

University of Southern Queensland

Faculty of Health, Engineering and Sciences

Identification of the effectiveness of various commercial
COVID -19 Masks using ANSYS software

A dissertation submitted by

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Abstract

The latest outbreak of Covid-19 has wreaked havoc in the world since its emergence in December 2019 and has been causing significant loss of life and economic loss globally. Various preventive measures and guidelines have been issued by health professionals to prevent the spread of the virus such as good hand hygiene, social distancing, cough and sneeze etiquettes, and most importantly face masks. To expand the scientific underpinning of such recommendations, Computational Fluid Dynamics can provide simulations-based analysis to emphasise the importance of face masks in reducing the community spread of corona virus.

Although virus can transmit through many modes, but airborne transmission of larger cough and sneeze droplets and aerosols is considered in this study which can carry virus laden particles through air. The aim of this project is to identify the efficacies of various commercially available face masks which is achieved by the computational fluid dynamics of human exhalation cough flow field. It is found that larger droplets fall on the ground and smaller particles remain suspended in the air for longer periods of time. The simulations are based on Reynolds Averaged Navier-Stokes (RANS) approach and $k-\epsilon$ model is used for CFD solver. The Lagrangian discrete phase model is used for exhaled particle tracking and identifying the suspended, evaporated and escaped particles through the masks.

Three different types of masks are used for comparison, fabric mask, surgical mask and N95 mask. It is identified that N95 mask is the most efficient mask of them all as it can block larger droplet nuclei as well as small finer aerosols which can carry the virus RNA and transmit in the surroundings. Surgical mask and fabric mask are also efficient in blocking the larger cough or sneeze droplets however, finer particles of size $< 5 \mu\text{m}$ can penetrate through their layers and escape in the surroundings. The larger droplets have higher viral content as compared to finer particles; therefore, any kind of mask can provide protection from airborne transmission.

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I certify that the ideas, designs and experimental work, results, analyses and conclusions set out in this dissertation are entirely my own effort, except where otherwise indicated and acknowledged.

I further certify that the work is original and has not been previously submitted for assessment in any other course or institution, except where specifically stated.

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Chapter 1. Introduction

1.1 Introduction:

Several infectious respiratory diseases have emerged in the recent past due to circulation of various viruses all around the continents such as influenza viruses, rhinoviruses, adenoviruses, respiratory syncytial viruses, boca viruses and coronaviruses (Boncristiani et al. 2009). The novel corona virus or COVID-19 is the latest in the list which has changed the course of the world since its emergence in Wuhan, China in December 2019. The ongoing deadly global pandemic due to coronavirus disease is the fifth pandemic after the 1918 Spanish flu pandemic with more than 238 million confirmed cases and more than 4.8 million confirmed deaths (Worldometer 2021). It was declared as a pandemic by the World Health Organisation as of March 11, 2020 (WHO 2020).

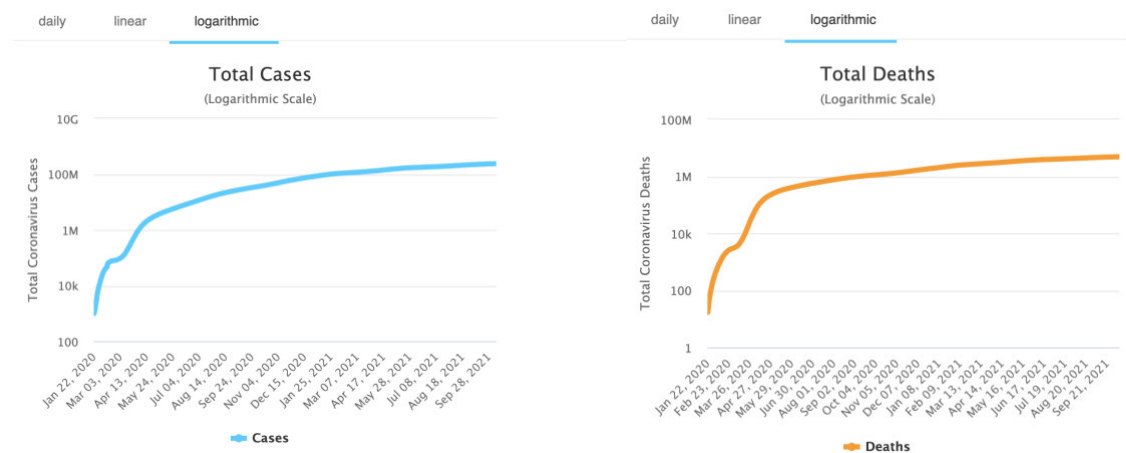


Figure 1: The total number of Covid-19 cases and deaths to date (Worldometer 2021)

The unfortunate event of the current pandemic has called for exceptional protection measures to stop the transmission of the airborne virus. Health professionals have recommended several preventive control measures such as hand hygiene, social distancing, quarantine of infected people, contact tracing, personal protective equipment, and face masks. Although social distancing and staying home can help reduce the spread but the world needs to move on and learn

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to live with this virus. Use of facial masks is the first protective measure which can be adopted to help reduce the risk of transmission. Research suggests that face masks can be very effective against airborne transmission as they can block the larger respiratory droplets and smaller aerosolized particles by blocking and resisting them through their filtration layers.

1.2 Background:

In Covid-19, Co stands for corona, vi for virus and d for disease, as this virus was first reported in 2019, hence it was named as Covid-19. Coronaviruses are a large family of viruses and are not new to humans. They cause upper-respiratory tract illness like the common cold, however the new strains of coronaviruses which emerged from animal reservoirs triggered serious illness and death. SARS coronavirus emerged in November 2002 and caused severe acute respiratory syndrome (SARS) and disappeared by 2004. Middle East respiratory syndrome (MERS) was caused by MERS coronavirus in September 2012 and transmitted from camels. Covid-19 is a new strain of already existed coronavirus which is believed to be present in animals specifically bats and jumped to human species through an intermediate domestic animal, however the source is still unknown.

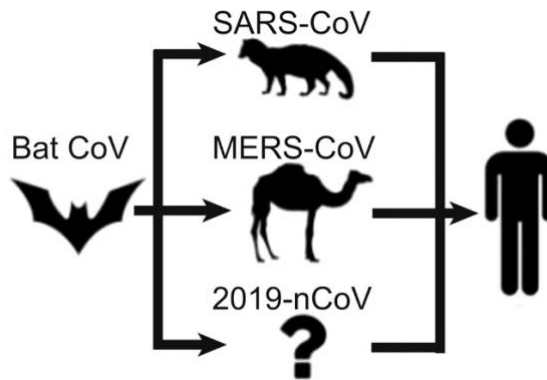


Figure 2: origin of coronavirus ((Adachi, 2020)

The infectious disease COVID-19 leads to respiratory problems, fever, and infection of lungs in serious cases. The symptomatology of patients infected with COVID-19 is highly variable, some show no symptoms at all whereas it can become life-threatening for others. The common symptoms include fever, dry cough, tiredness, sore throat, shortness of breath and chest pain in

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serious cases. It is transmitted from person to person primarily due to the transfer of virus-laden fluid particles from the nose or mouth of the infected person during breathing, talking, singing, sneezing, and coughing (Mowraska 2006). The respiratory exhalation can produce thousands of droplets with various sizes at a high velocity, which are transported by the flow field.

Infectious micro-organisms, including viruses, pathogens, bacteria, etc., are contained in the droplet nuclei. Several research studies show that the severe acute respiratory syndrome (SARS) in 2003 and the current COVID-19 global pandemic of coronavirus disease 2019, both transmitted by contact or through the airborne route (Beggs 2003). Besides the severe effect on human health, the pandemic has hit the global economy the hardest due to lock downs, border closures and quarantine requirements in several parts of the world. The figure below by PwC Australia shows the loss of GDP in US\$m due to this pandemic (Loughridge & Thorpe 2020).

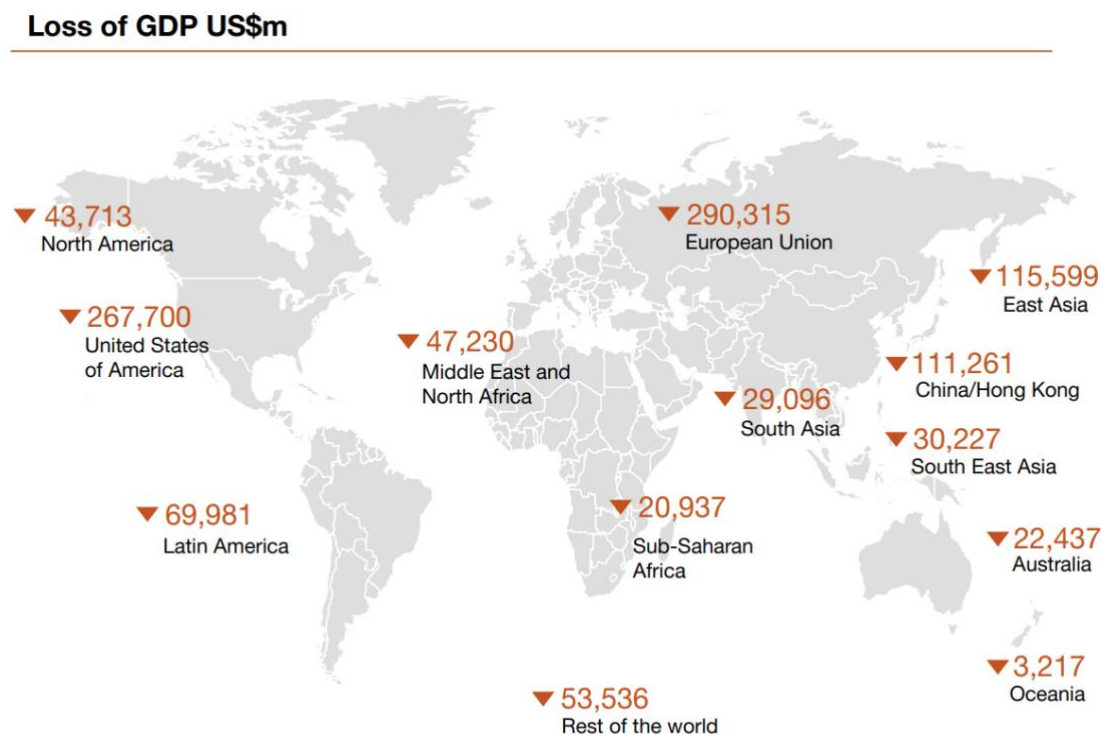


Figure 3: Loss of GDP all over the world (Loughridge, 2020)

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To study, predict and control the transmission of the infectious respiratory disease become highly significant due to the catastrophic impact on human health and global economy. Three modes of transmission have been identified by the researchers and health professionals.

- Direct contact: also known as person to person contact means when a healthy person touches the virus laden droplet released from an infected person directly. It can be avoided by using proper hand hygiene measures.
- Indirect contact: it means that a healthy person can get infected by touching the inanimate objects and surfaces which have infected particles deposited on them due to cough or sneeze of some infected person. Cough and sneeze droplets are heavy, and they fall on ground or adjacent surfaces rather than staying suspended in the air.
- Airborne transmission: the last mode of transmission is airborne transmission of virus laden aerosols which are released from the mouth or nose of an infected person while talking, breathing, singing, coughing, or sneezing. They are relatively smaller in size and travel large distances through the air carrying the infection with them.

1.3 Aims and Objectives:

The main aim of the project is to identify the effectiveness of various COVID-19 masks using ANSYS software and to determine their usefulness in preventing and slowing down the pandemic. To achieve the objective:

- Identify the need to use masks to prevent the inhalation of air-borne COVID-19 virus and to minimize the exhalation of virus-laden aerosols and droplets.
- Conduct detailed research on various commercial COVID-19 masks available in the market with different filtration efficiencies and breathability levels.
- Identify the level of effectiveness required for different mask users such as healthcare workers, aged care workers, patients etc.
- Develop a computational model including a face, upper airway and various masks using ANSYS software.

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- Analyse the airflows and droplets motions near the face when wearing different masks by numerically investigating the dynamic characteristics, such as the velocity variation, streamwise penetration, and particle deposition after flowing through the mask.
- Characterize the effect of mask filtration and resistance on the deposited aerosols and particles on face and upper airway.
- Differentiate the effect of particle size and inhalation flow rate in different masks by analysing the particle dosimetry.
- Analyse the deposition of particles in the upper airway for different flowrates and mask resistances.
- Validate the numerical results with the mask viscous resistance using Darcy's Law provided in the literature and evaluate the effectiveness of various masks using all the data.

1.4 Resource Requirements:

CFD analysis to understand the given challenge has a benefit of understanding the flow problems without the need of performing any actual physical testing or experimenting. Hence the most important resource required to successfully complete this project is to acquire and install the ANSYS software to perform the required modelling, simulation, and analysis. Student version of ANSYS software was provided by university of Southern Queensland (USQ) to complete the elective course in Computational Fluid Dynamics - MEC5100. To model the complex geometry, free software like Blender and Fusion 360 can be utilised.

Mesh generation is the most significant part of numerical analysis and chosen mesh can determine the success or failure of a flow problem in hand in achieving the satisfactory computational solution. Grid generation has become an entity by itself in CFD (Tu et al. 2018). Learning the modelling techniques, mesh generation, solution assessment and analysis are achieved in CFD course of MEC5100 where special consideration is given to specify a range of boundary conditions as required in this particular flow problem. The ANSYS software is available in USQ computer laboratory and can also be assessed remotely via VPN connection if it is required to work from home.

1.5 Project Organisation:

The dissertation project is organised in five chapters, an overview of the chapters is provided below.

1.5.1 Chapter 1. Introduction

Chapter 1 presents a general introduction about the coronavirus infection and its global impact. It highlights the effect this pandemic has caused globally on human health and economy. It gives a background knowledge about the origin of the pathogen and its modes of transmission in the community. The motive, scope, objectives, and organisation of the present study are provided in this chapter as well.

1.5.2 Chapter 2. Literature Review

Chapter 2 provides the details of the literature review of the previous studies conducted in terms of the experimental and numerical work. It presents the different modelling approaches adopted to track the human exhalation flow by different researchers and highlights the importance of CFD analysis to evaluate the airflow and particle dosimetry. It also provides an overview of the literature investigating the filtration efficiency through the masks by the mechanism of the aerosols penetration and simulations. Numerical as well as experimental work is studied to validate the results of the present project.

1.5.3 Chapter 3. Methodology

Chapter 3 discusses the modelling techniques used to develop the head model, mask models and droplet models. The complex geometry of the head model and mask model is developed using opensource blender software and fusion 360. Whereas the simulations are modelled in ANSYS Fluent by applying appropriate boundary conditions and turbulence models. The governing equations behind ANSYS CFD solver are also discussed in this chapter. The aerosols and droplet dispersion, deposition and divergence simulations are based on discrete phase model which is governed by Lagrangian equations. Boundary conditions used for the inlet, outlet and walls and the importance of turbulence model used for the simulations are presented as well.

1.5.4 Chapter 4. Results and Discussions

Chapter 4 presents the comparison of the CFD results of the different mask models based on same characteristics of human cough flow in terms of both the flow fields and the droplet counts. Different time-dependent cough velocities at the inlet mouth are simulated to compare the dispersion and deposition of different masks according to their filtration efficacies.

1.5.5 Chapter 5. Conclusion

Chapter 5 discusses the conclusions based on the analysis of the result of the present study. The validation of different mask efficiencies and consequential effect of the project are discussed. The risks associated to the project are also discussed in this chapter. The last part of the document presents the list of references and appendices containing the project timeline, specifications, resource planning etc.

Chapter 2. Literature Review

2.1 Introduction:

There is an extensive literature available describing the link of exhalation of corona virus from an infected person whether asymptomatic or symptomatic, to the spread of disease in the community because of its airborne nature. Airborne transmission is defined as the spread of an infectious agent caused by the dissemination of droplet nuclei (aerosols) that remain infectious when suspended in air over long distances and time. Virology and aerosol science has confirmed that the aerosols not only spread by coughing and sneezing but also by breathing, talking or singing (Asadi et al. 2020). The site of origin, reopening of small airways in the respiratory system and various other factors and physical mechanisms can affect the particle properties in the human exhaled breath (Bake, 2019).

In many cases, CFD and experimental studies have been conducted to examine the airborne transmission in simplified environment (Yu et al. 2004; Zhang & Chen 2006). Mohamed et al. (2017) and Dudalski et al (2018) experimentally studied the velocity field of the cough flow produced by influenza- infected human subjects through the Particle Image Velocimetry (PIV) and hot-wire anemometry (HWA) measurements. They also conducted experimental collection of nasal swab data to identify and quantify the species of the pathogen and the viral content (Dudalski, 2020).

The airborne nature of the corona virus encouraged scientists to figure out the preventive measures to reduce the spread of the disease. As suggested by the World Health Organisation (WHO) after social distancing and isolating, the next best thing is to use a face covering to block the droplets and aerosols as it can alter the airflow significantly (Xi et al. 2020). Face masks have become the universal symbol of this pandemic and various masks are available in the market for public use and medical use, such as N95 masks, surgical masks, and fabric masks. N95 mask is a type of respirator, and it provides more protection than a surgical mask because it can filter out both large and small particles. Surgical masks are loose fitting disposable masks and can filter out large particles while breathing in and out. A cloth mask is only effective if it is made of at least two layers of tightly woven fabric to stop droplets from passing through the mask (Mayo Clinic 2021).

2.2 Respiration and Transmission:

There are various studies conducted to analyse the size of droplets and aerosols produced by a person infected with COVID-19. It is important to study the fundamentals on the formation of exhaled droplets and aerosols to identify the effectiveness of filtration used in different face masks and their optimal use. The World Health Organization (WHO) and Centres for Disease Control and Prevention (CDC) postulate that the particles of more than $5\ \mu\text{m}$ as droplets, and those less than $5\ \mu\text{m}$ as aerosols or droplet nuclei (Jayaweera et al. 2020). It is identified that the deadly pathogen can be found in both large droplets and small aerosols. The studies show that the large respiratory droplets produced by coughing and sneezing are larger than $5\ \mu\text{m}$ and can be contained by proximity control. The desiccation of suspended droplets attribute to formation of infectious droplet nuclei which is less than $5\ \mu\text{m}$ in size, and they can remain airborne for a significant period of time and can deposit in the lower respiratory tract in humans (Fennelly 2020). Water droplets with diameter less than $50\ \mu\text{m}$ would evaporate in less than 3s before reaching the ground assuming an average 1.6 m initial height and still air. For mucus, such a drying process would yield left-over droplet nuclei which could potentially carry viruses. Hence, there is no fixed droplet size. Larger droplets $100\ \mu\text{m}$ in initial size, may become aerosol particles because of rapid drying (Vuorinen, 2020).

What happens at two metres when someone coughs?

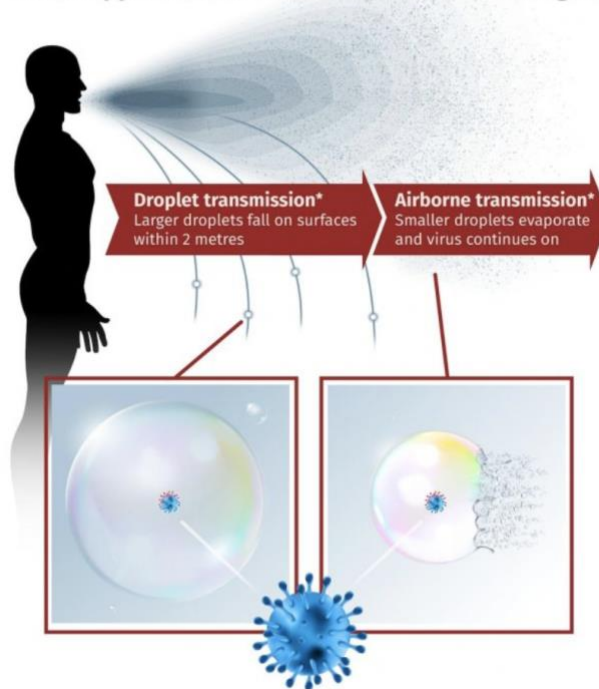


Figure 4: Transmission of coronavirus (CBC News)

Chapter 2. Literature Review

Coughing and sneezing can produce higher concentration of infected particles as compared to speaking and breathing. Thousands of droplets with various sizes at a high velocity are produced during this forced exhalation which are transported by the flow field. Infectious micro-organisms, including viruses, pathogens, bacteria, etc., are contained in the droplet nuclei (Beggs 2003). During coughing and sneezing, the diameters of most droplets produced from the mouth are around $10\ \mu\text{m}$ and some are even larger than $100\ \mu\text{m}$ (Duguid, 1946). These larger droplets fall to the ground or adjacent surfaces due to gravity while the smaller droplets propagate in the air with decreasing diameter and eventually evaporating after becoming droplet nuclei.

The airborne transmission can be considered as droplet transmission because any droplet size can be carried by air when the larger droplet dries up and convert into nuclei containing the pathogen. The virus laden fine aerosols of size less than $5\ \mu\text{m}$ or larger droplet nuclei released by an infected person are transmitted to a healthy person by inhalation. However, the finer aerosols can linger in the air for a considerable amount of time, whereas the larger droplets follow a ballistic trajectory and impact on or fall onto surfaces within a limited radius of the source. Leung et al. (2020) conducted a study on the efficacy of facial mask in reducing the risk of coronavirus transmission via droplets and aerosols, the viral RNA was detected in 30 percent of the larger droplets while 40 percent of smaller aerosols contained viral RNA.

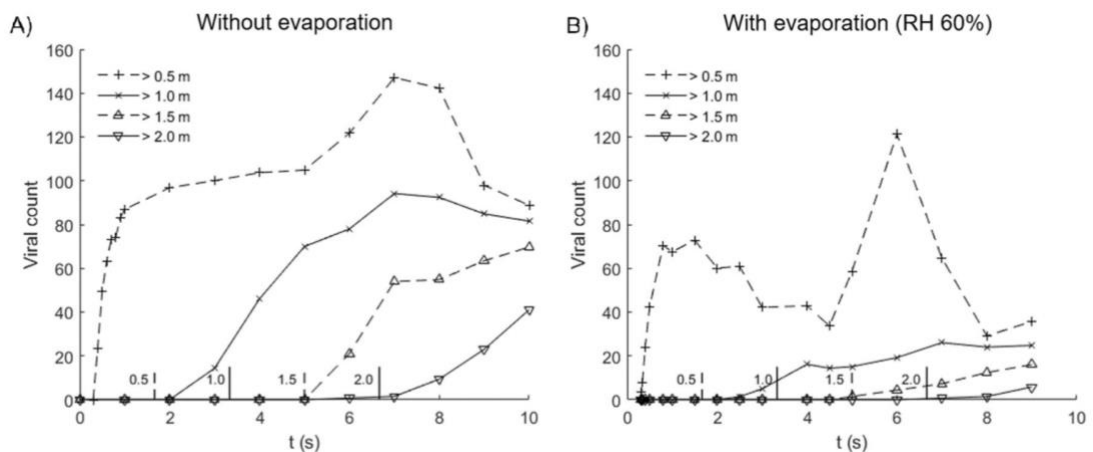


Figure 5: Evaporated droplets persist as droplet nuclei which may pose infection risk over extended distance and time scales (Li, 2021)

Chapter 2. Literature Review

Xi et al. 2020 conducted a study to investigate the inspiratory airflows and particle motion near the face when wearing a face mask in comparison to those without a mask to characterize the dosimetry of aerosols on upper respiratory system. The study quantified the number of aerosols deposited on the face and entering the lungs through upper airways. The results of the study provided significant information about particle dynamics and protection efficiency of face masks. The simulation study by Khosronejad et al. (2020) showed that use of masks can effectively limit the distance travelled by finer particles and settling velocity of $10\ \mu\text{m}$ particles can be reduced to reach the settling velocity of $5.5\ \mu\text{m}$ particle.

Infection control involves blocking any stage of the infection. Reducing the generation of virus in an infected person, using disinfection measures to kill the virus released in the atmosphere or simply isolating the infected person can be the methods adopted to reduce airborne transmission. Personal protection control pathway is to use face masks to prevent the distribution or inhalation of the pathogens.

2.3 Efficacy of face masks:

Several researchers have performed theoretical and experimental investigations of virus transmissibility through the facemasks and alternatives. (Stutt et al. 2020) developed the holistic mathematical frameworks for assessing the potential impact of facemasks in COVID-19 pandemic management. The results revealed that professional and home-made facemasks were highly efficacious to reduce exposure to respiratory infections among the public. In addition, when people wear the facemasks all-time at the public places, the certain epidemiological threshold, known as the effective reproduction number, could be decreased below 1, leading to the prevention of epidemic spread. (Ngonghala et al. 2020) developed a parametric model for providing deeper insights into the transmission dynamics and control of COVID-19 in a community. They used the COVID-19 data from New York state and the entire US to assess the population-level impact of various intervention strategies. The results suggested that the consistent use of facemasks could significantly reduce the effective reproduction number. The highly efficacious facemask, such as surgical masks with an estimated efficacy of around 70%, could lead to the eradication of the pandemic if at least 70% of the residents use such masks in public consistently. The use of low efficacy masks, such as cloth masks with an estimated efficacy of 30%, could also lead to a significant reduction of COVID-19 transmission.

Chapter 2. Literature Review

Several external parameters were identified by Tcharkhtchi (2021) which can alter the filtration efficiency of the mask, such as particle size, shape of the particles, flow rate, steady or transient flow, charge state of particle, frequency of respiration, humidity and temperature and loading time as shown in the table below.

Influence of external parameters on filtration efficiency.

External parameters	Filtration efficiency of the mask
Particle size	Decreasing particle size, decreases efficiency
Shape of particles	Low aspect ratio, decreases efficiency (rode shaped particles diffuse less than spherical shaped particles)
Face velocity (flow rate)	Increasing flow rate, decreases efficiency
Pattern of flow (Steady or cyclic)	Cyclic flow decreases efficiency compared to static flow
Charge state of particle	Efficiency decreases for uncharged particles
Frequency of respiration	Increasing frequency decreases the efficiency
Humidity and temperature	Increasing humidity and temperature decreases the efficiency
Loading time	Increasing loading time, increases the efficiency (However, there is the risk of virus accumulation)

Table 1: Influence of external parameters on filtration efficiency Tcharkhtchi (2021)

In the same study, bacterial leakage values were compared for the cases without mask and with different masks after clinical trials. The table below is reproduced to show the trial results.

Comparing the values related to the bacterial leakage for the case without the mask and with different masks

	No mask	cloth mask	surgical mask	N95 mask
Mean bacterial colony count per trial	209.6	33.18	9.36	8.54
Total bacterial colony count	10480	1659	468	427
Percentage of leakage	100	15.83	4.47	4.07

Table 2: Bacterial leakage with various masks Tcharkhtchi (2021)

Chapter 2. Literature Review

The three basic types of face masks are identified in the literature study. The basic cloth face mask is the simplest one made of different types of fabric. The quality of fabric material decides the filtration efficiency of a cloth mask such as packing density, fibre material etc.

3-layer cotton mask



Figure 6: fabric mask

The second type is the surgical mask which has a three layers structure. The middle layer is the filter media, inner layer absorbs moisture while outer layer repels water.

Surgical mask



Figure 7: surgical mask

The third type is the N95 face mask which contains filter and the word 95 indicates that at least 95 percent of aerosols of the size of $0.5 \mu\text{m}$ can filter out (Tcharkhtchi, 2021).



Figure 8: N95 respirator

2.4 Role of ANSYS:

Numerical approaches such as CFD techniques are relatively more efficient, economical and convenient to use as compared to experimental techniques (Kannan 2015). CFD approaches are extensively used in engineering to simulate physical phenomena and find the solution to practical problems by using a set of governing equations. They have a wide variety of applications such as aerodynamics, hydraulics, automobile industry, oil and gas industry, and ships etc. Various fluid phenomena, laminar and turbulent flows, radiation, and heat transfer etc. can be investigated and simulated using CFD techniques. The fluid dynamics-based numerical techniques have gained momentum in the field of the facemask research domain as well. The computational fluid flow models have shown their potentials in an improved prediction of the spreading of respiratory virus-laden droplets and aerosols, sensitive to the ambient environment and crucial to the public health responses (Kumar & Lee 2020). The advantages of using CFD analysis is that it allows characterization and measurement of any fluid property at all points in the flow and precise tracking of particle motions, sizes and locations (Leonard et al. 2020), whereas experiments only permit data to be extracted at a limited number of locations in the system (where sensors and gauges are placed). Most significantly, CFD allows solution of complex problem without the need to formulate a physical experiment reducing the risks associated with physical assessment. It allows great control over the physical process and provides the ability to isolate specific phenomena for study. While experimental studies are essential for the broad characterization and design evaluation of respiratory facemasks, further theoretical and numerical methods and algorithm-based investigations provide a better insight into the facemask's fluid flow dynamics (Kumar & Lee 2020).

Aliabadi et al (2011) used Unsteady Reynolds Averaged Navier-Stokes (URANS) approach to conduct a CFD simulation of the cough flow and analysed the impact of humidity on droplet dispersion, heat and mass transfer. In their study they used $k-\varepsilon$ model and the Lagrangian discrete phase model to solve the turbulence of the flow field and track the particles respectively. Khosronejad et al (2020) developed a numerical model to show that face masks can suppress the spread of Covid-19 in indoor environments. They solved the spatially filtered continuity and Navier–Stokes equations with the Boussinesq assumption to simulate the incompressible, stratified, turbulent flow of a dilute air–saliva mixture which satisfies the discrete continuity equation.

Chapter 2. Literature Review

Mittal et al (2020) used a mathematical framework for estimating risk of airborne transmission of Covid-19 by using face mask and social distancing. They used buoyancy effects and wall-modelled Large Eddy Simulations (LES) using Boussineq approximation. The LES method predicts the development of fluid flows more accurately as compared to URANS, or RANS technique since it resolves the large turbulence scales and only models the small scales through the sub grid-scale model (SGC) turbulence model. However, it has a very high computational cost whereas RANS approach is less time-consuming for the simulations.

The LES method separates and resolves the large eddies that contain most of the energy through the spatially filtered mass and momentum Navier-Stokes equations and models the small scales through the SGS model. The RANS equations are based on time averaged derivation of Navier-Stokes equations and the effect of turbulence is simulated through modelling the Reynolds stresses whereas, LES is spatial integration and only very small eddies are averaged on sub grid scale such as dissipation of kinetic energy. An LES simulation is always unsteady turbulent flow (ANSYS, 2020). The governing equations of LES are obtained by filtering the partial differential equations governing the flow field $\rho u(x, t)$.

After spatially filtering, the Navier-Stokes continuity equation is given as

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0$$

Equation 1

The Navier-stokes momentum equation after spatial filtering can be expressed as

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}_i}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}}{\partial x_j}$$

Equation 2

Where τ_{ij} represents the SGC stress tensor and \bar{p}_i is the filtered pressure field.

The term $\bar{u}_i \bar{u}_j$ causes the difficulty in LES modelling. It requires the knowledge of unfiltered velocity field, which needs to be modelled.

The stress tensor τ_{ij} is expressed as

$$\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j$$

Equation 3

Chapter 2. Literature Review

For the LES modelling, the central differencing discretization scheme is performed for momentum, water vapour species transport, and energy since it minimizes the numerical diffusion and provides the highest accuracy in resolving the large turbulence scales. Therefore, it is considered as the ideal choice for the LES method.

There is an exchange of momentum between the large resolved and small sub-grid stresses, and it needs to be modelled. Various SGS turbulence models are available including the kinetic energy SGS model, Smagorinsky-Lilly model, WALE model, and the dynamic Smagorinsky-Lilly model. The Dynamic Smagorinsky-Lilly turbulence model was adopted in the study by Mittal et al. (2020) and Ran Bi (2020), where the model constant C_s is used as a function of space and time over a wide range to avoid the damping of turbulent fluctuations.

The literature study has identified that it is essential to identify the size ranges and numbers of droplets to relate COVID-19 to airborne transmission and it is also necessary input for ANSYS simulations and result analysis. It is identified in the literature to clear the ambiguity among aerosols, airborne droplets and droplet nuclei to compare the size and time they linger in the air (Stutt et al. 2020).

Xi et al. (2020) studied particle dynamics at an inhalation rate of 30L/min with and without mask and measured the deposition of particles on mask for different particle sizes to account for larger droplets and smaller aerosols filtered by masks. They used low Reynolds number $k-\varepsilon$ turbulence model to simulate the inspiratory airflows based on its ability to accurately predict pressure, velocity, and turbulent flows. Spherical profile of particles was generated, and particle motions were tracked using a discrete phase Lagrangian algorithm.

Chapter 2. Literature Review

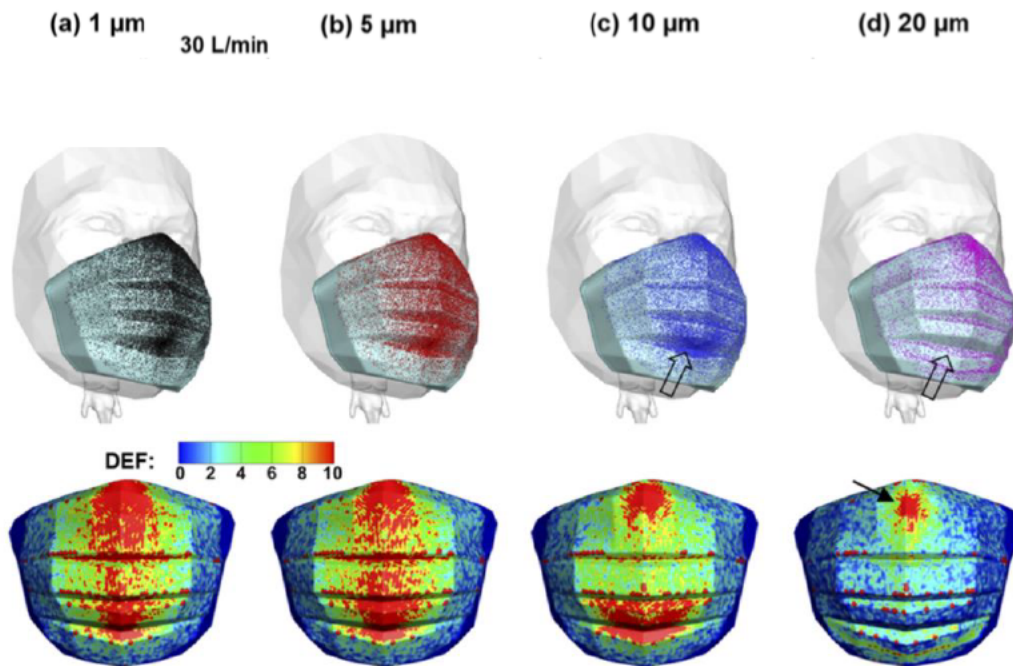


Figure 9: Various sized particles filtered by a mask Xi et al. (2020)

It is evident from the literature study that very less research has been conducted on the quality of face masks required for public and little evidence is provided to establish that normal fabric masks are safe enough to protect from virus laden aerosols. It was established in the research study that infected patients and their close contacts such as health care workers require extra protection as they are in high-risk close proximity whereas general public who can maintain a safe distance can rely on disposable masks or layered fabric masks as those can also filter out the large droplets and discerned droplets in normal situations.

Chapter 3. Methodology:

3.1 Introduction:

For expiratory activity, coughing is one of the common forced activities which plays a significant part in transmitting the airborne virus in the indoor environment. Human cough flow is generally considered as a multiphase incompressible turbulent free jet flow which consists of a flow field as a continuous phase and the droplets as a discrete phase (Bourouiba, 2014).

The transport characteristics of cough flow depends on several parameters such as flow rate, flow direction, mouth opening area, ambient temperature, and relative humidity (Gupta, 2009). While coughing, all sized particles are generated ranging from large droplets of size 20 μm to aerosols of size 0.3 μm . The speed of cough flow is around 80km/h and sneeze travels at almost double the cough speed (Olsberg, 2020). Cough is repetitive action and for respiratory diseases it is the most common symptom, hence for simulation of human exhalation, coughing is selected.

The main objective of this project is to numerically characterize the difference in the accumulation of droplets and aerosols on the face and nose with different masks, specifically N95 mask, surgical mask, and fabric mask. To achieve this objective simulation method is used to evaluate the fluid flow problem. Computational fluid dynamics using ANSYS Fluent can provide precise simulation results of the fluid flow near the face and through the mask. The evolution of the flow field of coughing is time dependent. So, the dynamic characteristics, including the velocity field and turbulence parameters, are varying with time. Therefore, the CFD simulations in the present study are conducted under a transient condition.

3.2 Introduction to ANSYS software:

ANSYS Computational Fluid Dynamics simulation software allows to predict, with confidence, the impact of fluid flows. The software's unparalleled fluid flow analysis capabilities can be used to visualise the flow characteristics for comparative study. Computational Fluid Dynamics is a branch of fluid mechanics which provides a qualitative prediction of fluid flows by means of mathematical modelling (partial differential equations), numerical methods (discretization and solution techniques) and software tools (solvers, pre- and postprocessing utilities).

Chapter 3. Methodology

Large Eddy Simulations (LES) and Direct Numerical Simulations (DNS) approaches are very popular and feasible due to the development of computational processing techniques (Bi, 2020). LES and DNS, both methods can predict very accurate results for specific flows as compared to RANS approach. However, DNS method has very high computational cost whereas LES method lies between DNS and RANS in terms of computational cost and accuracy for turbulent flows.

The human cough flow is transient and turbulent flow with a higher Reynolds number; hence LES approach can predict the flow characteristics more accurately as compared to RANS approach, but it is computationally more expensive and time consuming than RANS technique. The coughing flow field is time dependent and have dynamic characteristics. Therefore, the ANSYS simulations in the present study are conducted under a transient condition. The boundary conditions, and ambient conditions are kept the same for all models for a fair comparison.

(Kuzmin 2021) describes the versatility of CFD in order to solve a variety of complex problems ranging from; meteorological phenomena, heat transfer, combustion, complex flows to human body functions such as breathing. He explains that CFD analysis process involves:

1. Problem statement
2. Mathematical model
3. Mesh generation
4. Space discretization
5. Time discretization
6. Iterative solver
7. CFD software
8. Simulation runs
9. Postprocessing
10. Verification

3.3 Numerical theory behind ANSYS modelling:

The main theory behind RANS method is Navier-Stokes equations of which the velocity component is given as

$$u_i = \bar{u}_i + u_i'$$

Equation 4

Where \bar{u}_i represents the mean velocity and u_i' is the fluctuating velocity component.

The mass and momentum conservation equations are given as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho \bar{u}_i)}{\partial x_i} = 0$$

Equation 5

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_i}{\partial x_j} \right) \right] + \frac{\partial(-\rho \overline{u_i' u_j'})}{\partial x_j}$$

Equation 6

Where ρ is density, p is pressure, μ is molecular viscosity of the injected fluid and it is mixture of water vapour and air in the present study and x_j and x_i represent the cartesian coordinates. $-\rho \overline{u_i' u_j'}$ represents the turbulent Reynolds stress factor and it defines the effect of fluctuations and turbulence on the flow. This factor needs to be modelled to solve the equations.

3.4 The energy equation

The energy equation is required to solve the heat transfer between the exhalation flow and the surrounding ambient environment (Nijemeisland, 2004). The energy transport equation used by ANSYS Fluent is given below

$$\underbrace{\frac{\partial(\rho E)}{\partial t}}_{\text{unsteady}} + \underbrace{\nabla \cdot (u (\rho E + p))}_{\text{convection}} = - \underbrace{\nabla \cdot [k_{eff} \nabla T]}_{\text{conduction}} - \underbrace{\sum_j h_j J_j}_{\text{Species diffusion}} + \underbrace{\tau_{eff} \cdot u}_{\text{Viscous dissipation}} + \underbrace{S_h}_{\text{enthalpy}}$$

Equation 7

Where E represents the total energy and is given below

$$E = S_h + \frac{u^2}{2}$$

Equation 8

Where S_h , p , ρ and u are the enthalpy, pressure, density, and velocity of the fluid respectively.

3.5 The Lagrangian model for droplet evaporation and transport:

The exhaled particles can be modelled as N particles dispersed within airflow. The droplets are ruled by well-known Lagrangian set of equations.

$$\dot{X}_i = u_i + \sqrt{2}D_v \eta(t) \tag{Equation 9}$$

$$\dot{U}_i = \frac{u(\dot{X}_i(t), t) - U_i(t)}{\tau_i} + g \tag{Equation 10}$$

where N is the number of droplets, X_i is the position of the i -th droplet and U_i its velocity, and g is the gravitational acceleration. Each droplet is affected by a Brownian contribution via the white-noise process η_i .

3.6 Development of head model:

Blender 2.9 was used to develop the 3D human head model by using front and side reference images of a male model. Low topology plane mesh was developed to define the basic features of the model.

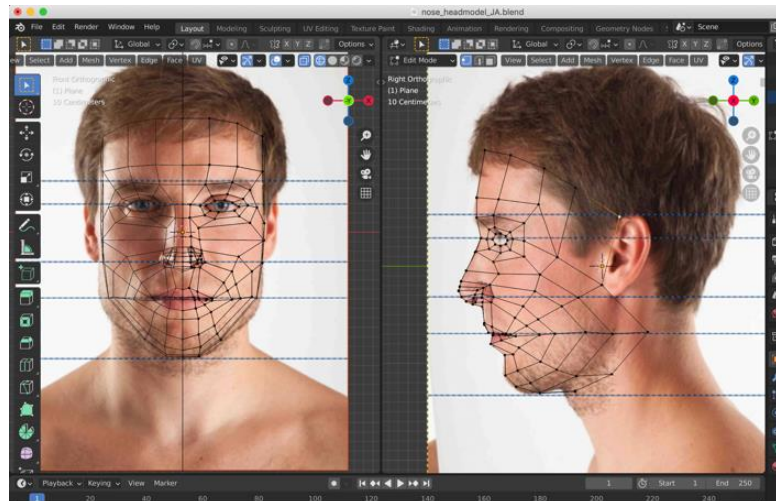


Figure 10: initial stage of modelling

Chapter 3. Methodology

It was refined later using subdivision surface modifier to increase the vertices on the mesh topology and refining the shape of the final head model.

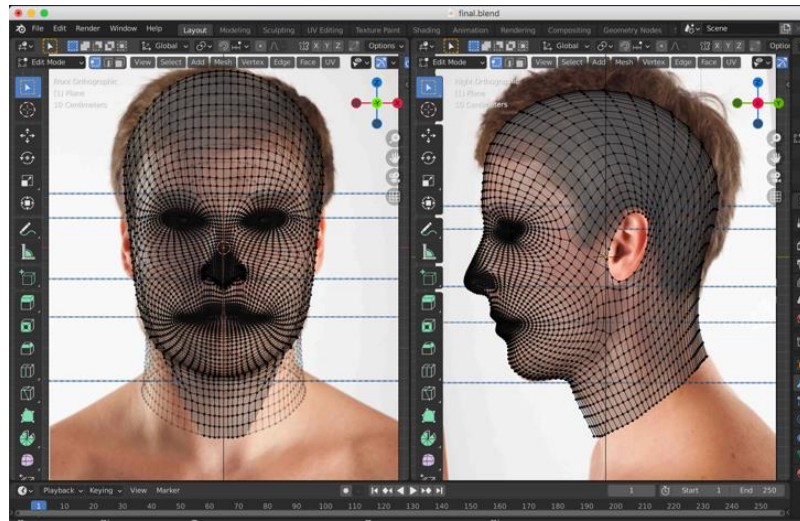


Figure 11: refined mesh with subdivision modifier

The final mesh was solidified using solidify modifier in blender.



Figure 12: front view of human head model



Figure 13: side view of human head model

3.7 Development of face mask:

The various masks can be modelled and assembled to the modelled face for comparison. The mask properties are obtained from the standard governing surgical masks, Australian Standard 4381:2015 and standard for N95 masks, AS/NZS 1716:2012 (Queensland 2020).

A mask model of N95 respirator was developed using Fusion 360 and it was appended to the head model in Blender as shown below.

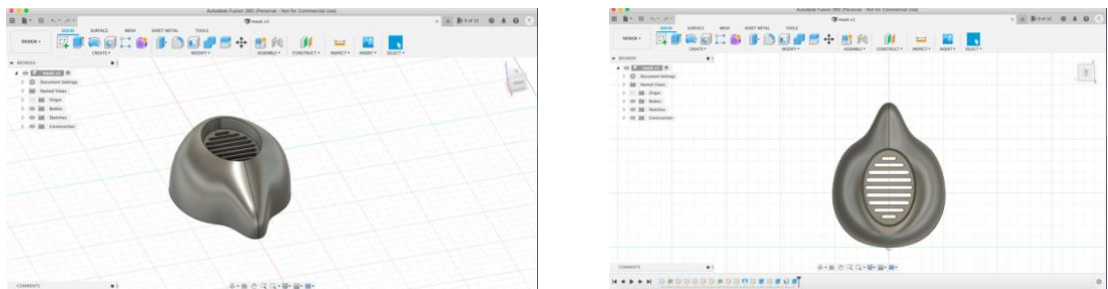


Figure 14: mask development

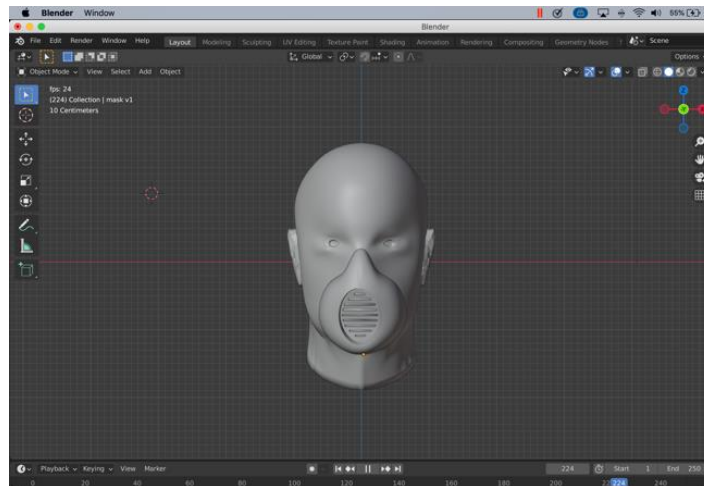


Figure 15: head model and mask appended together

The research study showed that the meaningful size of particles ranges from $0.1 \mu\text{m}$ to $100 \mu\text{m}$. It is highly unlikely for larger particles greater than $100 \mu\text{m}$ to penetrate through the mask as they cannot achieve a high velocity and falls down due to gravity whereas the particles smaller than $0.1 \mu\text{m}$ make up a very small fraction of the total particles and are likely to escape regardless of a mask and will remain airborne regardless of their velocity (Dbouk & Drikakis 2020).

3.8 Computational Domain:

A 3-dimensional computational domain was generated for the simulations, in the shape of a cubicle room to account for indoor environment. The dimensions of the room were $200 \text{ cm} \times 200 \text{ cm} \times 150 \text{ cm}$. The head is placed near a wall at an approximate height of 170 cm from the floor for an average male. The mouth was selected as velocity-inlet and all the walls of the room as pressure-outlet. The floor was selected as wall with trap boundary condition.

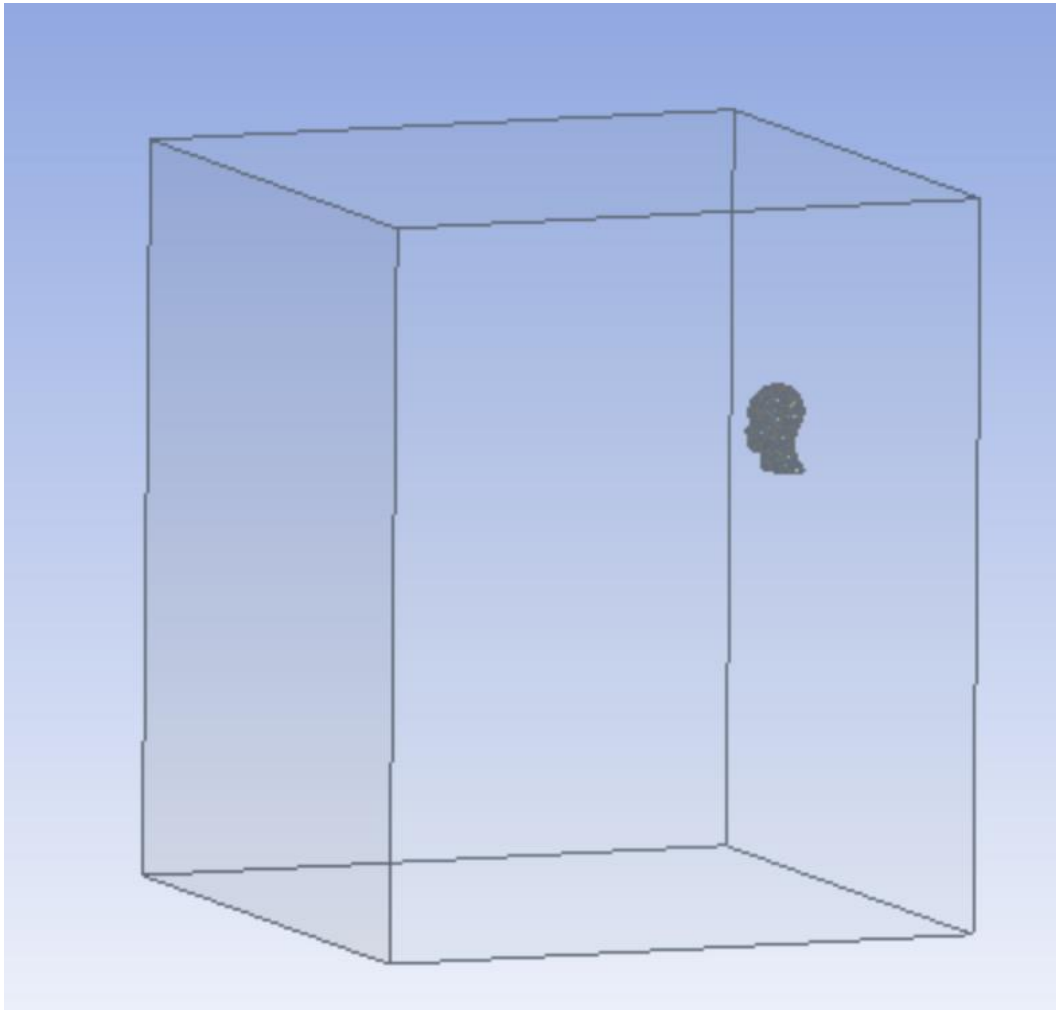


Figure 16: computational domain in ANSYS Fluent

3.9 Mesh Generation:

Mesh quality is an important consideration when undertaking a CFD analysis to provide accurate and reliable results. Generating a mesh often requires significant time and computing resources depending on the complexity and geometric configuration of the mesh required. It is however important to note that at this point the investment made in generating a good mesh pays greater dividends when it comes to generating a solution. Bakker, (2002) states that the mesh density should be high enough to capture all relevant flow features. Hexahedral meshes offer the best solution, with the accuracy of the solution becoming even greater when the mesh grid lines are

Chapter 3. Methodology

aligned with the flow. Quality of a mesh is defined by the following three features: Skewness, Smoothness and Aspect Ratio. Keeping the mesh quality high will ensure that solutions are as accurate as possible. The complex geometry of the model can be broken down into a mesh of discrete elements to increase the accuracy of the result. Although creating the mesh increases the accuracy of the solution but mesh count also increases simultaneously, thus increasing the computation time for simulation. Unstructured meshing technique was used because of the complex geometry.

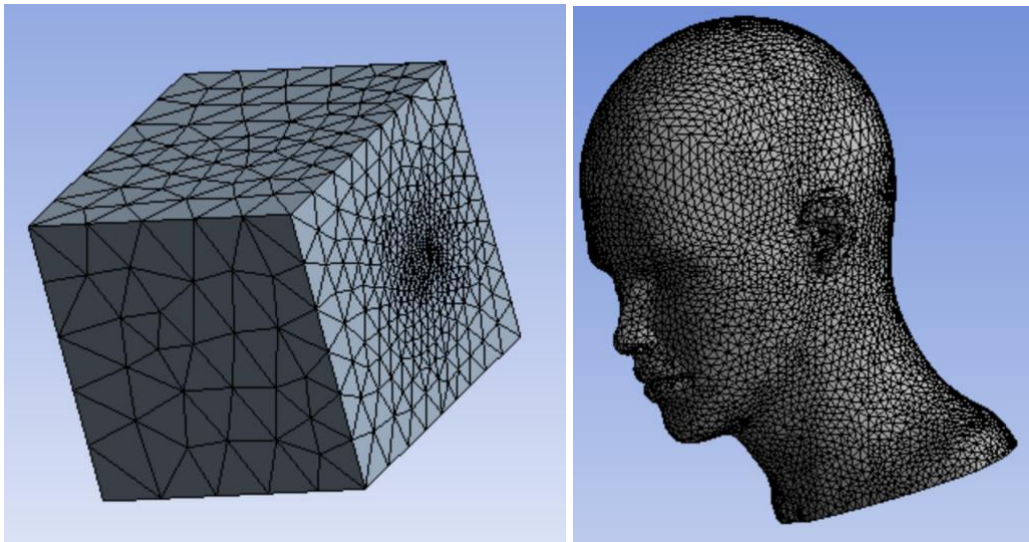


Figure 17: Initial mesh generation

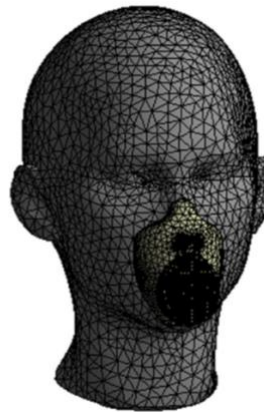
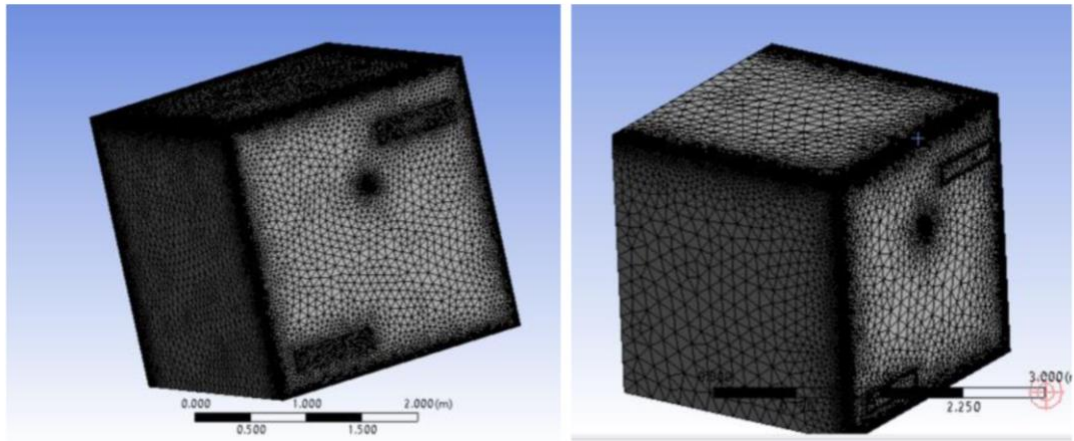


Figure 18: Refined mesh

3.10 Boundary Conditions:

Next step is to apply the boundary conditions and flow conditions such as flow inlets, outlets, and surface conditions. The mask elements were modelled as porous media with different filtration rates to account for different types of masks. The energy equation was turned on to account for temperature variations. Species transport model was turned on with diffusion energy source checked in. The discrete phase model was turned on with interaction with continuous phase and unsteady particle tracking. The number of volumetric species used were 3 containing water, oxygen and nitrogen to act as real air. The transient velocity profile imposed at the inlet is implemented as the inlet boundary condition to account for the time-dependent velocity of the flow at the human mouth. All the six walls of the domain were defined as no-slip adiabatic wall

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with DPM selected as reflective for five except floor. Floor's DPM was selected as trap. The fluid injected from the inlet is defined as water-air vapor which is usually considered as the flow caused by human exhalation activity.

Mask is modelled as a layer between surrounding air and face, it is modelled as a porous medium. For cotton mask, single layer is used, for surgical mask two layers of interface are used whereas for N95 respirator 3 layers of porous media are used to account for the filtration efficiency of the respective masks.

3.11 Turbulence Models:

The iterative solution can be achieved by applying the algorithm to solve the flow in each element based on the boundary conditions and flow conditions in the elements surrounding it. The employed algorithm is Reynolds-averaged Navier–Stokes' equations in conjunction with the $k-\omega$ turbulence model in the shear-stress-transport formulation for better convergence (Dbouk & Drikakis 2020). The selection of turbulence models depends on many factors, including the time and accuracy required, limitations of the model, the physics of the specific flow etc. The $k-\omega$ turbulence model is reliable in predicting a wide variety of flows, including aerofoils, pressure gradient flows, and shock waves (Bi et al., 2021). Therefore, the $k-\omega$ turbulence model is employed to predict the coughing flow field in this study. Two-way turbulence coupling with stochastic collision, coalescence and breakup of injected particles is used with Rosin-Lammer-Logarithmic spray of injected particles. Temperature of the particles is selected as 310 K and cough velocity is estimated as 22 m/s with a flowrate of 0.018kg/s.

Chapter 4. Results and Discussions:

For solution of simulations, pressure-velocity coupling method is used, pressure, momentum, water, oxygen, and energy are all selected second order upwind for better accuracy after hybrid initialization of the solution.

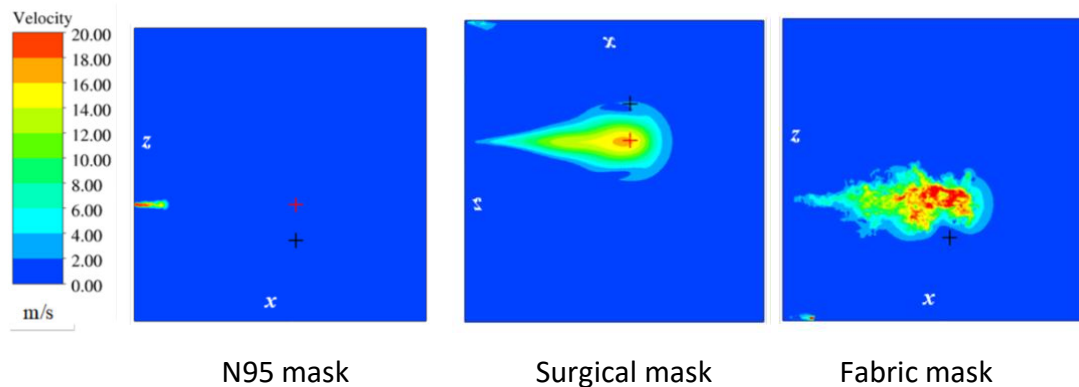


Figure 19: velocity simulations with different masks

The above simulations show that velocity of the particles released after exhalation is reduced when it passes through N95 mask because the filtration layers take away the turbulence and kinetic energy and reduce the speed of the particles, hence reducing the transmission. Whereas in surgical mask, the kinetic turbulence is reduced due to filtration although the particles travel a farther distance, but in case of fabric mask, the particles travel at a relatively higher speed with greater kinetic energy hence travel the farthest carrying the virus with them. Which suggests that N95 masks are much better in blocking and diverging the particles as compared to other masks due to their better filtration efficiency.

Wearing a mask can significantly distort the exhalation dynamics in terms of pressure distributions, velocity, contours, streamlines and vector fields as compared to no mask. A pressure-drop and velocity reduction is observed which indicates the usefulness of wearing masks to control the virus transmission.

Chapter 4. Results and Discussions

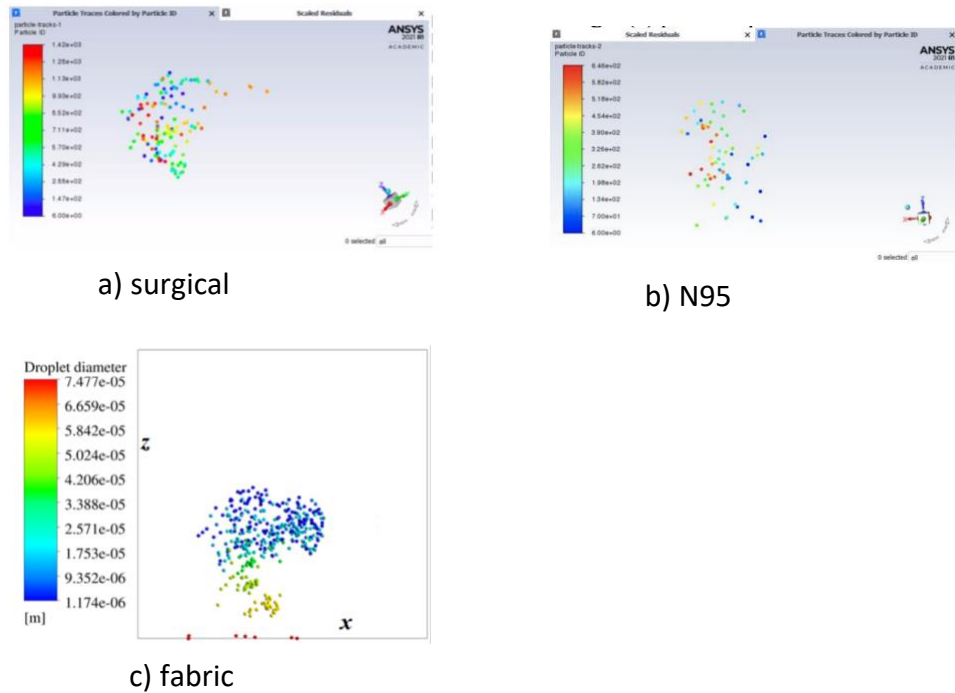


Figure 20: Particle tracking with various masks

The contours of droplet diameters give a clear visualization of the transient nature of the location of droplets in various sizes, which, in turn, provides a more graphic and easier understanding of the droplet dispersion process. The smaller droplets remain suspended for a longer time.

The table below shows the total particle released in the injection method and number of particles escaped, evaporated, and blocked by the three types of masks.

Particles	Released C_d	evaporated	escaped	Blocked C_u	lost	% Efficiency
N95 mask	412	13	29	364	6	88.3
Surgical Mask	616	28	67	498	23	80.8
Fabric Mask	372	38	96	192	46	51.6

Table 3: Mask efficiencies

Chapter 4. Results and Discussions

In the table above the mask filtration efficiency is calculated as

$$FE = (C_d/C_u) \times 100\%$$

Equation 11

where C_u , C_d are the particle count in the upstream feed prior to filtration and in the downstream filtrate, respectively.

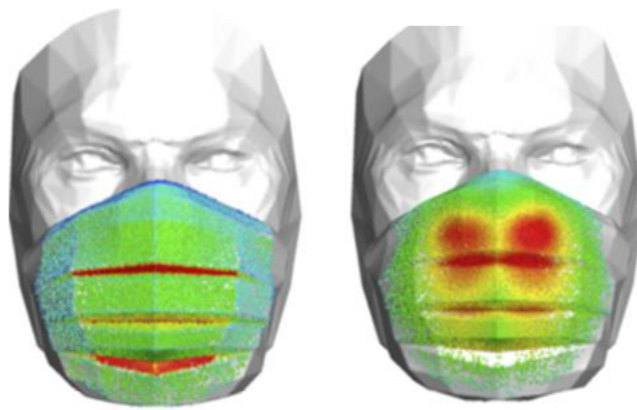


Figure 21: particle deposition in mask folds Xi et al. (2020)

Due to the mask resistance, the speed of both airflow field and particle motions notably decreased which decreased the chance of particles to escape through the mask after exhalation. All masks protect the wearer from larger droplets whereas the masks with higher efficiency can protect from smaller particle sizes as well.

Chapter 5. Conclusion and Recommendations:

5.1 Conclusion:

A numerical study has been carried out to simulate the human exhalation process and generation of cough droplets during the process. The Lagrangian discrete phase model is used to track the particles with the diameter range from $2e-6$ m. It was found that larger droplets were blocked by the masks whereas some of the smaller droplets escaped and evaporated. It was established that evaporation occurs immediately after the droplets were injected. The collision and coalescence have a great influence on the droplets sizes because they can change their size when they collide with each other. Initially droplets increase their sizes due to collisions and fall to the ground due to gravity which makes the number of suspended droplets fall.

It was evident that forced exhalation like coughing and sneezing can cause the droplets to escape from disposable and fabric masks but N95 can capture a large number of high speed and turbulent particles as compared to other masks. The gravity model used in ANSYS fluent indicated that the heavier particles sediment owing to their weight with negligible action of the airflow. However, the smaller particles travel a larger distance before evaporating due to inertial forces. Larger droplets greater than $75 \mu\text{m}$ contain even higher viral count per droplet, but they tend to settle rapidly and therefore present little airborne transmission potential except under strong wind conditions (Li, 2021).

It is apparent that face masks are very effective in protecting against infection from the spread of virus carrying exhaled cough droplets in the indoor environments, however finer aerosols can escape from the masks but most of the viral load is carried by heavy droplets. Various facemasks with different flow resistance show different efficacy but all of them block larger cough and sneeze droplets but fabric masks and surgical masks cannot block the finer aerosols which can escape through the filtration layers of the masks. Face masks are the new normal to live with the virus.

5.2 Recommendations:

Future study is recommended to investigate the behaviour of particles at different exhalation flow rate and exhalation speed. The size and speed of droplets can alter with changing flow rate and different mode of exhalation. Humidity also affects the behaviour of particles. It can change the sediment and evaporation rate of the exhaled particles. A future study related to different ambient conditions can be conducted to identify the behaviour of droplets and aerosols in different surroundings. Spherical profile of droplets is selected for simulation in ANSYS fluent, but particles may change their shape and behave differently when they collide initially. A future study can be conducted for outdoor conditions for different types and designs of masks. Particles were simulated in indoor ambient conditions in a closed confinement, whereas they can behave differently in outdoor conditions when wind is blowing in different conditions. Similar design of masks was considered for this study, but mask designs can be improved to identify the better efficient mask.

5.3 Consequential Effects:

The successful completion of the project provided sufficient evidence for the requirement of use of face masks for general public or essential workers in compromised situations. The world is facing this pandemic for more than a year now and there are very few countries which are safe from this contagion. Businesses are closing down, and unemployment rate is rising day by day. Although COVID-19 vaccine is available now, but it would take years to vaccinate the whole world population. The deadly virus can mutate itself to grow more dangerous and the only way is to learn to live with it by protecting yourself and the community. Along with other good hand and respiratory hygiene methods and social distancing, face masks in confined premises are the essential SOPs which can be followed to prevent the spread of this disease.

The main value of face masks is to protect the community. Face masks can be useful for both healthy and infected persons, it can protect the wearer from getting the infection or might prevent the wearer transmitting the airborne virus to others. The research studies based on CFD analysis of airflow while wearing a mask or without a mask, have shown that respiratory droplets and aerosols are diverted and filtered with the mask on and can significantly reduce the person-to-person transmission if masks are worn properly. The epidemiologic data from various studies to compare the COVID-19 growth rate before and after mask mandates in different countries, also

Chapter 5. Conclusions and Recommendations

suggest that the daily growth rate of community transmission slows down with the use of face masks.

The following two compelling cases suggest that face masks can reduce or prevent transmission in high-risk scenarios. In Missouri, in late May 2020, two infected hair stylists tested positive for corona virus and had close contact with the customers but none of the clients became infected as everyone wore a mask. In another case, a man flew from China to Toronto while unknowingly infected and wore a mask on the flight but all of the 25 passengers closest to him tested negative for COVID-19 (Bai 2020).

Couple of years ago masks were only used by very few communities but the rise of this pandemic has forced all the countries to make the use of masks a compulsion for some time for their citizens. Mostly, face masks are made of petroleum-based non-renewable polymers that are non-biodegradable, hazardous to the environment and create health issues (Dharmaraj et al. 2021). Use of disposable masks can give rise to increasing pollution as new ways need to be designed to recycle or safe disposal of the mask materials.

5.4 Associated Risks:

The execution of project involves research study and work on ANSYS software to perform the necessary numerical analysis, hence no hazardous risk is associated with completing this project. However, it carries some level of continuing responsibility.

- The research study and project evaluate the effectiveness of face masks and their role in prevention of airborne transmission; however, it is essential to wear the properly fitted mask, otherwise it will lose its effect and the risk associated to contract the virus will increase and mask will only provide a false sense of security.
- When wearing a mask, a person's speech become muffled and the people with hearing impairment can suffer as they rely on lip reading.
- There is a lack of non-verbal communication when wearing a mask which can make people mentally troubled or can arise psychological problems.
- Facial identification is hard when a mask is on which can give rise to crime rate.
- Masks need to be changed or washed regularly as breath can dampen the mask. The edges can lose the protective effect for both wearer and the environment (Matuschek et al. 2020).

Chapter 5. Conclusions and Recommendations

- Pathogens can accumulate on the surface of masks and if they are not exchanged regularly, the risk of spreading the disease can increase significantly.
- Surgical masks are disposable and should be used only once. The use of disposable masks by health workers and general public can give rise to environmental pollution as mostly the masks are made of vinyl and polymers which are hard to recycle or degrade.
- It can be an extra financial strain on already suffering economies.
- There can be an airflow obstruction when wearing a mask specially during physical exertion.

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APPENDIX A: Project Specification

For: Poonam Jawad
Title: Identification of the effectiveness of various commercial COVID -19 Masks using ANSYS software
Major: Mechanical Engineering
Supervisors: Belal Yousif
Enrolment: ENG4111- S1- 2021, Online

Project Aim: To identify the effectiveness of various COVID-19 masks using ANSYS software and to determine their usefulness in preventing and slowing down the pandemic.

Programme: Version 1, 17th March 2021

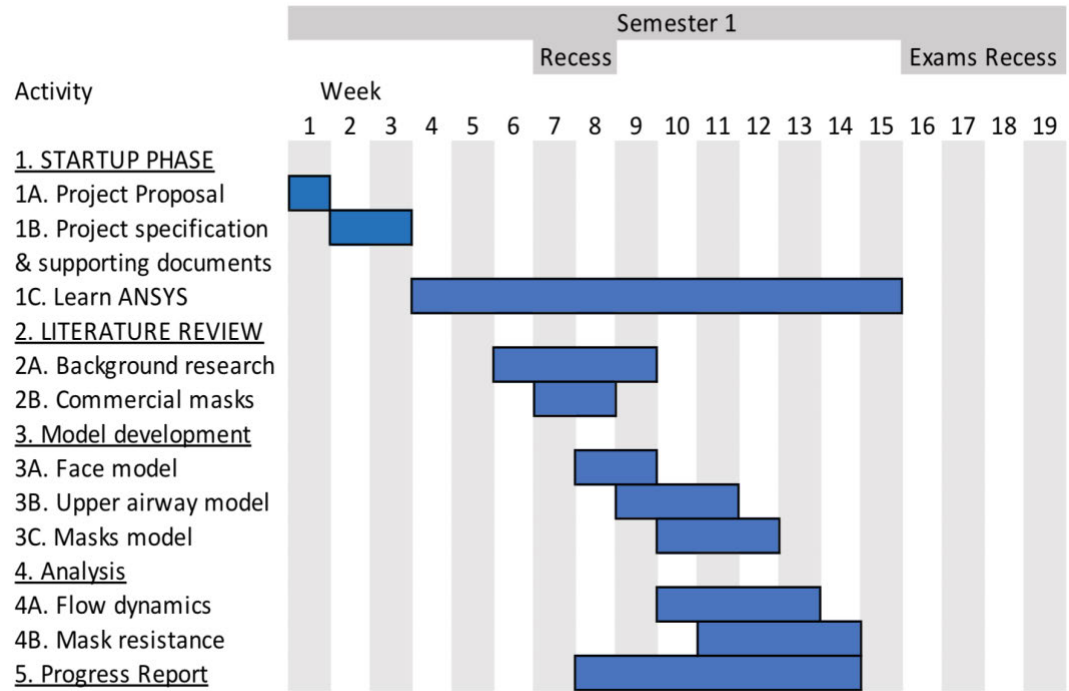
1. Identify the need to use masks to prevent the inhalation of air-borne COVID-19 virus and to minimize the exhalation of virus-laden aerosols and droplets.
2. Conduct detailed research on various commercial COVID-19 masks available in the market with different filtration efficiencies and breathability levels.
3. Identify the level of effectiveness required for different mask users such as healthcare workers, aged care workers, patients etc.
4. Develop a computational model including a face, upper airway and various masks using ANSYS software.
5. Analyse the airflows and droplets motions near the face when wearing different masks.
6. Track the particle motion using a discrete phase Lagrangian tracking algorithm for the flow and particle velocities.
7. Determine the mask viscous resistance using Darcy's Law.
8. Characterize the effect of mask filtration and resistance on the deposited aerosols and particles on face and upper airway.
9. Differentiate the effect of particle size and inhalation flow rate in different masks by analysing the particle dosimetry.

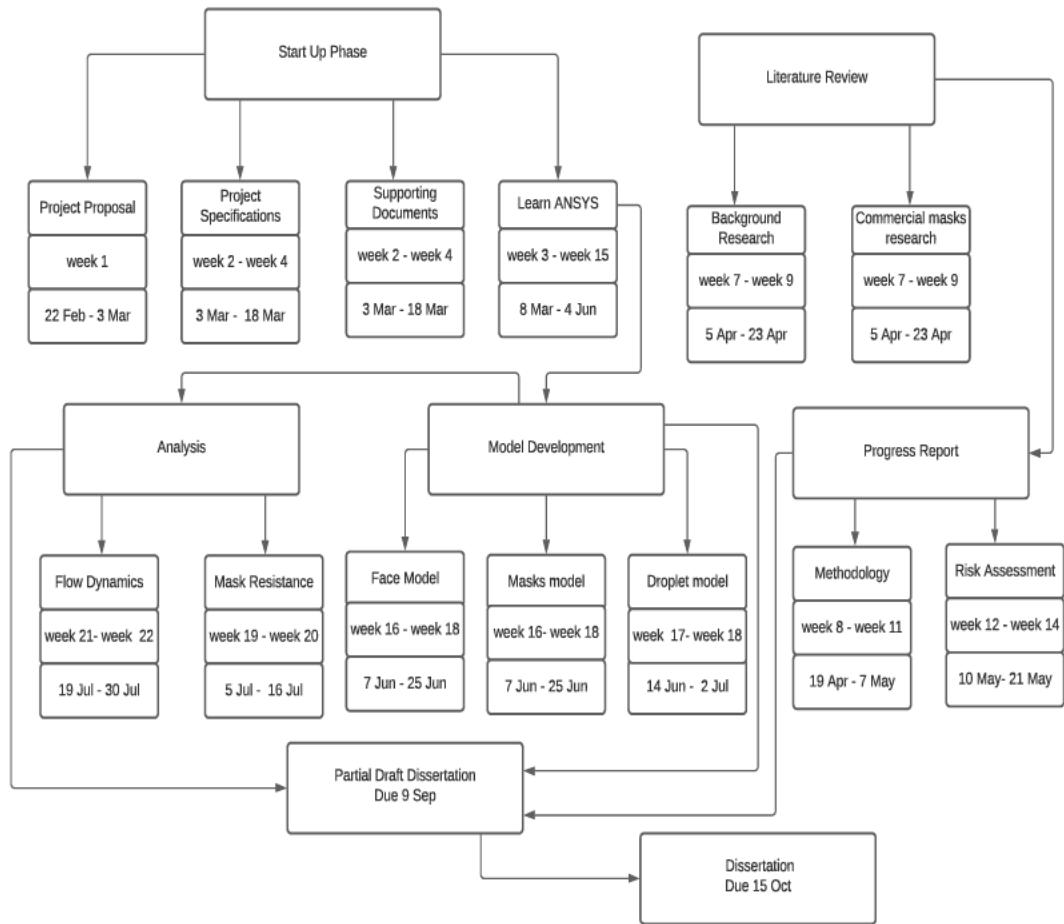
10. Analyse the deposition of particles in the upper airway for different flowrates and mask resistances.
11. Evaluate the effectiveness of various masks using all the data.

If time permits:

12. Investigate the fluid dynamics of the particles after a person coughs or sneezes in a mask as droplets shape, size and speed change considerably after such incident.

APPENDIX B: Project Research Timeline





APPENDIX C: Resource Requirement Plan

- Need to install ANSYS software.
- Need to learn and practice ANSYS software modelling and computations and simulations.
- Need access to USQ laboratory from time to time through VPN to work on ANSYS.
- The library database specially Science Direct to find relative journals and articles to conduct a detailed literature review.

APPENDIX D: Risk Management

Risk assessment is a process for developing knowledge and understanding about hazards and risks so that good decisions can be taken about controlling them. This project required use working on computer screen for long period of times, whether for researching the literature, computer modelling, simulations, or analysis. Therefore, the risk associated with this project is stress on eyes, headache, sleep problems, chronic neck and back pain etc. These risks can be managed by planning and organising the tasks appropriately, taking breaks and proper time management.