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Thermal Design Optimization of a Miniature Condensate Particle Counter

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By
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ABSTRACT

Condensate Particle Counters (CPCs) are used to measure particle number densities to ascertain nano-scale (30nm – 100 nm) particulate exposure to adults and children. An air sample is introduced in a supersaturated vapor environment maintained in the condensation chamber of the CPC to facilitate vapor condensation on the particle surface. The size of the condensate-immersed particle grows as the particle moves through the condensation chamber and eventually becomes sufficient large to detect by optical methods. In this thesis, the particulate-humid air two-phase flow in a micro-scale condensate particulate counter has been computationally modeled. The numerical model is based on a finite volume method where the mass, momentum, energy and species conservation equations are solved simultaneously with appropriate interface and boundary conditions. A parametric study is performed by considering various combinations of wall temperature, ambient temperature, air sampling rate, and geometry of the CPC. The design intent was to create a large super-saturated region of vapor-air mixture inside the condensation chamber which would result in required rate of growth at different ambient conditions for a range of particle sizes. Effects of different flow parameters, ambient conditions, and CPC geometry are delineated in the paper. The study showed that a low flow rate or low wall temperature would result in less super-saturation than required, whereas, a very high flow rate condition would restrict the supersaturated region close to the walls. The performance of two working fluid alternatives is compared with water under identical condition based CPC. The advantage and disadvantage of each working fluid and its interoperability is evaluated and documented based on the simulation of particle growth rate.
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NOMENCLATURE

$C_c$ Cunningham non-continuum correction factor

$C_D$ Coefficient of Drag

$D$ Coefficient of Mass diffusion

$K$ Coefficient of Thermal Conductivity

$K_r$ Kelvin Ratio

$M$ Molecular weight

$N_a$ Avogadro Number

$Le$ Lewis Number

$R$ Universal gas constant

$Re$ Reynolds Number

$S_r$ Saturation Ratio

$T$ Temperature

$W$ Humidity ratio

$V$ Velocity

$d_{h_{2}O}$ Diameter of a single water molecule.

$d_p$ Droplet diameter

$k$ Boltzmann constant

$m$ Mass of a vapor molecule $= \frac{M}{N_a}$

$mf$ Mass fraction of a particular species

$p$ Pressure
Arbitrary radius in cylindrical coordinate system

Molecular flux

Arbitrary length in cylindrical coordinate system

Sticking probability

Coefficient of Thermal diffusion

Particle relaxation time

Surface tension of the liquid phase

Arbitrary angle in cylindrical coordinate system

Mean free path

Coefficient of Viscosity

Density

Shear stress

**Superscripts**

\( \cdot \) Time derivative

**Subscripts**

1 Pertaining to the primary sample fluid (air)

2 Pertaining to the Working Fluid

\( atm \) Pertaining to atmospheric condition

c Pertaining to the Critical condition

d Pertaining to droplet surface
e  Pertaining to equilibrium
l  Pertaining to liquid phase
mix  Pertaining to the mixture
p  Pertaining to the particle
r  Pertaining to radial component
s  Pertaining to saturation condition
v  Pertaining to vapor
z  Pertaining to axial component

rr  Evaluated at ‘rr’ plane
rz  Evaluated at ‘rz’ plane
zz  Evaluated at ‘zz’ plane
θθ  Evaluated at ‘θθ’ plane
∞  Pertaining to asymptotic region from droplet

\{T\}  Evaluated at Temperature-T
CHAPTER 1

1. INTRODUCTION

1.1. MOTIVATION

One of the major concerns for human life sustainability in this earth that we inherit is the adverse effect of human activities on this environment. The earth’s atmosphere is getting more and more polluted through industrialization which is caused by our extensive use of fossil fuels as our primary source of energy. The global communities are now increasingly showing interest in studying various adverse effects caused by such pollutants on the flora and fauna and there by regulating its causes for sustainability of the eco system.

A considerable amount of atmospheric pollution is contributed by the emissions from automotive vehicles which use fossil fuels as the energy source. These automotive emissions can be broadly classified as gaseous combustion byproducts and organic particulate matter. Various gaseous combustion products like the NOx and Carbon Monoxide have been known to cause hazardous environmental phenomena like acid rain. The particulate matter emissions are observed to be less dangerous to human beings if they are of a considerable size, in the order of a few microns. This is because human nasal canal is generally capable enough to filter out them from entering the respiratory system [Kreyling et al., (2006)]. Whereas, recent studies have shown that ultra fine particles of the order of few nanometers will not be effectively filtered through our natural filtration system, which can lead to increased risk of respiratory deceases.
[Kreyling et al., (2006)][Pope et al., (1995); Seaton et al., (1995)]. The particulates emitted from diesel combustion are found to be in the order of ~30nm which falls in this category [Amann & Siegla, (1981)]. Currently, understanding the potential impact of particulate matter on human health is limited by the lack of knowledge of individuals’ exposures to particle size and accumulation. NIH’s (National Institute of Health) National Institute of Environmental Health Sciences (NIEHS) have taken initiative to study the exposure risk and identifying high risk zones in the daily life of children in American cities. This project is a part of NIESHS’s large scale interdisciplinary project named “Development and Field Test of a Positional Tagging Miniature Personal Sensor for PM1.0,” which aims research to develop a miniature particulate counting device that can be easily worn and carried around by children without affecting their daily activities. This project is an attempt to solve the major deficiency in using the commercially available particulate sensors; which is portability.

1.2. Scope

The objective of this particular study is to computationally model the particulate-humid air two-phase flow and optimize the thermal design of a water based condensate particulate counter and to analyze its performance in comparison with other fluids generally employed for such application. Optical laser-based methods are reliable in such particle detection and counting for larger particles; generally in micron sizes. However, particles in tens of nanometer size range which are of the primary concern here are too small to be detected by optical means. So in order to detect these tiny particles by a laser-based system, we need a mechanism to increase the particle size. This is achieved in a Condensation Particle Counter (CPC), also known as the Condensation Nucleate Counter (CNC), by condensation on the particle surface.
CPC is a device that operates on the principle of growth by condensation. Here, when a particle of nanoscale moves through a chamber which is kept at super-saturation level for water vapor, water starts to condense on the particle and thereby increasing its size to a countable measure for a laser counter. Here we consider the tube to be made of porous walls which is heated so that water supplied to it would evaporate in to the chamber, creating a supersaturated environment through which air containing particles are sampled. A schematic representation of the arrangement is given as Figure 1. The device is divided in to two regions, namely the ‘Preconditioning Chamber’ and the ‘Condensation Chamber’. The walls of this device are porous and water is allowed to fill the pores. The precondition chamber wall is non-heated, allowing natural water evaporation to increase humidity of the air entering the main condensation chamber. Walls of the condensation chamber are kept at elevated temperature which accelerates the evaporation and water vapor flows in to the chamber. This process could eventually result in an increased saturation level in the condensation chamber which is desired for the condensation of water on the particle that flows through [Brin & Fisenko, (2007)].

Figure 1        Schematic Diagram
Next chapter gives a brief background and account of the literature survey conducted in regards to this topic. The third chapter details the numerical modeling principles and equations considered for the computer aided calculations. Fourth chapter details the results and discussion based on the study, which is then followed by a summery and conclusion as the fifth chapter.
CHAPTER 2

2. BACKGROUND AND LITERATURE REVIEW

2.1. HISTORY AND CLASSIFICATION OF CONDENSATION NUCLEATE PARTICLE COUNTERS (CNC)

The history of Condensation Particle Counters (CPC) or Condensation Nucleate Counters (CNC) can be traced back to the early 19th century where various scientists started studying the cloud formation and rain drop initiation. A brief history of the scientific advancement in this area has been well described by McCurry (2000). His paper describes the experimental instrumentations devised by Espy (1841) and later the publications of Coulier (1875), where he discovers that the particles in the atmosphere are the epicenter of condensation and hence could be called as the “condensation nuclei”. This laid the basis of particle detection mechanism using the condensation nuclei counters (CNCs). During about the same time an experimental apparatus was devised by Aitken (1881) which was called the “Dust counters” which was later improved to “Pocket- Dust Counter”. There after a lot of scientists worked on the Aitken model dust counters which include Wilson (1897), Scholz (1931), Kassner et al (1968) and Jaenicke & Kanter (1976). According to McCurry, “Condensation is the only technique available for detecting neutral gas-borne particles that are too small for optical methods” [McMurry, (2000)].

Almost all of this development was done based on the condensation of vapor on particles through near adiabatic expansion of particle laden air containing vapor in a convergent divergent section. Another approach for the same instrument was to employ continuous flow chambers.
There are three basic types of such devices used based on the principle employed for obtaining supersaturation in the chamber.

They are

a) Laminar Flow Forced Convection Heat Transfer CNCs

b) Mixing Type CNCs

c) Segmented Thermal Diffusion Chamber

2.1.1. Laminar Flow Forced Convection Heat Transfer CNCs

These instruments utilize the forces convection heat transfer phenomena to create a supersaturated environment in the “cloud chamber” or the “growth tube”. Rosen et al., (1974) developed a steady flow thermal gradient diffusion cloud chamber (TGDCC) which used an annular space where the core is temperature controlled to a higher level while cooling the outer surface with an ice bath. The particle laden sample was then allowed to flow through this chamber. The temperature gradient from the core to the outer surface induces a supersaturation levels to the working fluid, which in this case was water. The particle flowing in this condition grows in size which was then measured using optical counting mechanisms. A schematic of this setup is given in Figure 2.

The more modern type of CNCs using this principle was fueled by the research conducted by Bricard et al (1976). The schematic given in the Figure 3 shows their instrument,
which utilizes alcohol as the working fluid and a Peltier cooler to create supersaturation, where the particle grows in size and which is ultimately counted through the optical counting setup.

They were perhaps the first to study the diffusivity of various fluids; the importance of diffusivity and vapor pressure characteristics of the working fluid in creating an elevated level of supersaturation which in turn would result in faster particle growth and hence improve detection. Other scientists like Sinclair (1974), Agarwal & Sem (1980), Wilson et al (1983), Stolzenburg & McMurry (1991), McDermott et al (1991), Saros et al (1996), Weber et al (1995), Keady (1988), Hameri et al (2002), Sem (2002) have done noteworthy research in this type of CNC and have significantly improved the performance of the counter.
Figure 2  Thermal Gradient Diffusion Cloud Chamber
[Rosen et al., (1974)]

Figure 3  Continuous Flux Condensation Nuclei Counter
[Bricard et al., (1976)]
2.1.2. Mixing Type CNCs

In this type of CNCs the Supersaturation in the condensation chamber is achieved by mixing cold and hot sample. Holl & Mühleisen (1955), Fuchs & Sutugin (1965), Cadle & Langer (1975), Kousaka et al (1982), Okuyama et al (1984) etc made some significant contributions to improve mixing type CNCs. The advantage of these types of CNCs is that the selection of working fluids becomes easier since the vapor diffusivity of the fluid plays a much lesser role because the super saturation is achieved through mixing and not through thermal diffusion through the working fluid vapor. A schematic of one mixing type CNC is given in Figure 5 which was developed by Kousaka et al (1982).

2.1.3. Segmented Thermal Diffusion Chamber

This particular variant of CNC was first developed by Hoppel et al (1979) which are shown as a schematic in Figure 4. It has got a cylindrical column with hot and cold segments that are saturated with water vapor. The aerosol transport through each segment is very short as compared to the time required for thermal/phase equilibrium but when the aerosol passes through a number such alternating sections, because of the exponential relation of vapor pressure with temperature, eventually the aerosol gains high degree of super saturation at the exit.
Figure 5  Schematic of Mixing Type CNC  
[ Kousaka et al., (1982) ]

Figure 4  Steady flow segmented thermal diffusion chamber  
[ Hoppel et al., (1979) ]
2.2. LITERATURE REVIEW

The laminar flow, water based condensate particulate counter in particular is considered for our study based on the intended application. Based on the study conducted by Agarwal and Sem (1980), it is clear that since water has a generally higher mass diffusivity as compared to alcohols, water would easily diffuse in to the sampled air as compared to them. This in turn would result in a failure for the instrument to generate a high supersaturated condensation chamber as compared to the alcohols. Kousaka (1982) was able to successfully employ water as medium but by utilizing a mixing flow model, which is much more complicated in design as compared to a continuous flow CPC.

Hering & Stolzenburg (2005) introduced a new CPC with water as a medium. Here the Water is allowed to pre-saturate in a pre-conditioning chamber and then enter the condensation chamber with walls kept at elevated temperatures and water being allowed to evaporate in to the flowing sample. This results in a higher supersaturation near the axis of the growth tube because, since the mass diffusivity of water vapor in air exceeds the thermal diffusivity of air; the flux of water vapor to the centerline is faster than the heat flux from the walls. This would results in maximum growth rate for the particle near the center line since it experiences the maximum saturation ratio, which has a direct correlation with the particulate growth. In this study they are able to predict the saturation distribution inside the growth tube using a computational model, but they do not take the prediction to the next level and predict the growth of particulate in such a saturation distribution. Further study is done on an experimental device and data presented. The computational saturation prediction also assumes a constant diffusivity for water in air. The
diffusivity model of water in air is a function of temperature and, in CPC we are dealing with considerable temperature gradients between the wall and the axis hence inclusion of this effect would further improve the model that Hering *et al* (2005) presented.

Kulmala *et al* (2007) have published a categorical analysis of the CPC efficiency improvement based on the temperature difference between the pre-conditioning wall and the condenser wall. The paper gives a comparison of the saturation plot and temperature plots inside the growth tube for various conditions and validated them through experiments. We have used these plots to verify our results. They have also given an accounted comparison of n-Butanol as a working fluid.

Stolzenburg & McMurry (1991) have presented their work on the Ultrafine CPC for counting particles less than 20nm. In this paper they present a comprehensive study on various design factors to be considered while designing a continuous flow CPC which is taken as a reference for our study. They include the inlet flow rate, condenser/saturator wall temperature, geometry in L/D ration and working fluids. But they have used and alcohol medium which could achieve supersaturation levels through, cold saturation and a relatively hot preconditioning chamber, where as in water based CPC, as in our case, the saturation wall are to be heated and the preconditioning walls should be kept at a relatively lower temperature.

Yang *et al* (2000) conducted a computational study of saturation and growth of particles in the growth tube for a convergent divergent nozzle arrangement. Since their equipment involves convergent divergent section where the sample expands, there would be a large difference in the
particle flow velocity to that of air. In a single growth tube with straight flow, the particle velocity would be effectively same as that of the sample flow especially since it tends to achieve a fully developed velocity profile while passing thorough the preconditioning chamber. An experimental study conducted by Gellar et al (2006) is an indicator for some preliminary indications that the increased flow rate and higher saturator temperature would give a significant improvement in the detection efficiencies. The optimum value for this application has to be determined here.

Regarding alternate liquids being used for CPC application, Iida et al (2008) published a comparative study of one Water Based CPC and Butanol based CPC. They conclude in the study that the counting efficiencies of Butanol based CPC is higher than that of water based one. The WCPC was using 10 times the flow rate sampling as compared to the BCPC to match the counting efficiency.

There are a number of publications available on the particle detection efficiencies based on the number concentration of the seed particles like the work done by Tsang & Brock (1983), Fitzgerald et al (1998), Kulmala (2004), Mordas et al (2008), Hämeri et al (2002). The single particle growth rate model done in this exercise can be further enhanced by considering these cases for a comparative study.
2.3. PROBLEM STATEMENT

For an optimized design for the equipment, some important design parameters to be considered are the length of the chamber that would make these particles to grow to the desired size, and the saturation ratio that has to be maintained for it. The variation of the supersaturation ratio in the condensate chamber is governed by the mass flow rate, wall temperature and humidity. For nano-scale particles, the partial pressure of vapor required for condensation is greater than the saturation pressure at the surface temperature. This is due to the curvature of the particle surface and it is known as the Kelvin effect [Hinds, (1999)]. If the length of the CPC is more than the desired value, it would expose the particle to a region of low vapor concentration and the water blanket formed through condensation can start evaporating and shrink the particle.

Since we are considering nano size particles which eventually grow to micron size, as per Seinfeld and Pandis (2006) the particle growth process has to be dealt as three separate regimes; which are kinetic, transition and continuum regimes respectively. As explained by Fuks (1959), when the condensation particle size is less the mean free path (\( \lambda \)), which for the air-water vapor will be in the vicinity of 0.120 \( \mu m \), Maxwellian (2003; 1890) solution of growth with continuum assumption completely fails. A free molecular regime obeying kinetic theory of gases is more applicable in this region. The region where the particle size is \( \lambda < d_p < \sim 10 \lambda \) could be considered as a transition zone, and there by leaving the higher sizes in the continuum zone.
Even though there are well defined theoretical explanations available for the particle growth in free molecular regime, as explained through kinetic theory of gases by Hirschfelder (1954), and in the continuum regime, as explored by Maxwell (1890); Clement (1985) or Wagner (1982), a solution for the transition regime is not available. In this study we have followed the two zone theory given by Hinds (1999) for our predictions with the Fuks’s correction factor to correct for the transition zone. The ambiguity in selecting the sticking probability ($\alpha$) which gives the fraction of incident vapor molecules that gets condensed are discussed elaborately by Barrett and Clement (1988) and the more probable value of $\alpha = 0.04$ was selected based on the observations by Hsu and Graham (1976) for the specific case of water vapor-air aerosols. The gravitational effect on the growing particle and the general sticking probability of the particle to the wall of the condensation chamber are not considered as a part of this study. A general modeling of above mentioned condition was carried out by Lin & Tarbell (1980) which was not considered in the scope of this study.

The same setup was then simulated for alcohols namely, n-Butanol and Isopropanol; which are the commercially available alternative for the fluid medium in equipments employing the same growth tube principle. The general advantage of using these liquids where analyzed based on the physical properties and then a prediction of particle growth was conducted to compare the results with the water based CPC.
The thermo physical properties of the liquids considered were obtained from the Yaws Handbook (1999) and Perry’s Handbook (1997). The factor that would play a major role in determining the growth rate of molecules in the kinetic regime is the sticking probability assumption for the case of the alcohols considered. A study from Rudolf et al (1998) and by Clement (1995) especially shows that the sticking probability of the alcohols is generally comparable to that of water at atmospheric conditions.
CHAPTER 3

3. NUMERICAL SOLUTION

The design problem was addressed in two separate theoretical parts. The first one concerning the optimized design configuration for achieving the right amount of supersaturated region within the condensation chamber and the second being the optimum value of the super saturation required to induce a study growth in particle size. The first part of the solution was considered as an elimination criterion for deciding the parameters to be considered for the growth rate confirmation.

For the initial part of the problem, the device was computationally modeled and by utilizing FLUENT® flow solver on various combinations of wall temperatures, air sampling rate, diameter and length, are evaluated and compared to arrive at the best combination. The design intent in this section was to create maximum region of super-saturation of water vapor inside the condensation chamber. The post processing of the results were done using Tecplot 360® module.

In the second section, the best two alternative designs selected through the first analysis were further investigated by modeling the particle growth in their respective solution. For this study, a stream of particle at four locations on the axis, and 25%, 50% and 75% of the radius from the axis with an incident inlet velocity was assumed to undergo growth by condensation from their initial size of 30nm. This mathematical analysis for particle tracking and particle growth was done by using the data of vapor concentration and velocities obtained from the previous simulation. The particle tracking formulation was coded in MATLAB ®.
The third section deals with the investigation of alternate working fluids. As discussed in the introduction, n-Butanol and Isopropanol were selected as the alternate working fluids to be tested. First the behavior of these liquids based on the working temperature, which in this case is the wall temperature is compared and its benefits are predicted. Lewis number (Thermal diffusivity to Mass diffusivity ratio) is plotted for various working temperatures. Based on this, the same equipment geometry finalized through the observations in the first two sections are used to study and compare the saturation distribution. Finally, Particle growth rate study was conducted using the same liquids both in axial locations and in terms of the exit particle diameters.

3.1. PART 1 - FLOW FIELD OPTIMIZATION

A schematic model of the device was created using GAMBIT© preprocessing module of Fluent 6.3©. Since the problem is axisymmetric, it was represented as a simplified 2D axisymmetric geometry with the preconditioning chamber, and the condensation chamber. The system is assumed to be in steady state and in incompressible laminar flow based on the flow parameters considered. All other physical properties like the density and coefficient of viscosity are also assumed to be following the mixing law based on the weighted mass fraction of the two species. Different combinations of the primary design variables were then analyzed individually to arrive at the optimum configuration. The system is then solved using Fluent 6.3© flow solver for mass, momentum, energy and species conservation; the expression for which are given below [Burmeister, (1983)].
Continuity:-
\[ \frac{1}{r} \frac{\partial (rV_r)}{\partial r} + \frac{\partial V_z}{\partial z} = 0 \]  
(1)

Radial Momentum:-
\[ \rho \left( V_r \frac{\partial V_r}{\partial r} + V_z \frac{\partial V_r}{\partial z} \right) = -\frac{\partial p}{\partial r} + \left( \frac{1}{r} \frac{\partial (r\tau_{rr})}{\partial r} + \frac{\partial (\tau_{rz})}{\partial z} - \tau_{\theta\theta} \right) \]  
(2)

Axial Momentum:-
\[ \rho \left( V_r \frac{\partial V_z}{\partial r} + V_z \frac{\partial V_z}{\partial z} \right) = -\frac{\partial p}{\partial z} + \left( \frac{1}{r} \frac{\partial (r\tau_{rz})}{\partial r} + \frac{\partial (\tau_{zz})}{\partial z} \right) \]  
(3)

Energy Eq
\[ \rho c_p \left( V_r \frac{\partial T}{\partial r} + V_z \frac{\partial T}{\partial z} \right) = k \left( \frac{1}{r} \frac{\partial \left( r \frac{\partial T}{\partial r} \right)}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right) \]  
(4)

Mass Diffusion Eq
\[ V_r \frac{\partial m_{f2}}{\partial r} + V_z \frac{\partial m_{f2}}{\partial z} = D \left( \frac{1}{r} \frac{\partial \left( r \frac{\partial m_{f2}}{\partial r} \right)}{\partial r} + \frac{\partial^2 m_{f2}}{\partial z^2} \right) \]  
(5)
For the inlet flow, sampling air was assumed to have 25% saturation and a temperature of 25°C. The pre-conditioning zone, which occupies the first 20 mm of the growth tube is considered to be an unheated porous wall with are slightly irrigated to obtain about 60% of saturation level for that temperature. Other boundary conditions applied for the problem is understandable from the schematic representation given in Figure 6.

\[ Wall , T_{atm} = 25^\circ C, \]
\[ mf_z = 60\% Sat @ T_{atm} \]

\[ Wall , T_{wall} , \]
\[ mf_z = 100\% Sat @ T_{wall} \]

\[ VelocityInlet = Vi \]
\[ T_{atm} = 25^\circ C, \]
\[ mf_z = 25\% Sat @ T_{atm} \]

Figure 6    Boundary Conditions

A pressure based implicit solver with multispecies transport simulation without any chemical reaction was selected for the CFD analysis. A SIMPLE based pressure-velocity coupling and second order upwind schemes were chosen as the solutions control parameters with standard under relaxation parameters considered in Fluent.

In the case of water vapor mixture, Fluent 6.3\textsuperscript{©} calculates the relative humidity of the medium as the ratio of the partial pressure of the water vapor content in the air-water mixture to the
saturation pressure of water vapor (Equation (11) at the mixture temperature calculated as per Equation (6) [Guide, (2007)])

\[
\ln \left( \frac{p_s}{p_c} \right) = \left( \frac{T_c}{T} - 1 \right) \sum_{i=1}^{8} F_i [a(T - T_p)]^{i-1}
\]

(6)

Where

\[
P_c = 22.089 \text{ MPa}
\]

(7)

\[
T_c = 647.286 \text{ K}
\]

(8)

\[
F_1 = -7.4192420, \quad F_2 = 0.29721, \quad F_3 = -0.1155286, \quad F_4 = 8.685635 \times 10^{-3}
\]

\[
F_5 = 1.0941 \times 10^{-3}, \quad F_6 = -4.34 \times 10^{-3}, \quad F_7 = 2.5206 \times 10^{-3}, \quad F_8 = -5.2185 \times 10^{-4}
\]

\[
a = 0.01
\]

(9)

\[
T_p = 338.15 \text{ K}
\]

(10)

\[
Relative \text{ Humidity} = \frac{p_v}{p_s}
\]

(11)

3.2. PART 2 – PARTICLE TRACKING AND GROWTH CALCULATION

In this section, a computational code was prepared for the particle growth rate prediction based on each regimes discussed in the introduction. Two of the most desirable alternatives were selected from the CFD analysis and the saturation ratio distribution on each grid point was used for simulating the particle growth.

The program is prepared for calculating the particle size at each time step based on the location of the particle computed using the axial component of the velocity solution. The corresponding saturation ratios, temperature etc were interpolated from the fluent solution matrix.
3.2.1. Particle Drift Velocity:

The particle in the sample flow experience drag force due to the flow of air media in which it floats. A general expression of drag force on a spherical particle at a constant fluid velocity is given by Equation (12) [Yang et al., (2000)].

\[
F_D = m_p \frac{dV_p}{dx} = \frac{\pi d_p^2}{4} C_D \frac{1}{C_c} \frac{1}{2} \rho_g (V_g - V_p)^2
\]  

(12)

Here \( m_p \) is the mass of the particle and \( C_D \) is the drag coefficient on the particle. Since here the Reynolds No on the particle is of the order \( Re_p < 0.1 \), the flow is in the Stoke’s flow regime and an expression for \( C_D \) is given by the Equation (13). Where, \( C_c \) is the Cunningham non-continuum correction given by Equation (14) where \( \lambda_g \) is the mean flow path for the sample gas (air) at that temperature and pressure.

\[
C_D = \frac{24}{Re_p}
\]  

(13)

\[
C_c = 1 + \frac{2 \lambda_g}{d_p} \left[ 1.257 + 0.4 e^{(-0.55 d_p/\lambda_g)} \right]
\]  

(14)

Here \( Re_p \) is the Reynolds No calculated for the particle given by the expression given in the Equation (15).

\[
Re_p = \left| V_g - V_p \right| \frac{\rho_g d_p}{\mu_g}
\]  

(15)
For Stokes’s flow the equation can be reduced in terms of the residence time evaluated at each \( x \) location is given by the Equation (16) [Yang et al., (2000)].

\[
\zeta \frac{dV_p}{dx} = V_g - V_p
\]

(16)

Where \( \zeta \) gives a measure of the residence time as given below

\[
\zeta = \frac{d^2 \rho}{18 \mu g} \frac{24 C_c}{C_d Re_p}
\]

(17)

Now based on this drag force, the distance covered by a particle at \( V_p = 0 \) initially to reach a velocity to near the velocity of the sampling air is calculated. This calculation is done for the maximum velocity at the axis of the finalized case (case 4) with an inlet flow rate of 0.3 lpm, this corresponds to the value- \( V_g = 3.183 \text{m/s} \). The calculation is also done for an average particle size of 1 \( \mu \text{m} \). The particle which is of the range of \( \sim 30 \text{nm} \) initially, when grows to the size of 1 \( \mu \text{m} \) would be dominated by the condensed water around it and hence the mass of the particle is calculated based on the properties of water. All properties are calculated for the maximum temperature attainable in this case, which corresponds to the wall condition with 65 °C and atmospheric pressure.

The relative velocity Vs time graph of the stagnant particle is given in Figure 7. It shows clearly that a stagnant particle of a considerable size of 1 \( \mu \text{m} \) itself would accelerate to the inlet flow velocity in 25 \( \mu \text{s} \) where the relative velocity seems to reduce to zero.
In this 25 μs, with this velocity of 3.183 m/s, the particle would have travelled ~80 μm through the channel. Since the device has a 20 mm preconditioning chamber, it is hence certain that all the particles that is coming with the flow would certainly be flowing with essentially the same velocity as that of the incident inlet velocity.

Based on the above observation we assume all the particles in the flow system to have the same inlet velocity as that of the sampling air. All proceeding particle growth rate calculation is done based on this assumption.
3.2.2. Free Molecular Regime:

Kinetic theory of gases approach can be applied to the system when the particle size is very small where the continuum approximation becomes invalid. Here, the condensation can be construed as an effect of random molecular collisions between individual vapor molecules. At this condition, an expression for the particle growth rate can be obtained by balancing the net rate of vapor molecule leaving from the droplet surface [Hirschfelder, (1954)] and the molecular influx of the vapor molecule [Barrett & Clement, (1988)].

A simplified expression for the growth rate for this regime is taken from Hinds (1999) which is given below.

\[
\frac{dp}{dt} = \frac{2Ma(p_d - p_{\infty})}{\rho_iNa\sqrt{2\pi mkT_{\infty}}}
\]  
(18)

Here both \(p_d\) and \(p_{\infty}\) are calculated based on the relation

\[
p_{\infty} = p_s\{T_{\infty}\}.Sr
\]  
(19)

\[
p_d = p_s\{T_d\}.Kr
\]  
(20)

The saturation pressure at for water any temperature \(T\) is evaluated based on the empirical relation given as Equation (21).

\[
p_s\{T\} = \exp\left(16.7 - \left[\frac{4060}{T - 37}\right]\right)
\]  
(21)
And the Kelvin ratio for each diameter $d_p$ is calculated as Equation (22)

$$Kr = \exp \left( \frac{4\gamma M}{\rho_t RT_d d_p} \right)$$  \hspace{1cm} (22)

The temperature at the surface of the droplet is evaluated using the empirical relation given as Equation (23) [Hinds, (1999)].

$$T_d - T_\infty = \frac{(6.65 + 0.345T_\infty + 0.0031T_\infty^2)(Sr - 1)}{1 + (0.082 + 0.00782T_\infty)Sr}$$  \hspace{1cm} (23)

3.2.3. Continuum Regime:

In this regime, the growth of the particle can be attributed at large to the diffusion of vapor molecule on to the particulate surface. Assuming a perfectly spherical particle, the growth rate through condensation can be evaluated by Equation (24) [Hinds, (1999)].

$$d_p = \frac{4D M}{R \rho_t d_p} \left( \frac{p_d}{p_\infty} - \frac{p_\infty}{T_d} \right) \phi$$  \hspace{1cm} (24)

Here, $\phi$ is the Fuks’s correction factor which is used to smooth the transition from the molecular regime to the continuum regime [Fuks, (1959)].

$$\phi = \frac{2\lambda + d_p}{d_p + \left( \frac{5.33\lambda^2}{d_p} \right) + 3.42\lambda}$$  \hspace{1cm} (25)
The mean free path $\lambda$ for water vapor at atmospheric pressure condition is calculated using the empirical formula given as

$$
\lambda = \frac{RT_\infty}{\sqrt{2\pi N_a d_{H_2O} p_{atm}}} \quad (26)
$$

The diffusion coefficient for water vapor at a particular temperature $\{T\}$ is calculated using the Chapman-Enskog correlation [Cussler, (1997)].

### 3.3. PART 3- ALTERNATE WORKING FLUIDS

Here, various alternative working fluids were analyzed for the intended application. The two fluids selected for this application are n-Butnol and Isopropanol. The advantage of these fluids over water is its slower mass diffusivity as compared to the thermal diffusivity. This can be analyzed using the non-dimensionalized parameter called the Lewis Number, which is the ratio of coefficient of thermal diffusion ($\alpha_T$) to the coefficient of mass diffusion ($D$). The properties for each liquid are calculated from properties defined as a polynomial function with respect to temperature as given in Perry’s data book (1997) and Yaw’s data book (1999). Based on this the Lewis number of the mixture is calculated based on the wall temperature and the mass fraction of each fluid required for obtaining a 100% saturation condition. The Table 1 gives the formulae used for the material properties for these liquids in pure form. The mixture properties are calculated based on the equations given in Equations (27) to (31) [Guide, (2007)].
These empirical equations for the properties are also used in Fluent® in order to calculate the saturation profiles in the flow field. The coefficient of mass diffusion for these cases are calculated by Fluent® using kinetic theory model which uses a modified Chapman-Enskog formulation [Guide, (2007)]. These saturation profiles are then compared with that of water in order to arrive at the comparative edge these fluids have when used instead of water. Later, like in the case of water, the saturation distribution for a sample problem is imported to MATLAB® and the particle tracking algorithm is run with the properties of the corresponding fluid to get the particle growth prediction at various radius locations. An exit profile of particle diameters across the cross section is also obtained and compared with that of Water.

The most important parameters that have to be evaluated in this case are the saturation ratio. Unlike the case of water vapor, the saturation ration in the case of these liquids is not calculated internally by Fluent®. It is calculated using the custom field functions option in Fluent® to load
the equation used for the saturation ratio of each fluid based on its partial pressure obtained through the mass diffusion solution and the vapor pressure calculation obtained from the empirical equation given in the data book as the expression in the Table 1. The Saturation ratio in these cases is calculated based on the equations given as Equations (32)-(34) [ASHRAE, (1997)].

\[
W = \frac{mf_2}{mf_1} \quad (32)
\]

\[
W_s = \frac{M_2}{M_1} \frac{p_v}{(p_{atm} - p_v)} \quad (33)
\]

\[
Sr = \frac{W}{W_s} \quad (34)
\]

The saturation ration hence calculated throughout the domain is then exported to MATLAB® for implementing the particle tracking algorithm. In the algorithm for particle growth calculation the saturation pressure \(p_s\) calculation given in Equation (21) is replaced with the polynomial function for the vapor pressure correlation as given by the data book which is quoted in Table 1.
### Table 1
PROPERTIES OF ALTERNATE LIQUIDS DEFINED WITH RELATION TO THE TEMPERATURE

<table>
<thead>
<tr>
<th>Working Liquid</th>
<th>Parameter</th>
<th>Molecular Mass ( {M} ) (kg/mol)</th>
<th>Heat Capacity ( {C_p} ) (J/kgK)</th>
<th>Thermal Conductivity ( {\alpha_T} ) (W/mK)</th>
<th>Gas Viscosity ( {\mu} ) (Pa.s)</th>
<th>Vapor Pressure ( {P_v} ) (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>n-Butanol</strong></td>
<td>Equation</td>
<td>Constant</td>
<td>( \frac{A + BT + CT^2 + DT^3 + ET^4}{M} )</td>
<td>( A + BT + CT^2 )</td>
<td>( A + BT + CT^2 )</td>
<td>( 133.32 \times 10^{A+\frac{B}{T}+C \log_{10}T+DT+ET^2} )</td>
</tr>
<tr>
<td>( A )</td>
<td></td>
<td>8.157</td>
<td>1.7830 ( \times 10^{-2} )</td>
<td>(-10.867 \times 10^{-7})</td>
<td>39.6673</td>
<td></td>
</tr>
<tr>
<td>( B )</td>
<td>74.123 \times 10^{-3}</td>
<td>4.1032 ( \times 10^{-1} )</td>
<td>(-4.1032 \times 10^{-5})</td>
<td>0.2828 ( \times 10^{-7})</td>
<td>(-4.0017 \times 10^{3})</td>
<td></td>
</tr>
<tr>
<td>( C )</td>
<td></td>
<td>(-2.2645 \times 10^{-4})</td>
<td>1.6334 ( \times 10^{-7})</td>
<td>(-4.716 \times 10^{-12})</td>
<td>(-1.0295 \times 10^{1})</td>
<td></td>
</tr>
<tr>
<td>( D )</td>
<td></td>
<td>6.0372 ( \times 10^{-8})</td>
<td>(-)</td>
<td>(-)</td>
<td>(-3.2572 \times 10^{-10})</td>
<td></td>
</tr>
<tr>
<td>( E )</td>
<td></td>
<td>(-6.280 \times 10^{-12})</td>
<td>(-)</td>
<td>(-)</td>
<td>8.6672 ( \times 10^{-7})</td>
<td></td>
</tr>
<tr>
<td><strong>Isopropanol</strong></td>
<td>Equation</td>
<td>Constant</td>
<td>( \frac{A + BT + CT^2 + DT^3 + ET^4}{M} )</td>
<td>( A + BT + CT^2 )</td>
<td>( A + BT + CT^2 )</td>
<td>( 133.32 \times 10^{A+\frac{B}{T}+C \log_{10}T+DT+ET^2} )</td>
</tr>
<tr>
<td>( A )</td>
<td></td>
<td>25.535</td>
<td>0.07775</td>
<td>(-10.859 \times 10^{-7})</td>
<td>38.236</td>
<td></td>
</tr>
<tr>
<td>( B )</td>
<td>60.096 \times 10^{-3}</td>
<td>2.2103 ( \times 10^{-1} )</td>
<td>(-3.6017 \times 10^{-4})</td>
<td>3.0873 ( \times 10^{-8})</td>
<td>(-3.551 \times 10^{3})</td>
<td></td>
</tr>
<tr>
<td>( C )</td>
<td></td>
<td>5.3492 ( \times 10^{-5})</td>
<td>5.7593 ( \times 10^{-7})</td>
<td>(-4.8098 \times 10^{-12})</td>
<td>(-1.0031 \times 10^{1})</td>
<td></td>
</tr>
<tr>
<td>( D )</td>
<td></td>
<td>(-1.4727 \times 10^{-7})</td>
<td>(-)</td>
<td>(-)</td>
<td>(-3.474 \times 10^{-10})</td>
<td></td>
</tr>
<tr>
<td>( E )</td>
<td></td>
<td>4.9406 ( \times 10^{-11})</td>
<td>(-)</td>
<td>(-)</td>
<td>1.7367 ( \times 10^{-6})</td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER 4

4. RESULTS AND DISCUSSION

4.1. GRID DEPENDENCY EVALUATION

A sample case was considered here to check the grid dependency of the numeric solution provided by Fluent® CFD solver. This is done for a sample case where the wall temperature was kept at 65°C and the flow rate is kept at 0.1 lpm. Four incremental grids where used to solve the case with the same boundary conditions and solver parameters. The comparative plots of the resulting temperature contours are given in Figure 8 and the saturation ratio solution is given in Figure 9. The four grids considered here are 10(r) × 175(L), 25(r) × 350(L), 50(r) × 700(L), 100(r) × 1400(L).

The results clearly show comparable results as given by Hering et al (2005) for the distribution of temperature and saturation along the axis of the growth tube which starts from ‘0’ location in the X-axis. They also show that the results are not grid dependant because all four curves lie over each other showing minimal change in the solution of these critical parameters for this study. In the second part of the study, where we analytically predict the size of the particle along the flow direction, it is required to locate the particle at each definite time step and interpolate the values of temperature and saturation ratio around the particle at that moment, which forms the basis for the growth rate calculation for that moment. Hence, though a courser grid seem to numerically acceptable solution, a significantly fine grid of 50(r) × 700(L) is selected for further analysis in order to get adequate data for the interpolation and growth rate & diameter calculated thereafter.
Figure 8  Comparison of Temperature Plots along the axis for different grid sizes.

Figure 9  Comparison of Saturation Ratio Plots along the axis for different grid sizes.
4.2. **PART 1 - FLOW FIELD OPTIMIZATION**

For the study, a number of variables were selected which would give influence in a variety of conditions were selected. Given below is a table illustrating different variables considered for the study.

<table>
<thead>
<tr>
<th>Cases Considered</th>
<th>$L/D$ Ratio</th>
<th>Inlet Flow Rate ($lpm$)</th>
<th>Condensation Wall Temperature ($^\circ{C}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>25</td>
<td>0.1</td>
<td>45</td>
</tr>
<tr>
<td>2</td>
<td>25</td>
<td>0.1</td>
<td>55</td>
</tr>
<tr>
<td>3</td>
<td>25</td>
<td>0.1</td>
<td>65</td>
</tr>
<tr>
<td>4</td>
<td>25</td>
<td>0.3</td>
<td>65</td>
</tr>
<tr>
<td>5</td>
<td>25</td>
<td>0.5</td>
<td>65</td>
</tr>
<tr>
<td>6</td>
<td>25</td>
<td>0.7</td>
<td>65</td>
</tr>
<tr>
<td>7</td>
<td>15</td>
<td>0.3</td>
<td>65</td>
</tr>
</tbody>
</table>

The results obtained from the CFD analysis of various important combinations of design variables are presented in Figure 10 thru Figure 22. Plots of temperature distribution, isotherms, saturation ratio distribution and saturation ratio contours are presented in an absolute scale where the temperature is colored from $298K$ to $338K$ and saturation ration from 0 to 2. The region with X co-ordinates from $-0.02m$ to 0 is the preconditioning chamber where the walls are kept
wet but unheated to maintain a constant saturation of 60% RH as the entry condition for the condensation chamber.

4.2.1. Condenser Wall Temperature

Figure 10 shows the results for the first case considered for $L/D = 25$ model with inlet flow rate of 1 $lpm$ and the condensation chamber wall kept at $45^\circ C$. The results clearly indicate that a generally uniform temperature and saturation region is obtained with in the first $\sim 25 mm$ of the condensation chamber itself. There after a $Sr$ of nearly 1 is maintained as shown by the last saturation contour colored in green. The super saturation region with $Sr > 1.25$, which is generally desirable for a steady and fast growth of the particle through condensation is the region with yellow and redder color tones which is practically absent in this case.
Figure 10  Case 1  (45°C, 0.1 lpm, L/D = 25) - Plots
Figure 11 shows the results for Case 2 considered with the same $L/D$ model and inlet flow rate of 1 lpm, but by elevating the wall temperature to 55°C. Here, the temperature profile gets developed in the ~20mm of the condensation chamber just as in the case 1. This is because the inlet velocity and geometry was unaltered giving the same entrance length for the temperature. The elevated temperature condition in the condensation chamber improves the diffusion of vapor molecules from the walls and increases the humidity ratio there by results in a region with higher saturation ratios. But even in this case, the region that is marked with yellow or redder tones is negligibly small. A particle flowing through this region will get very less time to grow in this region; which on reaching the large area with $Sr\sim1$ will start to diminish in size through back evaporation of the condensate. For the device to work effectively, even higher wall temperature would be desirable considering the improvement achieved from Case 1 to Case 2.

Further increasing the wall temperature to 65°C, achieving the pragmatic limit the device considering the portability and energy consumption, Case 3 was considered and the solution is presented in the Figure 12. Continuing the trend observed in the previous case, it produced a better distribution of saturation ratio. The $Sr$ contours show a significant improvement in the region of super saturation and thus arriving at the best possible configuration for the wall temperature variable out of three cases considered so far.
Figure 11  Case 2  (55°C, 0.1 lpm, L/D = 25) - Plots
Figure 12  
Case 3  
(65°C, 0.1 lpm, L/D = 25) - Plots
Figure 13 shows the comparative super saturation zones in the three cases considered so far. The super saturation cutoff value was set as $Sr = 1.1$ based on a preliminary calculation which suggested that in all the sizes of particles considered ranging from 30 nm to a few Microns, the Kelvin ratio will always be below 1.05 indicating that the particle will always grow through condensation. Now, it is again clear from this comparison that as the wall temperature is increased, the super saturation zone is enlarged and the degree or super saturation is also elevated.

On a closer look in to the axis region alone would give a temperature and saturation plot as given in the Figure 14 and Figure 15. These results are comparable to the plots given by Kulmala et al (2007). This analysis also helps us to finalize the conclusion that Case 3 with the wall temperature of 65°C would give the best possible saturation distribution and the maximum level of super saturation among the cases considered so far.

All Subsequent analysis was done with the condensation wall temperature fixing at a value of 65°C. Next set of evaluation was carried out to check the effect of sample inlet velocity or the sample flow rate. It is evident that the increased inlet velocity would delay the development of temperature profile. This further would be handy in generating a larger region with higher saturation ratio.
Figure 13  Comparison of Super Saturated Zone (Sr>1.1) Case 1, Case 2, & Case 3
Figure 14  Comparison of Temperature along the axis for Case 1, 2 & 3

Temperature Plot Along the Axis for Cases 1, 2 & 3
(0.1 pm, L/D-25)
Figure 15  Comparison of Saturation Ratio along the axis for Case 1, 2 & 3
4.2.2. Sample Inlet Flow Rate

Case 4 (Figure 16) is with inlet volume flow rate of 0.3 lpm. The temperature distribution clearly shows an elongated temperature profile and isotherms. It is also noted that the sample temperature reaches the wall temperature only at the end of the device. The saturation contours show a much improved region of super saturation thus almost maintaining a supersaturated zone required to induce a continuous growth for the particle.

A further increment in inlet flow rate as in the case of case 5 and 6 shown in Figure 17 & Figure 18 which are cases evaluate with inlet flow rate of 0.5 lpm and 0.7 lpm respectively. It can be clearly noted that an increase in the inlet flow rate of the sample greatly affects the temperature distribution inside the growth tube making it cooler in the inner core as compared to the region close to the wall. It is also interesting to note that in case 5 and case 6, the temperature near the central axis doesn’t reach the wall temperature at all and hence could be construed as thermally underdeveloped.

The underdeveloped temperature profiles make the central core cooler and hence its capacity to hold water vapor is lesser as compared to the previous cases. This results in higher super saturation conditions near the center line. It is clearly visible from these figures that the saturation profile is more extended in the case of a higher flow rate as compared to a relatively slower sample flow. This means that for a higher flow rate, a larger area or volume of the growth tube would be in supersaturated condition than compared to slower ones.
Figure 16. Case 4 (65°C, 0.3 lpm, L/D = 25) - Plots
Figure 17  Case 5  (65°C, 0.5 lpm, L / D = 25) - Plots
Figure 18  Case 6  (65°C, 0.7 lpm, L/D = 25) - Plots
A comparative plot of the super saturation ($Sr > 1.1$) is represented in Figure 19. It is inferred from this plot that case 4 with 0.3 lpm clearly shows an improved saturation distribution as compared to the case 4 with 0.1 lpm flow rate. Both 0.5 lpm and 0.7 lpm flow rates also show further improvement in super saturated region but an incremental positional delay in reaching super saturation can be noted especially in the central region. This effect is clearly evident from the Figure 21 which plots the saturation ratio along the axis; this is also in coherence with the observations made by Yang et al. (2000). This would mean that a particle at the axis or any region for that matter would experience a higher super saturation zone worthy enough to cause condensation and growth, much early inside the growth tube in the case of a reduced flow rate. Whereas the degree of super saturation the same particle would experience inside the growth tube would be significantly larger in the case of a higher flow.

Another important implication of higher inlet velocity is that a particle flowing in with the sample with a high velocity would get comparatively lesser time in a region of higher saturation. This means that even though higher velocities would result in a better saturation distribution, a careful analysis has to be done so that the particle won’t go out of the region of interest too quickly that it won’t get enough time for condensation and there for increase in its size.

Volume flow requirement has got other implications on the overall engineering of the device as well. A higher sampling rate would require a higher motor power. Also the heat removal rate from the condensation wall will be faster; thus increasing the energy requirement for maintaining the wall at a near constant temperature. Thus an optimum value of sampling rate, as considered in Case 4 (0.3 lpm) is concluded to be the best possible option among those considered so far.
Comparison of Super Saturated Zone ($Sr > 1.1$) Case 3 (0.1lpm), Case 4 (0.3lpm), Case 5 (0.5lpm) & Case 6 (0.7lpm)

Figure 19  Comparison of Super Saturated Zone ($Sr > 1.1$) Case 3, Case 4, Case 5, & Case 6
Figure 20: Comparison of Temperature along the axis for Case 3, 4, 5 & 6
(65 deg C, L/D - 25)
Figure 21  Comparison of Saturation Ratio along the axis for Case 3, 4, 5 & 6
4.2.3. Geometry- \((L/D \text{ ratio})\)

A final variant was also considered with a reduced \(L/D\) ratio in an attempt to miniaturize the design to the maximum extent possible. Instead of \(L/D\) of 25, a value of 15 is evaluated in Case 7. This is achieved by changing both the diameter and length of the device in an attempt to not lose the advantage of creating an increased volume of region with desired super saturation. All other parameter like wall temperature \(65^\circ C\) and the flow rate of 0.3 \(lpm\) as concluded above is considered here and resulting graphs are given in Figure 22.

Comparing case 7 with the best possible case concluded before i.e. Case 4 for the region of super saturation \(Sr > 1.1\), it can be easily noted that there is a significant improvement in the region or volume of super saturation. On a closer look it can be identified that there is only marginal difference between these cases in terms of the degree of super saturation. This becomes evident in the axial temperature and saturation plot given in Figure 24 and Figure 25. Here it becomes clear that eventually, in terms of temperature development and super saturation Case 7 can be considered as a Case 4 with shortening of the growth tube.

Because of this, like in the case of high inlet flow rate, the shortening of the device also has a disadvantage in terms of the time available for the particle to grow in the super saturated zone; however the increased diameter would reduce the flow velocity given the volume flow rate is maintained the same. A best solution out of these two would call for further analysis in terms of particle growth rate to arrive at the best possible option. This is carried out through numerical particle tracking in the next section.
Figure 22  Case 7  (65°C, 0.3 lpm, L/D = 15) - Plots
Figure 23  Comparison of Super Saturated Zone (Sr>1.1) Case 4 (L/D=25) & Case 7 (L/D=15)
Figure 24  Comparison of Temperature along the axis for Case 4 & 7

Temperature Plot Along the Axis for Cases 4 & 7
(65 deg C, 0.31pm)
Figure 25  Comparison of Saturation Ratio along the axis for Case 4 & 7
4.3. PART 2 – PARTICLE TRACKING AND GROWTH CALCULATION

The growth rate of 4 particles all with initial size of 30nm located across the cross section of the device was numerically calculated based on the saturation and temperature distribution results obtained through CFD Simulation for Case 4 and Case 7. Figure 26 gives a plot of growth rate in these particles along the length of the device for various seeding points. If we just look at the growth rate shown for a particular geometry for example Case 4 which is represented by the solid lines, it can be noted that the particles flowing further away from the axis of symmetry grows to a higher size than the corresponding particle flowing through the axis. This is because of the developing flow profile which imparts a higher velocity to the particle near the centerline. The particles in the faster zone, even though experiencing the best saturation rations in the respective case, gets comparatively lesser time to grow, hence exiting the device with the minimum size in the distribution.

Now, looking at both the cases together, it becomes evident that the growth rate is higher in Case 7. The is because, here were are comparing the same inlet flow rate of 03 lpm condition in two different diameters; with the Case 4 being smaller in diameter than Case 7, the inlet velocities would be higher in Case 4. This is further illustrated through a vector plot of the velocities for both the cases shown as Figure 27. Now, even though the results discussed in the earlier section with Figure 24 and Figure 25 shows that both the geometries given almost the same temperature and saturation ration, the particles in Case 7 is slower compared to Case 4, giving additional time for the particle in a supersaturated condition to grow in size. This is the reason why the entire particle seeds in Case 7 show a higher growth rate as compared to the smaller variant considered in Case 4.
Figure 26  
Particle Growth rate along length

Case 4 \(65^\circ C, 0.3 lpm, \frac{L}{D} = 25\) with Case 7 \(65^\circ C, 0.3 lpm, \frac{L}{D} = 15\)
Figure 27  Velocity Vector Comparison of Case 4 & Case 7
Figure 28 shows the comparison of the particle size at the exit of the device across the cross section from the axis to a region very close to the wall. Since both the variants considered here are with different diameters, the diameter variable is normalized with growth tube diameter in each case for comparison. Since the flow velocity is very close to zero because of the no-slip wall condition, the particles in that zone would take a very long time to come out of the growth tube. Moreover, most of this particle would be in a region of very high levels of saturation susceptible enough to always impart condensation of the fluid on to the particle. This in turn would result in very high particle diameters at the outlet. The slower the flow, the larger would be this effect. Moreover the probability of particle sticking together due of its larger size, near to null velocity and proximity of the wall is really high. Hence to have a realistic comparison only 90% of the radius is considered here for comparison.

It can be easily agreed up on that, the particle exiting the shorter variant, which in this study is Case 7 would barely reach 1\textmu m target size near the axis; whereas in Case 4, it reaches a much comfortable size of 2\textmu m at the center line. The higher size of particle in Case 7 near the wall point exits are justified considering a larger diameter of the device in comparison to Case 4 thereby resulting in a comparatively lesser velocities for the same flow rate.

This study helps us to decide that, since most of the particle would be flowing through the central region of the growth tube, Case 4 would result in a better counting efficiency than that of the shorter Case 7 version. These results can further be enhanced by taking in to effect, the inter-particular interactions and gravity.
Figure 28  
Comparison of exit particle size 

Case 4 \( (65^\circ C, 0.3tpm, \frac{L}{D} = 25) \) with Case 7 \( (65^\circ C, 0.3tpm, \frac{L}{D} = 15) \)
4.4. **Effect of Inlet Parameters - Inlet Temperature and Inlet Humidity**

In this section, the finalized case from the previous analysis was further checked for its performance with varying inlet conditions. In the previous sections the inlet conditions were assumed to be at 25°C temperature and 25% RH. Here, the inlet conditions are evaluated independently by first changing the incident sample humidity was varied from 0% to 75% and then the sample inlet temperature from 15°C to 35°C. These values are consistent with the normally occurring weather conditions where the device would be finally used. The parameters considered for this study is listed below in Table 3.

<table>
<thead>
<tr>
<th>Cases Considered</th>
<th>L/D Ratio</th>
<th>Inlet Flow Rate (lpm)</th>
<th>Condenser Wall Temperature (°C)</th>
<th>Inlet Humidity (%)</th>
<th>Inlet Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>25</td>
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<td>65</td>
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<td>25</td>
<td>0.3</td>
<td>65</td>
<td>0</td>
<td>25</td>
</tr>
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<td>0.3</td>
<td>65</td>
<td>50</td>
<td>25</td>
</tr>
<tr>
<td>10</td>
<td>25</td>
<td>0.3</td>
<td>65</td>
<td>75</td>
<td>25</td>
</tr>
<tr>
<td>11</td>
<td>25</td>
<td>0.3</td>
<td>65</td>
<td>25</td>
<td>15</td>
</tr>
<tr>
<td>12</td>
<td>25</td>
<td>0.3</td>
<td>65</td>
<td>25</td>
<td>35</td>
</tr>
</tbody>
</table>

Table 3 **Cases Considered with the Inlet Variations**
4.4.1. Inlet Humidity Variations

The inlet humidity can vary from really dry condition with near 0% RH to considerably humid ambient condition with 75% RH. The results for the case with 0% RH is given in the Figure 29 and Figure 30 and Figure 31 respectively shows the temperature and saturation distribution and contours for the cases with 50% RH and 75% RH respectively. It can be inferred from the graphs that the inlet humidity would not play any major role in changing the supersaturation region inside the condensation chamber. This become clear by looking at the supersaturation plot comparison given in the Figure 32 which does not show any major variation between the cases considered. On a closer look at the saturation distribution along the axis, given in the Figure 34, the saturation levels of the condenser chamber are slightly shifted by the inlet humidity parameter, but this change is very small.

It can be further observed that the preconditioning chamber which is intended to bring the inlet sample to a uniform 60% RH condition appears to be adequate for all humidity conditions considered here. So based on the above observations, it can be concluded that the device would perform satisfactorily as predicted in the normally occurring ambient humidity ranges.
Figure 29  Case 8  (65°C, 0.3 lpm, L/D = 25) with Inlet Humidity of 0% RH - Plots
Figure 30  Case 9  (65°C, 0.3 lpm, L/D = 25) with Inlet Humidity of 50% RH - Plots
Case 10- "0.3 lpm" Flow Rate & "65 deg" Saturation Wall Condition L/D = 25 with 75 % inlet RH

Figure 31 Case 10 (65°C, 0.3 lpm, L/D = 25) with Inlet Humidity of 75% RH - Plots
Figure 32  Comparison of Super Saturated Zone (Sr>1.1) Case 4, 8, 9 & 10
Figure 33  Comparison of Temperature along the axis for Case 4, 8, 9, & 10
Figure 34  Comparison of Saturation Ratio along the axis for Case 4, 8, 9 & 10
4.4.2. Inlet Temperature Variations

Next set of simulations are done for varying inlet temperatures. During the device application, the inlet temperature can vary based on the weather and season from $15^\circ C$, to $35^\circ C$. This study is conducted considering the same inlet saturation level of $25\%$ RH and the preconditioning chamber feeding vapor to the flow which tries to bring the saturation level up to $65\%$ RH.

Case 11 solutions with $15^\circ C$ inlet temperature condition are given by the Figure 35. It shows that at lower working inlet temperatures the super saturation inside the condensation chamber significantly improves. The super saturation levels reached in this conditions are well above $Sr \sim 2.5$. So the device would eventually perform better by increased condensation resulting in the particle growing to higher diameters. This is because of the higher $\Delta T$ between the inlet flow and the condenser wall temperature. Case 12 shown in Figure 36 corresponds to a higher level of inlet temperature of $35^\circ C$ than what was considered so far in the previous section. In this case, even though the region of supersaturation doesn’t seem to reduce considerably, the level of supersaturation drops. A comparison of the supersaturation levels with the inlet temperature of $15^\circ C$ (Case 11), $25^\circ C$ (Case 4), $35^\circ C$ (Case 12) is given in Figure 37. It clearly shows that the supersaturation levels are significantly increased with reducing temperature and reduces with increased inlet temperature condition. Figure 38 and Figure 39 shows a comparison of the temperature and saturation distribution along the axis of the cases considered here.

Based on this analysis we can say that the device with finalized parameters as in Case 4 would perform well at lower ambient conditions but its efficiency would be compromised at higher inlet temperatures.
Figure 35  Case 11  (65°C, 0.3 lpm, L/D = 25) with Inlet Temp of 15°C - Plots
Case 12 - "0.3 lpm" Flow Rate & "65 deg." Saturation Wall Condition L/D = 25 with 35 deg inlet

Figure 36  Case 12  (65°C, 0.3 lpm, L/D = 25) with Inlet Temp of 35°C  - Plots
Comparison of Super Saturated Zone (Sr>1.1) Case 4, 11 & 12

Figure 37  Comparison of Super Saturated Zone (Sr>1.1) Case 4, 11 & 12
Figure 38  Comparison of Temperature along the axis for Case 4, 11, & 12

Temperature Plot Along the Axis for Cases 4, 11 & 12
(65 deg C, 0.3 lpm, L/D - 25, 25 % Rh Inlet)
Figure 39  Comparison of Saturation Ratio along the axis for Case 4, 11 & 12

Saturation Ratio Plot Along the Axis for Cases 4, 11 & 12
(65 deg C, 0.3 lpm, L/D - 25, 25 % Rh Inlet)
4.5. **PART 4- ALTERNATE WORKING FLUIDS**

In this section, we extend our studies on to other alternate working fluids such as n-Butanol and Isopropanol. The advantage of using these alcohols is its ability to give higher saturation ratios at lower temperatures. In order to explore this behavior the Lewis numbers of these fluids at various temperatures are compared in the Figure 40 and are compared with the water vapor. This chart shows that the Lewis numbers for both n-Butanol and Isopropanol reduces sharply with temperature as compared to water vapor, with Isopropanol always showing significantly smaller values as compared to the other two. What this indicates is that, for a given temperature more than 45° C, both these alcohols will have mass diffusion predominance over thermal diffusion. So, for a given condition, thermal profiles in the case of these fluids would develop slower than that of water. This is would result in a higher supersaturated regions in the flow field for these fluids as compared to that of water.

To confirm this, now we would consider a sample case with a sampling rate of 0.1 lpm and the wall temperature maintained at 100% saturation with a wall temperature of 45°C, 55°C & 65°C are analyzed for a L/D ratio of 25. The same case is analyzed by changing only the working fluid for condensation in the condensation chamber. In comparison to earlier cases, the inlet flow is assumed to have 0% concentration of working fluid because both n-butanol and Isopropanol is not a naturally occurring constituent of the atmospheric air sample. To get a one to one comparison with the water vapor condenser, the boundary conditions are adjusted accordingly. The updated boundary conditions are schematically represented in Figure 41. Table 4 shows the case variable matrix considered for this section.
Lewis No Variation with Temperature for Various Liquids Considered

Figure 40 Lewis Number comparison of working fluids Vs Condenser wall temperature
Updated Boundary Conditions for Working Fluid Study

Table 4  CASE SETS CONSIDERED FOR WORKING FLUID STUDY

<table>
<thead>
<tr>
<th>Cases Considered</th>
<th>L/D Ratio</th>
<th>Inlet Flow Rate (lpm)</th>
<th>Condensation Wall Temperature (°C)</th>
<th>Working Fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>I-i</td>
<td>25</td>
<td>0.1</td>
<td>45</td>
<td>WATER</td>
</tr>
<tr>
<td>I-ii</td>
<td>25</td>
<td>0.1</td>
<td>45</td>
<td>n-BUTANOL</td>
</tr>
<tr>
<td>I-iii</td>
<td>25</td>
<td>0.1</td>
<td>45</td>
<td>ISOPROPANOL</td>
</tr>
<tr>
<td>II-i</td>
<td>25</td>
<td>0.1</td>
<td>55</td>
<td>WATER</td>
</tr>
<tr>
<td>II-ii</td>
<td>25</td>
<td>0.1</td>
<td>55</td>
<td>n-BUTANOL</td>
</tr>
<tr>
<td>II-iii</td>
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<td>0.1</td>
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<td>ISOPROPANOL</td>
</tr>
<tr>
<td>III-i</td>
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<td>0.1</td>
<td>65</td>
<td>WATER</td>
</tr>
<tr>
<td>III-ii</td>
<td>25</td>
<td>0.1</td>
<td>65</td>
<td>n-BUTANOL</td>
</tr>
<tr>
<td>III-iii</td>
<td>25</td>
<td>0.1</td>
<td>65</td>
<td>ISOPROPANOL</td>
</tr>
</tbody>
</table>
4.5.1. Comparison of Saturation Levels

4.5.1.1. Case Set I with 45°C Condenser Wall Temperature

The first set of cases were analyzed for a saturation wall temperature of 45°C which for the working fluids, water, n-Butanol, Isopropanol are represented by Case (I-i), Case (I-ii) and Case (I-iii) respectively. Earlier we have analyzed the Lewis no for a particular temperature so as to get a general idea of the working fluid behavior to give the desired saturation levels. Now since, inside the growth tube, there will be a temperature distribution; it would be a good idea to keep a track of the Lewis number distribution also. Figure 42 shows the Lewis no distribution for the case I set with 45°C. The distribution shows a nearly constant Lewis number for water and considerably higher values for both the alcohols. This is consistent with the behavior obtained earlier for this temperature zone.

The saturation profiles for the cases Case (I-i), Case (I-ii) and Case Case (I-iii) are presented in the Figure 43 and Figure 44 is a plot of the supersaturated zone for these cases which are of our interest here. The supersaturation curves indicate a better spread of supersaturation region for the cases of alcohols in comparison with that of water vapor. It also indicates that the maximum supersaturation is in fact obtained in the case of Water. This phenomenon can be explained through the Lewis no plots from Figure 42, which gives an indication that at lower temperatures the mass diffusivity of alcohols are not that predominant over the thermal diffusivity hence resulting in lesser vapor molecule penetration through a relatively hotter zone in the centre of the growth tube; which is much less in magnitude to obtain a super saturation lever for that temperature.
LEWIS NUMBER DISTRIBUTION FOR CASE I (45 deg C) TRIALS WITH VARIOUS FLUIDS

Inlet Diameter := 2mm  Inlet Air Temp := 25 deg C  Pre Conditioning Temp := 25 deg C  Condensor Wall Temp := 45 deg C
Inlet Air Flow Rate := 0.1 lpm  Inlet Air Humidity := 0%  Pre Conditioning Humidity := 60%  Diffusion Model := Kinetic Theory

Figure 42     Lewis No Distribution in Case I Trials with Various Fluids for 45°C
Figure 43  Saturation Ratio Distribution in Case I Trials with Various Fluids at 45°C
SUPERSATURATION REGION (Sr>1.1) FOR CASE I TRIALS (45 deg C) WITH VARIOUS FLUIDS

Inlet Diameter : = 2 mm  Inlet Air Temp : = 25 deg C  Pre Conditioning Temp : = 25 deg C  Condensor Wall Temp : = 45 deg C
Inlet Air Flow Rate : = 0.1 lpm  Inlet Air Humidity : = 6%  Pre Conditioning Humidity : = 80%  Diffusion Model : = Kinetic Theory

Figure 44  Super Saturation Region in Case I Trials with Various Fluids at 45°C
4.5.1.2. Case Set II with 55°C Condenser Wall Temperature

The next set of results represents the cases- Case (II-i), Case (II-ii) and Case (II-iii) which differ from the previous set only by an elevated saturation wall temperature of 55°C. From Figure 40, it was noted that it is near this temperature where n-Butanol will start to have a lesser Lewis no in comparison to that of water. Where in the case of Isopropanol, this difference is largely evident and hence the characteristics observed in Figure 42 is justified.

Figure 43 and Figure 44 show a much more predominant improvement in supersaturated zones in the case of the alcohols. It is also noted that the n-Butanol (Case (II-ii)) shows the largest saturation values as compared to that of water in this case set. Figure 44 which shows the zone of supersaturation indicates clearly that the alcohols provide a better environment for the particle to grow in size through condensation than in the case of water vapor at the same conditions.

The most important point noted from these results is the relative shift in the supersaturated zone in the case of Isopropyl alcohol (Case (II-iii)) in comparison to that of both n-Butanol and water. This would have a profound effect in the particle growth rate, because this means that the particles are exposed to a higher saturation levels relatively late in the growth tube for Isopropanol. The effect of this behavior would become evident during the next stage when the particles are tracked.
LEWIS NUMBER DISTRIBUTION FOR CASE II (55 deg C) TRIALS WITH VARIOUS FLUIDS

Inlet Diameter := 2 mm  Inlet Air Temp := 26 deg C  Pre Conditioning Temp := 25 deg C  Condenser Wall Temp := 65 deg C
Inlet Air Flow Rate := 0.1 lpm  Inlet Air Humidity := 0%  Pre Conditioning Humidity := 60%  Diffusion Model := Kinetic Theory

Figure 45  Lewis No Distribution in Case II Trials with Various Fluids at 55°C
SATURATION RATIO DISTRIBUTION IN CASE II (55 deg C) TRIALS WITH VARIOUS FLUIDS

Inlet Diameter := 2 mm  Inlet Air Temp := 25 deg C  Pre Conditioning Temp := 25 deg C  Condenser Wall Temp := 55 deg C
Inlet Air Flow Rate := 0.1 lpm  Inlet Air Humidity := 0%  Pre Conditioning Humidity := 60%  Diffusion Model := Kinetic Theory

Figure 46  Saturation Ratio Distribution in Case II Trials with Various Fluids at 55°C
SUPER SATURATION REGION (Sr>1.1) IN CASE II (55 deg C) TRIALS WITH VARIOUS FLUIDS

Inlet Diameter := 2 mm  Inlet Air Temp := 25 deg C  Pre Conditioning Temp := 25 deg C  Condensor Wall Temp := 55 deg C
Inlet Air Flow Rate := 0.1 lpm  Inlet Air Humidity := 0%  Pre Conditioning Humidity := 60%  Diffusion Model := Kinetic Theory

Figure 47 Super Saturation Region in Case II Trials with Various Fluids at 55°C
4.5.1.3. Case Set III with 65°C Condenser Wall Temperature

Further increment in the condenser wall temperature follows the previously observed trend and results in further better supersaturation zone and degree of supersaturation in the case of alcohols in comparison to water. Here Case (III-i), Case (III-ii) and Case (III-iii) are compared in the Figure 45 to Figure 47.

The Lewis No plot for the Isopropanol Case (III-iii) now shows significantly low values since the temperature has increased by another 10°C to 65°C, but the values for n-Butanol and water are comparable in magnitude. This effect is clearly reflected in the saturation distribution chart (Figure 46), which shows comparable saturation profiles for water and n-Butanol. Even though the saturation profiles are comparable, the highest degree of supersaturation in the case of n-Butanol is close to 2 whereas for water it is more in the range of 1.8.

The Supersaturated zone with $Sr > 1.1$ given in Figure 47 shows that almost entire condensation chamber is supersaturated in the case of Isopropanol. The shift in the supersaturation zone, especially in the case of Isopropanol, is clearer in this condition. To understand how much of an impact this would bring about, the particle tracking algorithm used in the previous part is modified for calculating the particle growth along the axis and across the radius of the condensation chamber and is explained in the next section.

In general, this study is sufficient enough to prove that the considered alcohols would perform better at temperatures more than 45°C as compared to that of water, Cēterīs paribus.
LEWIS NUMBER DISTRIBUTION FOR CASE III (65deg C) TRIALS WITH VARIOUS FLUIDS

Inlet Diameter := 2mm  Inlet Air Temp := 25 deg C  Pre Conditioning Temp := 25 deg C  Condenser Wall Temp := 65 deg C
Inlet Air Flow Rate := 0.1 lpm  Inlet Air Humidity := 9%  Pre Conditioning Humidity := 60%  Diffusion Model := Kinetic Theory

Figure 48  Lewis No Distribution in Case III Trials with Various Fluids at 65°C
Figure 49  Saturation Ratio Distribution in Case III Trials with Various Fluids at 65°C
SUPER SATURATION REGION (Sr > 1.1) IN CASE III (65 deg C) TRIALS WITH VARIOUS FLUIDS

Inlet Diameter := 2 mm  Inlet Air Temp := 25 deg C  Pre Conditioning Temp := 25 deg C  Condenser Wall Temp := 66 deg C
Inlet Air Flow Rate := 0.1 lpm  Inlet Air Humidity := 0%  Pre Conditioning Humidity := 80%  Diffusion Model := Kinetic Theory

Figure 50  Super Saturation Region in Case III Trials with Various Fluids at 65°C
4.5.2. Particle Tracking and Growth Calculation for Alternate Fluids

The particle seeded at four radial locations are tracked from the condensation chamber entrance to exit with the same algorithm used for the water vapor condenser in the previous part and the results are presented in the Figure 51. This figure shows the particle growth for the case set no 2, ie with the condenser wall temperature maintained at 55°C. The particles in the water medium are represented with dashed lines, n-Butanol with chained lines and Isopropanol with solid lines. Each radial location is differentiated with the line color.

The graph shows a remarkable improvement in the particle growth in the alcohol medium as compared to that of water. One important observation is how quickly the growth regime changes from kinetic regime to continuum. Since the Alcohol molecules are almost triple or more in size as compared to water molecules, the mean free path (λ) value is significantly small, nearly reaching the 30nm size of the seed particle. So, in the case of both alcohols, the growth rate would be significantly large in early stages as compared to that of water medium.

It is interesting to observe that n-Butanol medium would result in a larger particle at the end of the growth chamber even though Isopropanol has higher saturation levels and supersaturation spread. An exit particle contours across the cross section of the growth tube is given in Figure 52 which verifies that in 90% of the region, n-Butanol results in a higher exit particle diameter as compared to both the other liquids. This could be because of two reasons. n-Butanol average molecular diameter being largest of the lot, collision frequency would be higher resulting in higher rate of condensation.
Figure 51  Particle Growth rate along length for Case (II-I), Case (II-ii) & Case (II-iii)
Figure 52  Comparison of exit particle size for Case ( II-I ), Case ( II-ii ) & Case ( II-iii )
Particle growth in Isopropanol medium shows that there is a considerable delay in the growth during the initial stage, even though they have a better saturation spread. This could because of the delay observed in reaching high degree of supersaturation along the axis due its diffusion characteristics. This could be confirmed by looking at the growth profiles of particles in the Isopropanol vapor medium alone. The particles near the axis were this delay in predominant clearly shows a slower growth rate initially as compared to the ones away from the center line. But when the particle experiences higher degree of supersaturation later in the growth tube, the particle begins to grow rather quickly.

It can be conclusively commented from this study that, both n-Butanol and Isopropanol working fluids will significantly improve the growth rate of the sample particle as compared to that of water and its feasibility as an alternative to water in the same equipment is worth exploring. But, these alcohols being hazardous in nature, it is very important to have a recovery system to separate out the fluid downstream.
CHAPTER 5

5. SUMMARY & CONCLUSION

5.1. SUMMARY

The study showed that a low flow rate or low wall temperature would result in less supersaturation than required, which in turn reduces the particle size through re-evaporation. Whereas, a very high flow rate condition would restrict the supersaturated region close to the walls. This would result in undersized particles at the exit since the particles will get less time in a supersaturated environment to grow to the required size. The study also showed a distinct distribution of particle sizes at the exit across the cross section clearly indicating that the particle exiting the device near the axis will be smaller compared to the particles flowing near to the wall.

It can be concluded from this study, that Case 4 with 65°C wall temperature, 0.3 lpm inlet flow rate, and a $L/D$ ratio of 25 is the best design option among the range of parameters considered here.

The technical feasibility of two alternate working fluids namely n-Butanol and Isopropanol is conducted and the saturation distribution and growth rate tracking calculations clearly indicated that these alcohols would certainly perform better than water for the intended application, but its practical applicability has to be decided based on the peripheral needs of recovery system for the purpose of safety and reduced consumption rate, which may not be a necessary condition if water is used.
5.2. Suggestions For Future Work

The effect of gravity is not considered in this study for simplicity and an improved prediction of particle size and inter-particle interactions can be modeled as performed by Lin & Tarbell (1980), and Ray & Dronamraju (1982), which could be considered as an improvement to the study conducted here.

An empirical growth equation has been developed by Kulmala (1993), which calculates the time required for an aerosol to grow to a particular size at a particular saturation level. This equation could be implemented in tandem with the saturation distribution to improve the growth model.
**CHAPTER 6**

6. REFERENCES


