of semicircle is  $4c$ , and 190000 hexahedral meshes.



Computational Domain



Meshing for aerofoil without appendage



Meshing for aerofoil with appendage

## 2.2 Initial Conditions

Table 1 shows the initial conditions of all the four cases respectively. Since, this is 2-dimensional simulation so the boundary and initial conditions are empty on front and back surfaces.

S. No.	Quantities	Values
1	K	Inlet: turbulentIntensityKineticEnergyInlet; intensity = 2%; value =0.018
		Outlet: zeroGradient
		Airfoil: krqWallFunction
		Top and bottom: krqWallFunction
2	Omega	Inlet: turbulentMixingLengthFrequencyInlet
		Outlet: zeroGradient
		Airfoil: zeroGradient
		Top and bottom: zeroGradient
3	alpha. water	Inlet: fixed value = 1
		Outlet: zeroGradient
		Airfoil: zeroGradient
		Top and bottom: zeroGradient
4	Phi	Inlet: zeroGradient
		Outlet: internalField
		Airfoil: zeroGradient
		Top and bottom: zeroGradient
5	Phi_rgh. orig	Inlet: zeroGradient
		Outlet: fixedValue (20300 m <sup>-1</sup> s <sup>-2</sup> )
		Airfoil: zeroGradient
		Top and bottom: zeroGradient
6	U. orig	Inlet: fixedValue (7.9695 m/s, 0.69724 m/s, 0 m/s)
		Outlet: zeroGradient
		Airfoil: no slip
		Top and bottom: zeroGradient

Table 01: Initial Conditions

Table 02 shows some of the constant properties that I have used for the simulation of all the four cases.

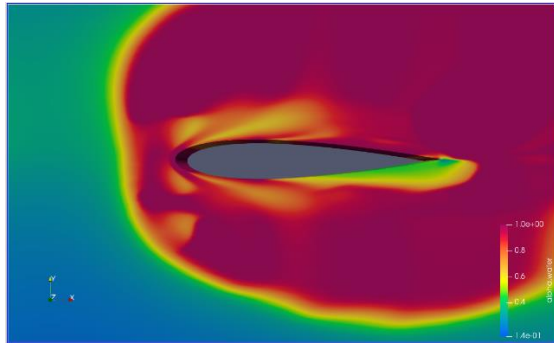
S. No.	Parameters	Values
1	Saturation pressure	2300 pa
2.	Sigma	1.2
3.	Schnerr and Sauer Coefficients	n = 10e12
		dNuc = 1e-5
		C <sub>c</sub> = 1
		C <sub>v</sub> = 1

Table 02: Constant properties

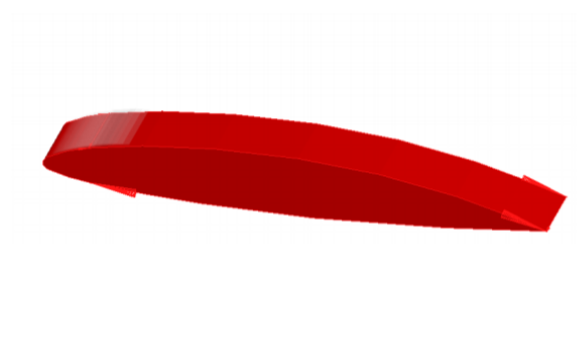
### 3. RESULTS

#### 3.1 Validation

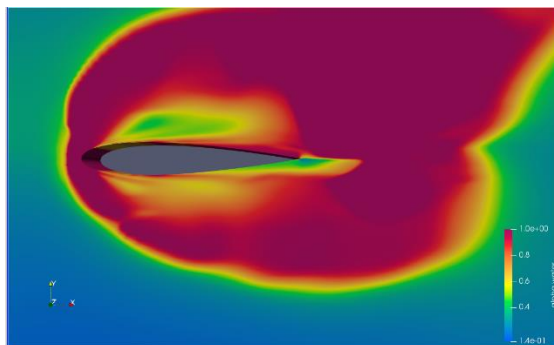
I have tried to capture the physics of originating, propagating and scattering of cavitation sheet on the aerofoil; and I present the physics of cavitation flow over aerofoil as the validation work (Case 1) for this project, and I have used V. H. Hidalgo et. al, 2013<sup>2</sup> to compare my results.



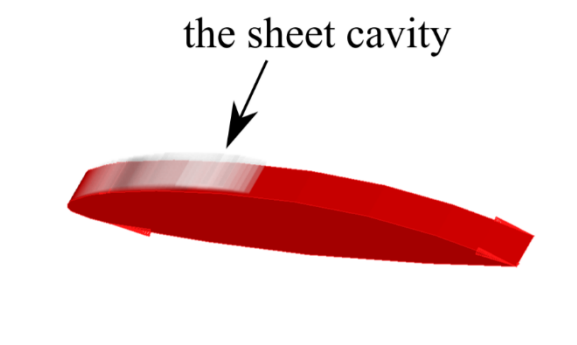
Cavitation begins from the front of the aerofoil  
(at 0.004 s)



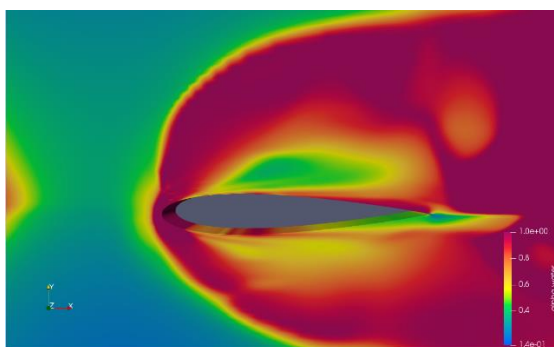
Cavitation sheet starts from the front of the aerofoil  
( V. H. Hidalgo et. al, 2013<sup>2</sup> )



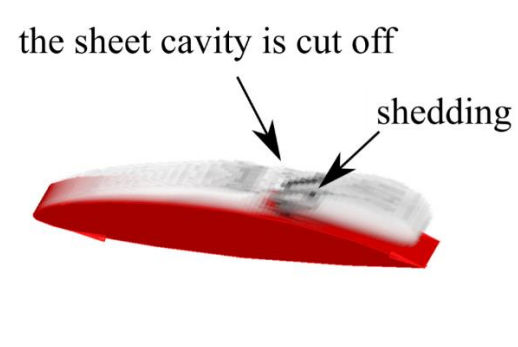
Development of cavitation along the suction side  
(0.076 s)



Development of cavitation along the suction side  
( V. H. Hidalgo et. al, 2013<sup>2</sup> )



Cavitation sheet cuts off  
(0.089 s)



Cavitation sheet cuts off  
( V. H. Hidalgo et. al, 2013<sup>2</sup> )

## 1. Without Appendage

Cavitation on the suction side of the aerofoil has been shown in figure 2 to figure 7 at different time. It can be seen from the figures that the cavitated area on the suction side vary with time, and the cavitation at a position also varies and keeps repeated after certain interval of time which is the most deleterious effect of the cavitation.

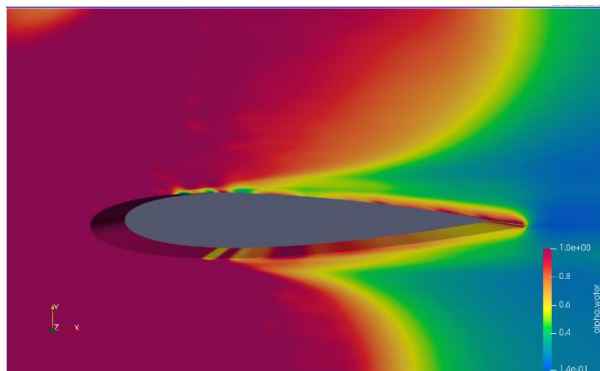


Fig. 02: Cavitation at 0.03 s

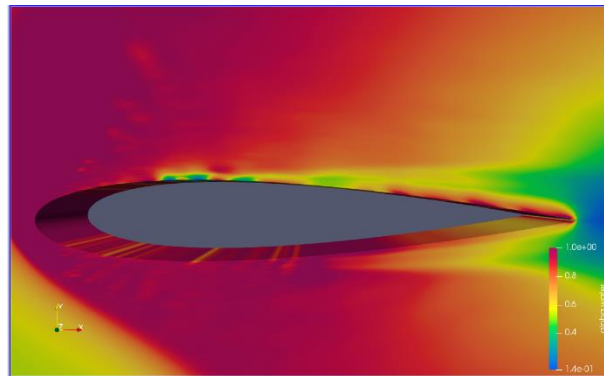


Fig. 03: Cavitation at 0.04 s

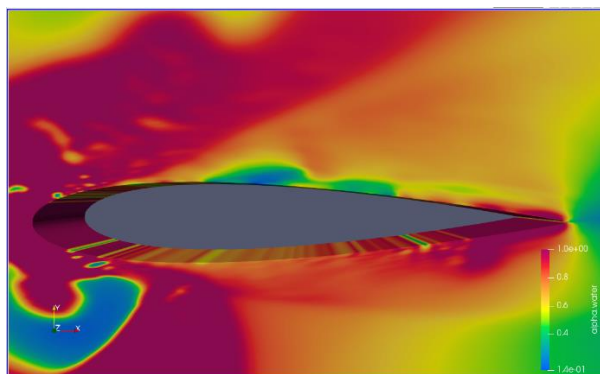


Fig. 04: Cavitation at 0.05 s

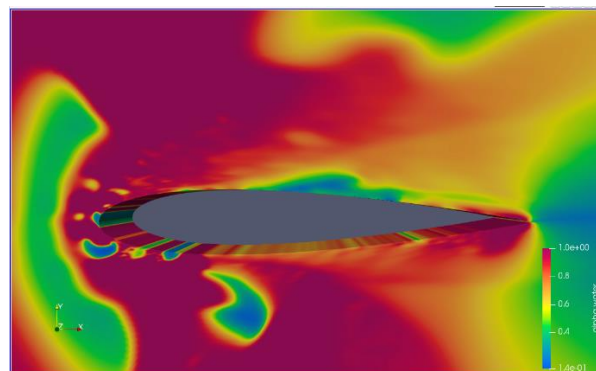


Fig. 05: Cavitation at 0.067 s

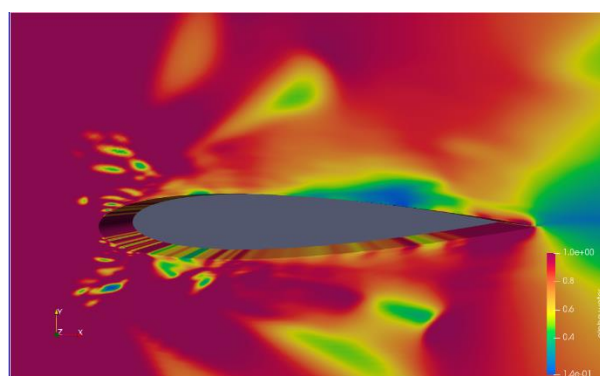


Fig. 06: Cavitation at 0.0798 s



### Case 2. With Appendage at 0.295c of height 0.0015 m

The appendage has been added at 0.295c on the suction side of the aerofoil. It has vertical height of 0.0015 m. Through figure 8 to 12, It can be seen that the cavitation is more stabilized, especially just behind the appendage. The variation has been stopped so the detrimental effects of the cavitation has also been reduced.

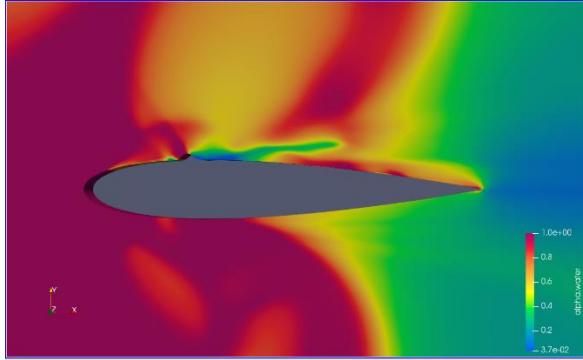


Fig. 08: Cavitation at 0.03 s

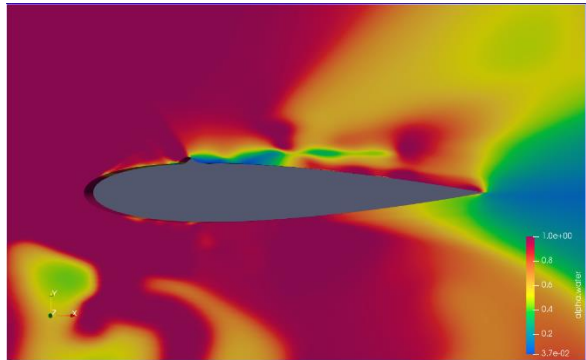


Fig. 09: Cavitation at 0.04 s

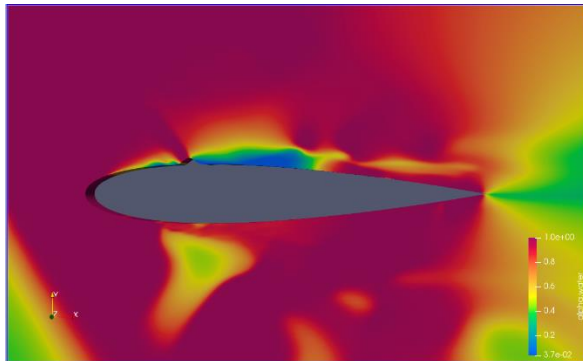


Fig. 10: Cavitation at 0.05 s

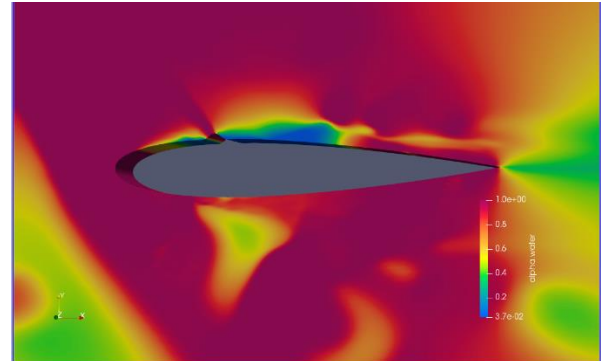


Fig. 11: Cavitation at 0.067 s

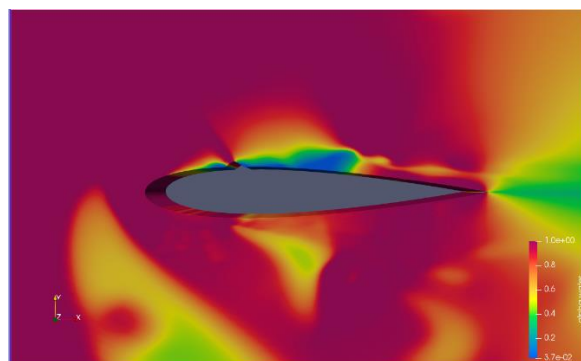


Fig. 12: Cavitation at 0.0798 s

### Case 3. With Appendage at 0.295c of Height 0.0025 m

This case has been simulated to show the influence of size of an appendage on cavitation. The appendage has been added at 0.295c on the suction side of the aerofoil. It has vertical height of 0.0025 m. Through figure 13 to 17, it can be seen that the cavitation is more stabilized, especially from appendage to the tail along the suction side. The variation of cavitation has been almost stopped for longer length than that of the previous case so the detrimental effects of the cavitation has also been reduced.

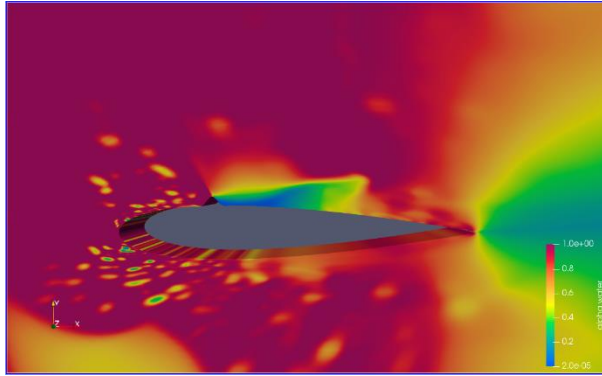


Fig. 13: Cavitation at 0.03 s

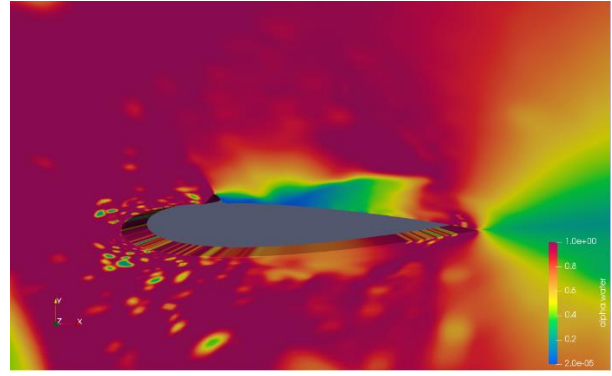


Fig. 14: Cavitation at 0.04 s

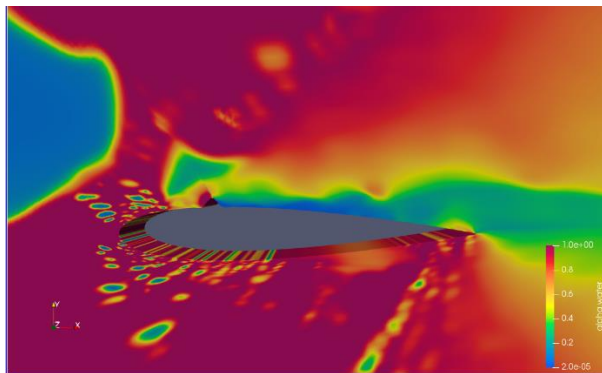


Fig. 15: Cavitation at 0.05 s

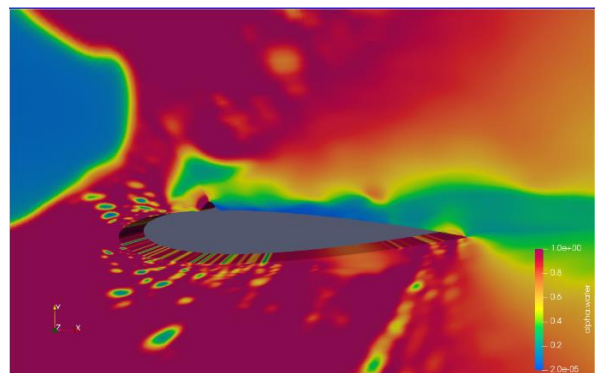


Fig. 16: Cavitation at 0.067 s

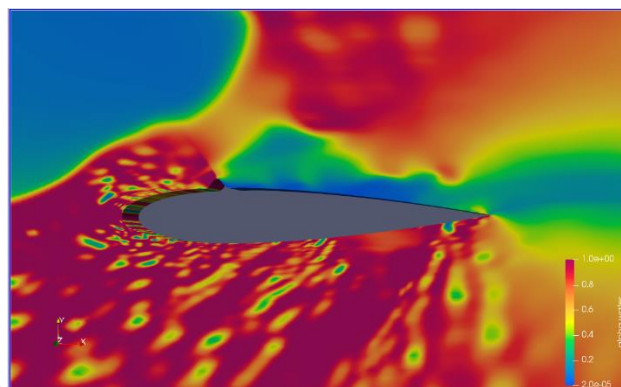


Fig. 17: Cavitation at 0.0798 s



#### Case 4. With appendage at 0.18c of height 0.0015 m

This case has been simulated with the aim to show the influence of position of appendage on cavitation. The 0.0015 m appendage has been added at 0.18c. Clearly, it can be understood from figure 18 to 22 that the cavitation pattern is different than that of case 2. The appendage at 0.18c of height 0.0015m, for the conditions given, reduce the pressure fluctuation on the suction side of the foil.

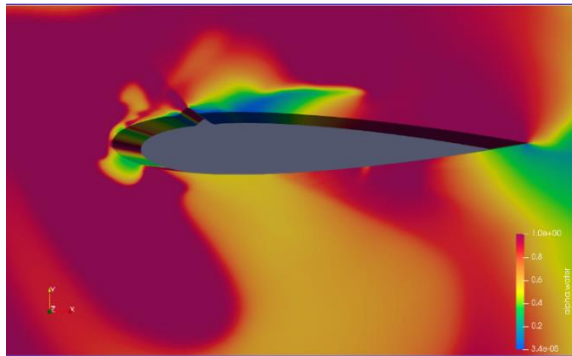


Fig. 18: Cavitation at 0.03 s

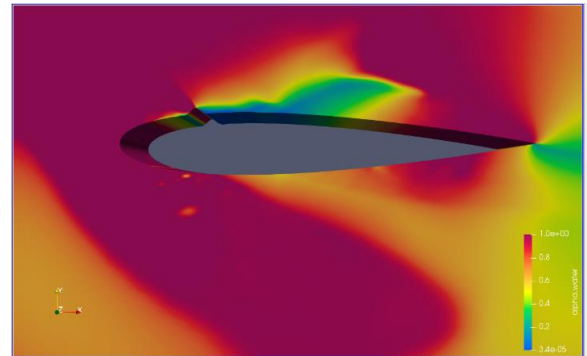


Fig. 19: Cavitation at 0.04 s

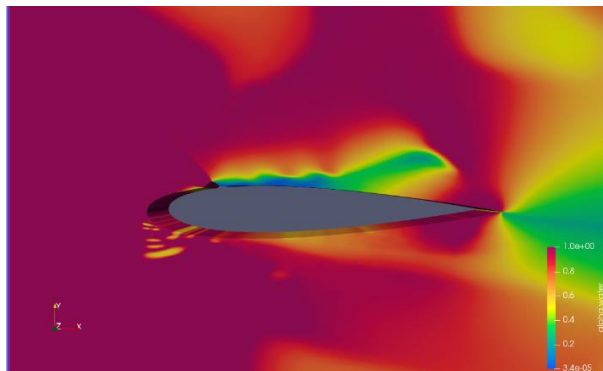


Fig. 20: Cavitation at 0.05 s

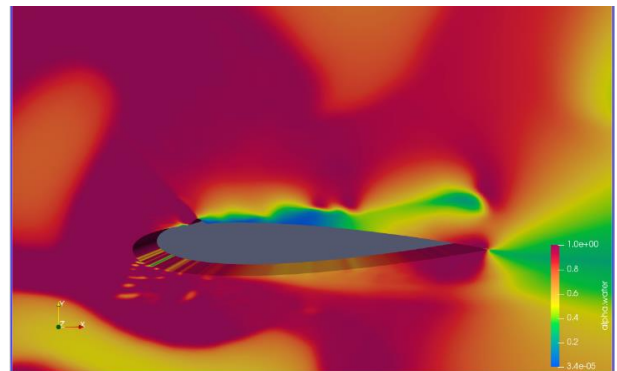


Fig. 21: Cavitation at 0.067 s

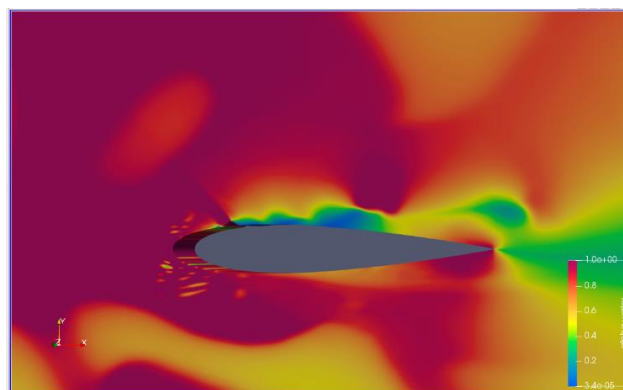


Fig. 22: Cavitation at 0.0798 s

#### 4. CONCLUSION

It can be inferred that adding an appendage reduces the periodicity of pressure fluctuation (figure 6 to 22) . As I am concerned about the cavitation at 0.3c of the aerofoil on the suction side, so in my opinion the appendage at 0.295c of height 0.0015 m is better than the first case: In third case, the appendage creates permanent cavitation in the whole area behind the appendage in the suction side, even in the places where it was not required. I find second case and fourth case equally suitable for generating artificial cavitation at 0.3c but due to the size of appendage in fourth case is smaller so it creates very thin layer of artificial cavitation; so, I find the case the appendage location and size in second case the most suitable for my problem setup.

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