

Design, Simulation and Experimental Validation of a Minor Flow Channel Based Virtual Impactor to Generate Mono-Disperse Aerosols

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ABSTRACT

The controlled release of mono-disperse aerosols can lower pollution and improve the environment and public health in Bangladesh, a developing country in South Asia. Different aerosol generation systems, such as conventional and virtual impactors (VI) mostly jet impactor, rectangular jet virtual impactor, slot-in-line virtual impactor, dichotomous virtual impactor and cascade impactor have been identified so far for the aerosol research based on condensation, penetration, atomization, and diffusion. To ensure uniformity in the dispersed or suspended aerosols, both conventional and virtual impactors can be used. The virtual impactors substitute a fake area of the slowly drifting air for the impaction region. Mono-disperse aerosol can be produced using a variety of techniques and methods, however the virtualized mono-disperse aerosol generating system with impaction plate might be a viable choice with many application domains. In order to address issues like the re-suspension of impacted particles, a virtual impactor has been designed, and the flow of aerosol particles inside the impactor has been simulated. By dividing the flow streams, the impaction surface is in this instance substituted by a minor collecting flow, giving rise to the concept virtual. Particles that are too small to be collected in the minor flow are carried out of the side of the virtual impactor by the "major flow," which is the bigger proportion of the flow. In this study, a virtual impactor with a single air intake, a minor stream channel that is inclined at 45° degrees to the inlet aerosol flow path, and a particle generator are designed, numerically analyzed, and tested for performance. The intended impactor's distribution of velocity profile, distribution of pressure, tracking of particles, and erosion contour have all shown simulation results. Wall losses of the virtual impactor have also been analyzed. The liquid mixture of 80% ethanol and 20% olive oil is used to create the mono-disperse aerosol. The minimum GSD (Geometric Standard Deviation) for this aerosol has been found to be 1.22 at an air flow rate of 56.6 lpm to the virtual impactor, and the NMAD (Number Mean Aerodynamic Diameter) has been determined to be 0.475 μm. For a minor flow of 13.28%, the monodisperse aerosol has been produced. A comparative study has been done between different types of impactors of aerosol generation systems with the designed and simulated virtual impactor based on design, mono-disperse aerosol generation and performance.

Keywords: Virtual Impactor, Conventional Impactor, Numerical Analysis, Minor Flow, Geometric Standard Deviation.

1. Introduction

Researchers primarily used both poly-disperse and monodisperse aerosols to examine the deposition of particles, despite the fact that polydisperse aerosols have been linked to negative health effects. Aerosol particles with a narrow distribution and a geometric standard deviation (GSD) of less than or equal to 1.25 are known as monodisperse aerosols. Dispersion is one of the aerosol's physical properties [1]. In the testing lab, mono-disperse aerosols with equally sized particles can be created. Particle sizes vary in aerosols of the polydisperse colloidal system type. For a controlled flow field with regard to velocity profiles, turbulence intensities, and a tight band scale particles distribution, laboratory test aerosol conditions are required. Aerosol generation system installation is complicated because of the lack of appropriate aerosol technology. The production of mono-disperse test aerosol has been carried out using a variety of tools and methods, but an active possible system with the broadest range of applications can be the impaction surface based mono-disperse aerosol generation system. Applications for monodisperse aerosols include the experimental testing of models, filter testing, and aerosol instrument calibration. It is crucial for researchers to create

monodisperse aerosols using the best possible aerosol generation impactors.

1.1 Impactors

An impactor is a device that uses selective collection or impaction to separate particles based on their inertia. The aerosol of interest is introduced into the impactor through a nozzle, creating a jet of particles that are directed towards a flat impaction plate that is parallel to the flow. When a particle's inertia surpasses a specific threshold, it will strike or collide with the plate. Only a small fraction of the particles will be able to follow the gas streamlines and escape the instrument. Gravimetric analysis of the impaction plates can be used to determine the particle size distribution. Impactors have the benefit of being straightforward in both design and use, and as a result, they have developed into a staple tool in aerosol science.

1.1.1 Conventional Impactors

A subclass of the conventional impactor is the virtual impactor. The typical impactor accelerates a stream of air that it directs towards an impaction plate using a nozzle. Particles with enough inertia will be

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removed from the air stream by the impactor, and they will then strike the impaction plate [2].

1.1.2 Virtual Impactors

A collection probe takes the place of the impaction plate as a virtual impactor. It separates the air stream inside the collection probe from the particles that would otherwise gather on the impaction plate of a traditional impactor and flushes them out of the collection probe with a small portion of the overall flow. Greater inertia large particles follow the streamlines of the primary flow and are carried upward. Smaller, less inertia-intensive particles deviate from the flow directions and continue to travel axially along the collecting probe with the minor path of flow. [2].

1.2 Atomizer

The air blast type dual (twin) fluid atomizer has been used in the experiment so that liquid can be sucked into it and that it is fed with compressed air. When using the atomizer, Bernoulli's principle has been taken into account. The pressure of the liquid is atmospheric. There is a pressure differential because the atomizer's constricted area has a lower pressure than the surrounding air. The atomizer is then filled with the liquid via a siphon. These are subsequently transported to the exit part after dissolving into tiny, fine droplets. The three components that make up the atomizer are an air inlet, a main body, and an exit nozzle [3].

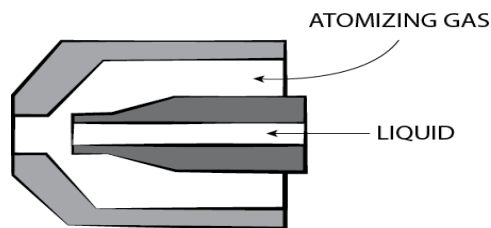


Fig.1 Air blast type twin fluid atomizer [3].

2. Design Criteria

Design criteria is an important factor for the design of anything. For our design, we also have to consider some important factors for the cross section and acceleration nozzles based on pattern of the spray and it's impact, droplet size, aerosol mass distribution and flow rate at different sections. One air intake, or inlet, and one minor flow channel where the minor flow channel is in inclination at 45° to the inlet aerosol flow path make up the virtual impactor as shown in the Fig.2(a) and Fig.2(b).

Table 1. The following data are required to design a virtual impactor.

Name of the properties	Values
Sample flow velocity at air inlet, aerosol inlet & nozzle for design	0.01, 5 & 17.95 m/s
Flow rate of aerosol & air (at ambient temperature & pressure)	1.121×10^{-7} & $3.94 \times 10^{-6} \text{ m}^3/\text{s}$
Stokes number ($St \ll 1$, fluid will flow along the streamline)	$1.4 \times 10^{-4} \text{ stks}$

Bernoulli's principle with pressure differential	$P_1 - P_2 = \frac{1}{2} \rho (v_1^2 - v_2^2)$
Particle diameter as expected	1.5×10^{-6}
Density & viscosity of aerosol solution (5% olive oil + 95% ethanol)	800 kg/m^3 & $2 \times 10^{-3} \text{ Ns/m}^2$

2.1 Design parameters

Table 2. Design parameters of constructed Virtual Impactor.

Name of the properties	Values
Diameter of air inlet	22.40 mm
Diameter of aerosol inlet	22.80 mm
Diameter of inlet nozzle	4.00 mm
Diameter exit nozzle	4.00 mm
Suction height of virtual impactor	125 mm

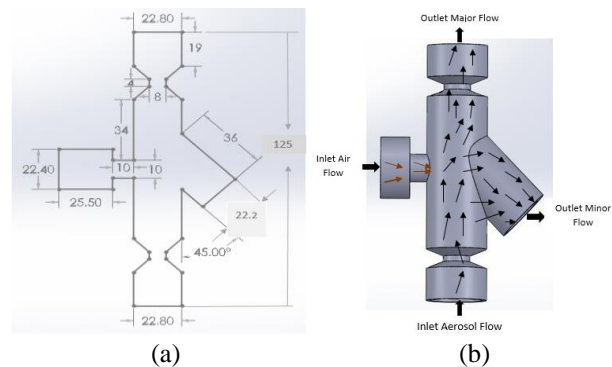


Fig.2 (a) A cross sectional and (b) 3D view of the designed minor flow channel based virtual impactor with dimensions.

3. Virtual impactor modelling and characterization

Mono-disperse aerosols are separated from poly-disperse to mono-disperse by an impaction principle followed as virtual rather than conventional by a virtual impactor. An atomizer is emulated to generate poly-disperse aerosol from the solution of (Ethanol + Olive oil) and is about to pass through an accelerating nozzle so that it can increase it's velocity and instead of impaction through a flat plate as of conventional impactor.

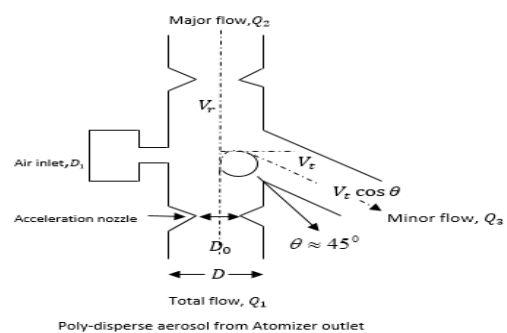


Fig.3 Simplified Impactor Model with circular area of major flow and minor flow.

The Stokes number, a dimensionless parameter can be used as the governing equation for the suggestion of whether a particle will strike the body of impaction or will follow the air stream-lines out of the region of impaction and form airborne particles. The characteristics of virtual impactors have been quoted by numerical solution of Navier-Stokes equation and of particles motion equation and reported the existence of a significant inner surface loss of the collection probe at the cut off size has also been reported [4].

V_i and V_r are velocities of major and minor portion of the flow. Q_1 , Q_2 and Q_3 are the denotation of total flow rate, major flow rate and minor flow rate respectively. Fig.3 dictates a simplified impactor model with circular area of major flow and minor flow along with some important parameters. Centrifugal force is the prime factor of travelling the particles along a circular streamline of major flow and causing it to move towards the collection probe.

Assuming the particle concentration (C) to be constant over the whole cross section, the collection efficiency E_1 , the fraction of entering particles that are collected is given by,

$$E_1 = \frac{\rho_a^2 D_{pa}^3 V_i^2}{70.3 \mu^2 D^2} \left[\frac{(\frac{B}{D})^2 J + KN + (\frac{Q_2}{Q_1})^2}{(\frac{B}{D})^2 J + KN} \right]^2 \quad (1)$$

Where,

ρ_a = Density of aerosol particle, D_{pa} = Particle aerodynamic diameter, $(B=D=d)$, $J = \{4(\frac{S}{D})^2 + (D-d)^2\}$, $K = \frac{Q_2 B}{Q_1 D}$, $N = \sqrt{4(\frac{S}{D})^2 + (\frac{d}{D} - 1)^2}$. The Stokes number is thus expressed as;

$$stk = \frac{\rho_a V_i C D_{pa}^2}{9 \mu D_0} \quad (2)$$

Where, V_i =Velocity of inlet aerosol, C =Correction Factor= $1 + \frac{2.52 \lambda}{D_p}$, λ = Mean free path of aerosol particle.

A mathematical model which is found most preferable is the well-known Gaussian distribution equation law. The Gaussian or normal distribution law is illustrated as:

$$Y'' = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[\frac{-(x-\bar{x})^2}{2\sigma^2} \right] \quad (3)$$

Where, x = Particle diameter, \bar{x} =Arithmetic mean particle diameter, σ =Arithmetic standard deviation.

$$Y' = \frac{1}{\ln \sigma_g \sqrt{2\pi}} \exp \left[\frac{-(\ln x - \ln M)^2}{2 \ln^2 \sigma_g} \right] \quad (4)$$

Where, M =NMAD = Number mean aerodynamic diameter, σ_g = Geometric Standard Deviation (GSD).

More, simplified form of equation (4) is;

$$Y = \frac{\sum n_i}{2.303 \log \sigma_g \sqrt{2\pi}} \exp \left[\frac{-(\log x - \log M)^2}{2 \log^2 \sigma_g} \right] \quad (5)$$

Where, n_i = Number of particles within size interval Δx ,

Y'' , Y' , Y = Probability density (frequency function).

Next, the two parameters M and σ_g can be expressed in terms of the following equation as below;

$$\log M = \frac{\sum n_i \log X_i}{\sum n_i} \quad (6)$$

$$\& \log \sigma_g = \sqrt{\frac{\sum n_i (\log X_i - \log M)^2}{\sum n_i}} \quad (7)$$

The numerical values for M and σ_g are properly expressed by these equations irrespective of the

logarithmic base employed since all conversion constants will be cancelled [4].

4. Numerical Study in ANSYS workbench

Numerical study has been done of a virtual impactor which significantly consists of single air inlet and single minor flow path or channel stream where channel of minor flow which is inclined at 45° to the inlet aerosol flow channel. The critical dimensions such as virtual impactor height, acceleration nozzle diameter, inlet and outlet diameters used in the numerical study have been taken for the geometry of the simulation. A software platform called Workbench supports our analytical (finite element analysis) duties. In essence, finite element modeling technique can be used to numerically resolve problems related to stress assessment, heat exchange or transfer, flow properties of fluid, as well as other engineering challenges. Ansys Workbench is the name of the finite element modeling program used in collaboration with CAD systems [5].

4.1 ANSYS workbench parameters

Ansys Workbench 2019 R2 is the simulation program utilized for the numerical analysis of the virtual impactor. Fluid analysis is the simulation's analysis system (fluent). For the numerical analysis in ANSYS, the essential 2D geometry of the virtual impactor has been visualized and deciphered using Solidworks software.

Table 3. Basic simulation parameters

Properties Name	Values
Flowing Model (Viscous)	K-epsilon (2 equations)
K-epsilon Model	Realizable
Near wall treatment	Enhanced
Total Flow Rate	0.426 kg/sec
No of iterations	200
No of particles tracked	184

Table 4. Mesh parameters

Properties Name	Values
Mesh Method	Triangle
Element Size Function	Adaptive
Smoothing Zone	High
Center of relevance	Fine
Transition	Slow
Element Adaptive Size	0.001m

4.2 Simulation criteria

The entrance and outflow parts of the virtual impactor that have been numerically examined are present. The aerosol inlet section of the impactor has been utilized to pass aerosol which are poly disperse made from an ethanol and olive-oil solution. The simulation takes into account factors such droplet diameter range, acceleration nozzle size and shape, liquid solution density, viscosity, and concentration.

By utilizing the analytical theories of Bernoulli's principle, Navier-Stokes equation in terms of velocity flow field, equation of collection efficiency, and sample and side flow velocities, the simulation dimensions of

inlet and outlet parts and acceleration nozzle have been determined.

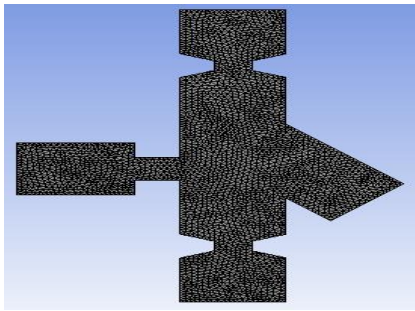


Fig.4 Mesh of the virtual impactor.

4.3 Mesh

The mesh structure of the virtual impactor has been shown in Fig. 4. The element size of mesh is kept 10^{-3} m for the virtual impactor. 3143 nodes and 5807 elements have been generated in the simulation software.

4.4 Boundary conditions

Table 5. Boundary Conditions

Properties Name	Esteems
Inlet Aerosol Velocity	0.5 ms^{-1}
Air Velocity	0.02 ms^{-1}
Minimum Diameter of droplet	$0.2 \text{ }\mu\text{m}$
Maximum Diameter of droplet	$180 \text{ }\mu\text{m}$
Convergence limit	0.0001
Mean diameter of droplet	$50 \text{ }\mu\text{m}$

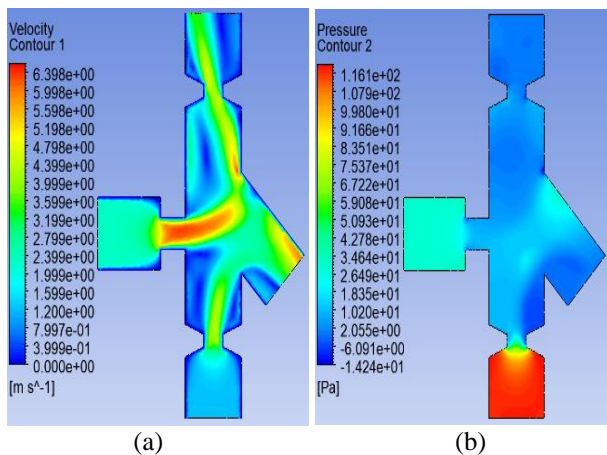


Fig.5 (a) Velocity distribution and (b) pressure distribution of the virtual impactor.

The distribution profile of velocity and pressure of the virtual impactor have been shown in the Fig.5(a) and Fig.5(b). The velocity distribution shows the impaction of fresh air on aerosol flow and separates in two flows. The outlet gauge pressure is set 0 in the fluent. The colors show the magnitude of velocity and pressure in regions of virtual impactor. Number of contours are set 100. Particle tracking of aerosol spray is done by discrete phase modeling (DPM) in fluent. The solution of ethanol and olive oil is used as aerosol material. Fresh air is used for impaction on aerosol flow.

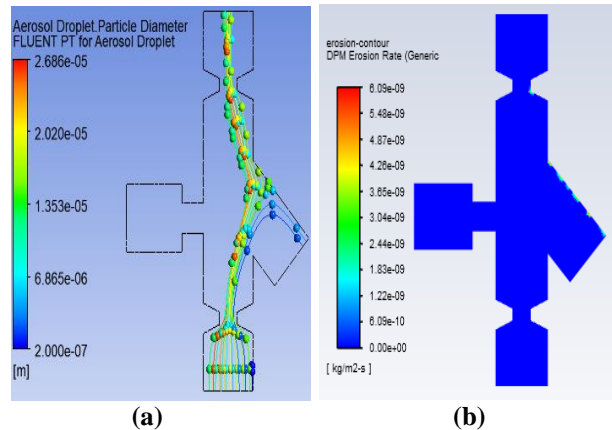


Fig.6 (a) Aerosol particle tracking and (b) erosion contours of the virtual impactor.

Particle tracking of aerosol spray is done by discrete phase modeling (DPM) in fluent. The solution of ethanol and olive oil is used as aerosol material. Fresh air is used for impaction on aerosol flow. Rosin-Rammler distribution is set as the diameter distribution. Particle tracking in virtual impactor has been shown in the Fig.6(a) and Fig.6(b). The particle diameters are indicated by colors. Erosion contour is obtained by enabling wall type trap in the fluent and erosion/accretion as the physical model. The erosion contours of the virtual impactor have been shown in the Fig.6. Here, the erosion rates are so much less that they can be neglected. But the erosion contours help to know the regions where the particles are trapped and to make decisions.

5. Methodology for producing mono-disperse aerosol using the virtual impactor

The experimental setup has been shown in the Fig.7. The virtual impactor has been fabricated from the designed data and simulation results and the material used for the fabrication was stainless-steel. The virtual impactor was placed at desired position. An air compressor was used to provide air to the atomizer and atomizer was placed at the bottom of the virtual impactor. Liquid solution made of was syphoned to the atomizer and aerosol was produced with the help of compressed air which was poly-disperse aerosol. The poly-disperse aerosol was then directed to the aerosol inlet of the virtual impactor and made mono-disperse by separating the droplets in major and minor flows. Larger aerosol droplets exited through the major flow. Smaller aerosol droplets were collected as mono-disperse aerosol from the minor flow. The minor flow was kept 5%-15% of total flow to obtain mono-disperse aerosol [41]. Discharges through different flows were measured by rotameters. Finally, the particles size of fine aerosol droplets was demonstrated by an optical particle counter (OPC) and Geometric Standard Deviation (GSD) and Number Mean Aerodynamic Diameter was calculated.

- Composition 1 —◆— (5% Olive Oil, 95% Ethanol)
- Composition 2 —■— (10% Olive Oil, 90% Ethanol)
- Composition 3 —▲— (15% Olive Oil, 85% Ethanol)
- Composition 4 —✱— (20% Olive Oil, 80% Ethanol)

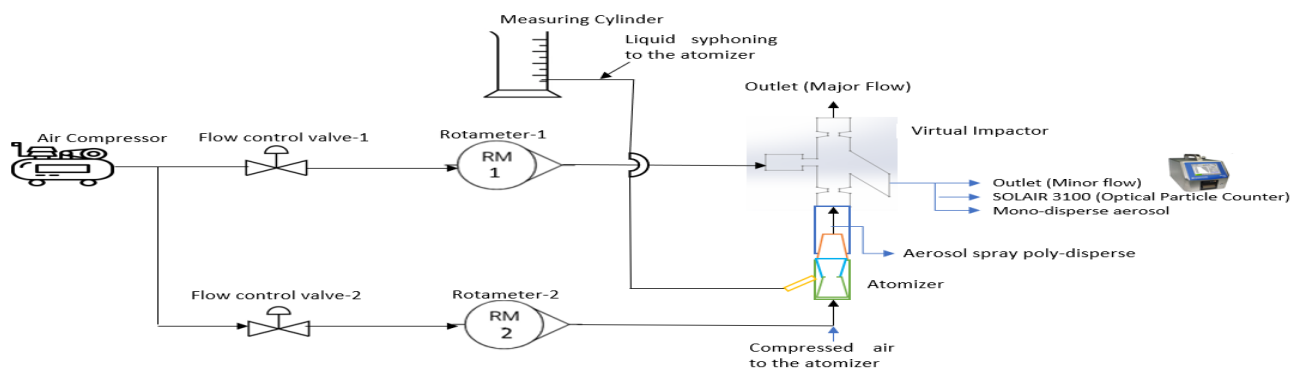


Fig.7 Schematic diagram of Experimental Setup for producing mono-disperse aerosol using the designed virtual impactor.

6. Results and discussion

The designed and simulated virtual impactor has a driving parameter called air flow rate. The impaction of poly-disperse aerosol from atomizer inside the impactor depends on air pressure and liquid consumption rate. Air flow rate is responsible for the design values of the variables used for the impaction. The air flow rate to the virtual impactor is directly proportional to liquid consumption rate and NMAD (Number Mean Aerodynamic Diameter), but inversely proportional to the GSD for different air flow rates to the atomizer.

Table 6. Variation of liquid consumption, NMAD and GSD with air flow rate to atomizer for 56.6 lpm air flow rate to virtual impactor for composition 04

Air flow rate to atomizer (lpm)	Solution Concentration	Liquid Consumption (ml/hr)	NMAD (μm)	GSD
22	20% Olive oil + 80% Ethanol	277	0.435	1.89
24		353	0.444	1.78
26		397	0.451	1.70
28		457	0.462	1.56
30		499	0.475	1.22

Table 7. Variation of liquid consumption, NMAD and GSD with air flow rate to atomizer for 56.6 lpm air flow rate to virtual impactor for composition 03

Air flow rate to atomizer (lpm)	Solution Concentration	Liquid Consumption (ml/hr)	NMAD (μm)	GSD
22	15% Olive oil + 85% Ethanol	290	0.420	1.93
24		367	0.427	1.88
26		401	0.431	1.71
28		469	0.440	1.66
30		502	0.452	1.50

Table 8. Variation of liquid consumption, NMAD and GSD with air flow rate to atomizer for 56.6 lpm air flow rate to virtual impactor for composition 02

Air flow rate to atomizer (lpm)	Solution Concentration	Liquid Consumption (ml/hr)	NMAD (μm)	GSD
22	10% Olive oil + 90% Ethanol	310	0.418	2.01
24		380	0.421	1.88
26		415	0.425	1.70
28		490	0.430	1.68
30		530	0.433	1.52

Table 9. Variation of liquid consumption, NMAD and GSD with air flow rate to atomizer for 56.6 lpm air flow rate to virtual impactor for composition 01

Air flow rate to atomizer (lpm)	Solution Concentration	Liquid Consumption (ml/hr)	NMAD (μm)	GSD
22	5% Olive oil + 95% Ethanol	420	0.410	2.09
24		510	0.431	1.82
26		580	0.435	1.64
28		640	0.442	1.61
30		710	0.449	1.56

The above data has been taken with respect to the different conditions of the experiment. From the results, different effects of various parameters have been observed for various compositions of liquid solution.

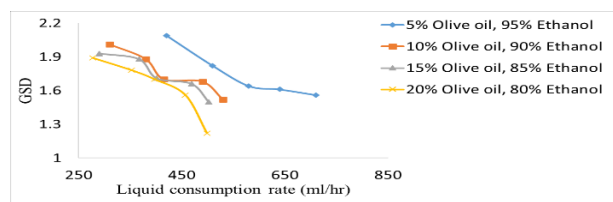


Fig.8 Effect of liquid consumption rate on GSD for different composition for 56.6 lpm air flow rate to virtual impactor.

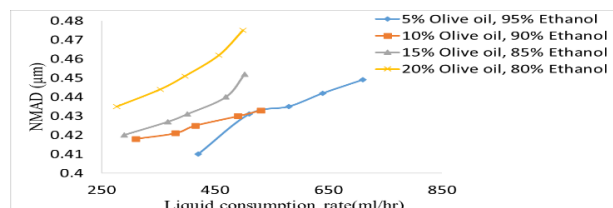


Fig.9 Effect of liquid consumption rate on NMAD for different composition for 56.6 lpm air flow rate to virtual impactor.

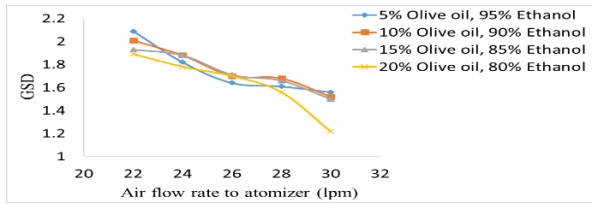


Fig.10 Effect of air flow rate to atomizer on GSD for different composition for 56.6 lpm air flow rate to virtual impactor.

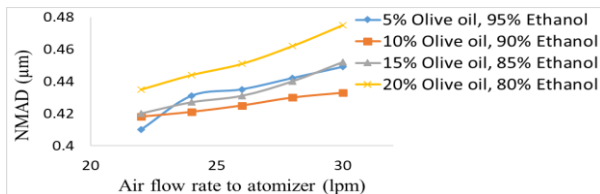


Fig.11 Effect of air flow rate to atomizer on NMAD for different composition for 56.6 lpm air flow rate to virtual impactor.

Table 10. Observation of particle tracking and escaping and experimental validation of simulation

Medium of study	Number of particles tracked	Number of particles escaped	Number of particles trapped	Percentage of particle trapped
Experimental	397927	357179	40748	10.24%
Numerical	1242	1135	107	8.61%

7. Comparison with the existing conventional and virtual impactors based on the literature

Various conventional and virtual impactors such as simple jet impactor, rectangular jet VI, slot-in-line VI, dichotomous VI, counterflow VI and cascade impactor have been used so far for sampling aerosol droplets based on their size using common or virtual impaction surfaces. The jet impaction is done using virtual space of slit type rectangular jet where slit width ratio is 0.5 with jet width 1mm and 50% separation efficiency. An inverted dual cone impaction surface is used in a slot-in-line VI with a circumferential slot of definite width and length for causing the flow instabilities in the major flow region [6]. In counterflow VI, inertial impaction is used to separate large droplets from the surrounding air with an adjustable cut size in the size range from 9 to 30 μm diameter, rejecting droplets smaller than the cut size and catching droplets larger than the cut size [7]. Dichotomous VI use acceleration nozzle and aerodynamic particle outpoint whereas cascade impactor uses electrical low pressure for measuring particle number concentration and particle number size distribution in real time. The ideas in this research were adapted from Chen, H. Y., and Huang, H. L. (2016), *Journal of Aerosol Science*, 94, 43–55. Sample flow, side flow, sheath flow, outlet (minor flow), and outflow are characteristics of virtual impactors utilized in this literature (main flow) [8]. To reduce the complexity of aerosol separation, however, we have not included the sheath flow section in our design. We have come to the point that the virtual impactor produces mono-disperse

aerosols with fewer particles trapped by comparing the separation efficiency based on the minor flow with the wall losses of the current study.

8. Conclusion

From the numerical analysis done by us, the percentage of particle trapped has been found 8.61% for 1242 no. of particles being tracked. From our experimental study, the percentage of particle trapped is 10.24% and at an air flow rate of 56.6 lpm to the virtual impactor, the lowest GSD for trapped aerosol has been found 1.22, and the NMAD has been found to be 0.475 μm . In the experiment, the monodisperse aerosol has been obtained for 13.28% minor flow which is similar to the literatures. The difference in between the no. of particles trapped in both simulation and experiment study in this research is only 1.63%. Therefore, we have concluded that the designed virtual impactor is actively suitable for mono-disperse aerosol generation of vast applicable fields based on both numerical and experimental study.

9. References

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NOMENCLATURE

GSD : Geometric Standard Deviation
 NMAD : Number Mean Aerodynamic Diameter

