LA-UR-12-24026
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Title: Rosin-Rammler Distributions in ANSYS Fluent

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Intended for: Report

1.0 INTRODUCTION

In Health Physics monitoring, particles need to be collected and tracked. One method is to predict the motion of potential health hazards with computer models. Particles released from various sources within a glove box can become a respirable health hazard if released into the area surrounding a glove box. The goal of modeling the aerosols in a glove box is to reduce the hazards associated with a leak in the glove box system.

ANSYS Fluent provides a number of tools for modeling this type of environment. Particles can be released using injections into the flow path with turbulent properties. The models of particle tracks can then be used to predict paths and concentrations of particles within the flow.

An attempt to understand and predict the handling of data by Fluent was made, and results iteratively tracked. Trends in data were studied to comprehend the final results. The purpose of the study was to allow a better understanding of the operation of Fluent for aerosol modeling for future application in many fields.

2.0 DATA

The data given here is an example of particles captured inside of a health-hazard environment, and the theory behind simple aerosol physics is described herein.

2.1.0 Cascade Impactor

A method of aerosol size measurement is a cascade impactor. A cascade impactor works by flowing air around turns to collect certain particle sizes. Depending on the radius of the turn and the mass of the particle, it will either continue around the turn, or become attached to the impaction plate. Larger particles resist changes of directions more than smaller particles do because of higher inertia in larger particles. Because of this larger particles are collected in the first stages, and smaller particles stay with the flow until later stages. The 'cutoff' in a cascade impactor is the smallest diameter collected in an individual stage. Using multiple impactors in series allows the mass of the particles to be sampled based on their size. After the air has been sampled, the impactor plate from each stage is weighed. The experiment is performed multiple times and an error is calculated from the differences in masses between trials.

2.2.0 Data Tables

The data format from a cascade impactor is given as a table with columns of: cutoff, bin center, mass concentration, and error (mass concentration) as shown in Table 2.2.1. The experimental data for mass and error came as a mass concentration (mass/volume). So in this case it was necessary to multiply both the mass and the error by the internal volume of 0.12 m^3 to obtain the mass for each stage. After the mass was converted from a concentration, the data was shifted down one row to coincide with the pre-filter for the original data acquisition. Because of integration, the total value of mass in each section was assigned to the upper limit of the impactor. A pre-filter is used to filter out particles larger than expected for the experiment. The final form of the data before modifications is shown in Table 2.2.2.

Table 2.2.1

Bin Center (µm)	Cut Point (µm)	Mass (µg/m^3)	Error ± (µg/m^3)
31.83	21.07	21490.385	55.694271266
18.02	14.97	19467.213	39.6746023808
12.37	9.77	26948.006	42.7633453287
7.88	5.98	30930.087	89.4944649644
4.74	3.50	14394.737	52.7046276695
2.51	1.53	15836.227	57.5342088256
1.22	0.90	8986.254	6.8041381744
0.72	0.53	1318.743	13.6082763488
0.31	0.10	14236.111	25.4587538609

Table 2.2.2

Bin Center (µm)	Cut Point (µm)	Mass (µg)	Error ± (µg)
0.31	0.1	0	0
0.72	0.53	1708.33332	3.055050463
1.22	0.9	158.24916	1.632993162
2.51	1.53	1078.35048	0.816496581
4.74	3.5	1900.34724	6.904105059
7.88	5.98	1727.36844	6.32455532

12.37	9.77	3711.61044	10.7393358
18.02	14.97	3233.76072	5.131601439
31.83	21.07	2336.06556	4.760952286
-	42.6	2578.8462	6.683312552

3.0 ANALYSIS

3.1.0 Aerodynamic Diameter

The data, as shown in Table 2.2.2, was inverted to increasing order to allow the data to be plotted. It is important to note that all the size data used in plots is the aerodynamic diameter rather than the physical diameter. The aerodynamic diameter (d_a) is defined as an equivalent diameter "… for a particular particle, as the diameter of the spherical particle with a density of 1000 kg/m^3 [1 g/cm^3] (the density of water)…(Hinds 53)." This means that all particles within a given aerodynamic diameter will settle at the same velocity, regardless of physical diameter.

> "A correction factor called the *dynamic shape factor* is applied to Stoke's law to account for the effect of shape on particle motion. The dynamic shape factor defines how "irregular" or how un-like a sphere a particle is and allows the irregular properties to be referenced as a spherical particle. The dynamic shape factor is defined as the ratio of the actual resistance force of the nonspherical particle to the resistance force of a sphere having the same volume and velocity as the nonspherical particle. The dynamic shape factor χ is given by
>
> $$\chi = \frac{F_D}{3\pi\eta V d_e}$$
>
> where d_e, called the equivalent volume diameter, is the diameter of a sphere having the same volume as that of the irregular particle (Hinds 51)."

To convert equivalent diameter (d_e) to aerodynamic diameter, the following formula is applied:

$$d_a = d_e \left(\frac{\rho_p}{\rho_o \chi}\right)^{1/2} \quad \text{(Eq. 3.1.01)}$$

where ρ_p is the particle density and ρ_0 is the density of water.

3.2.0 Mass Fraction

The plot in Figure 3.2.1 is a histogram of aerodynamic diameter vs. mass fraction. Mass fraction is the percentage of the total mass from each bin, given in Figure 3.2.1. The bin centers are shown with red dots over the middle of each bin. The last bin had an error while being plotted and does not extend as far as it should.

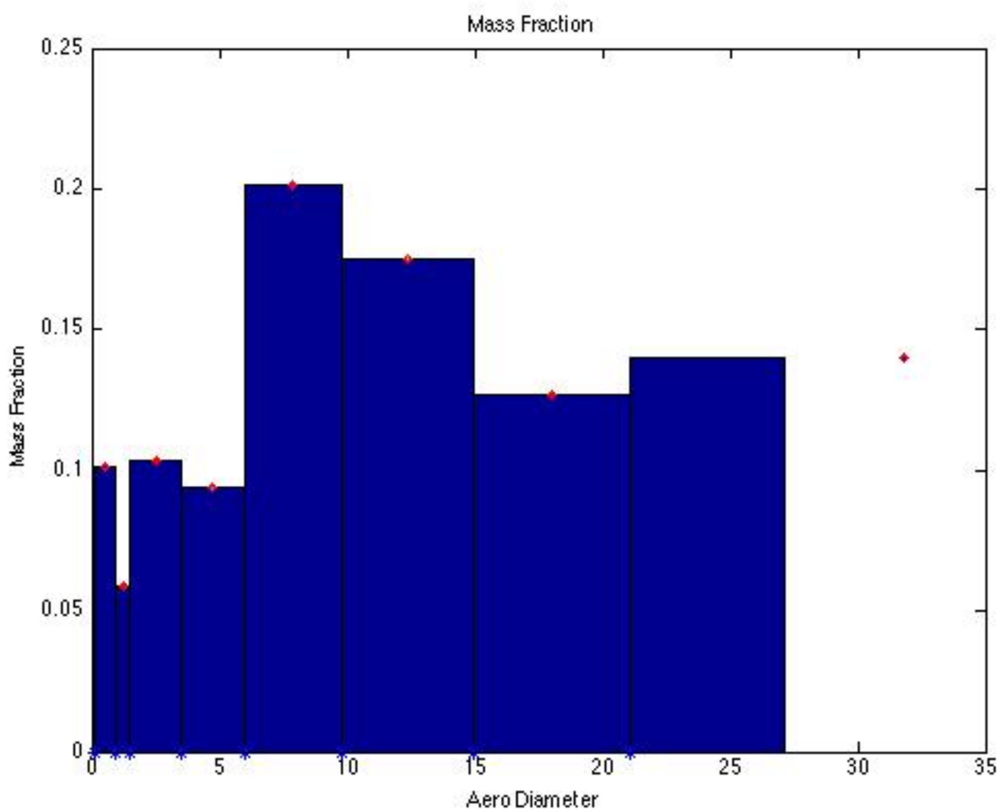

Figure 3.2.1

Included in Figure 3.2.1 are error bars, shown as “whiskers” at the Bin Centers of the histogram. For the data given, the errors were quite small; the largest relative error was less than 1%. To illustrate how small the error was, a close up of the error bars is shown in Figure 3.2.2.

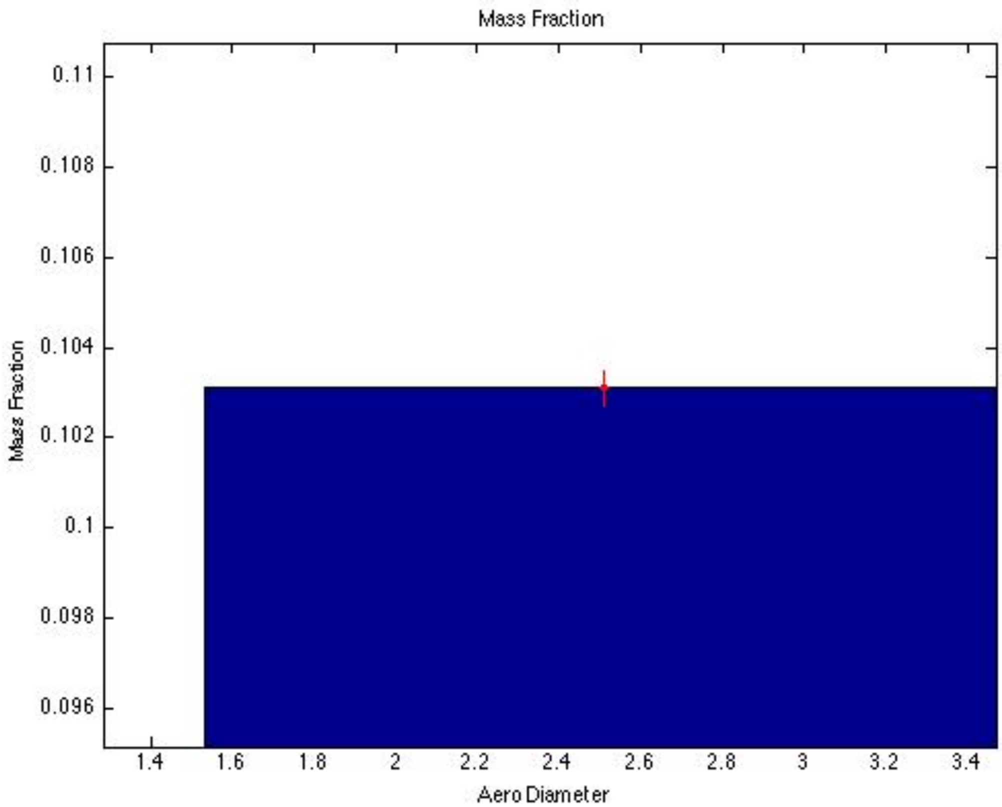

Figure 3.2.2

In order to see the "whiskers" on the plot, it was necessary to zoom a great deal to produce the detail seen (note the scales on the axis'). This was a visual confirmation of how miniscule the relative error was.

3.3.0 Differential Mass

It was necessary to standardize the bins after the initial plot by creating a mass differential plot. In order to create a mass differential, the fractional mass was divided by the difference of the bin widths. This created a second histogram of mass differential, as shown in Figure 3.3.1.

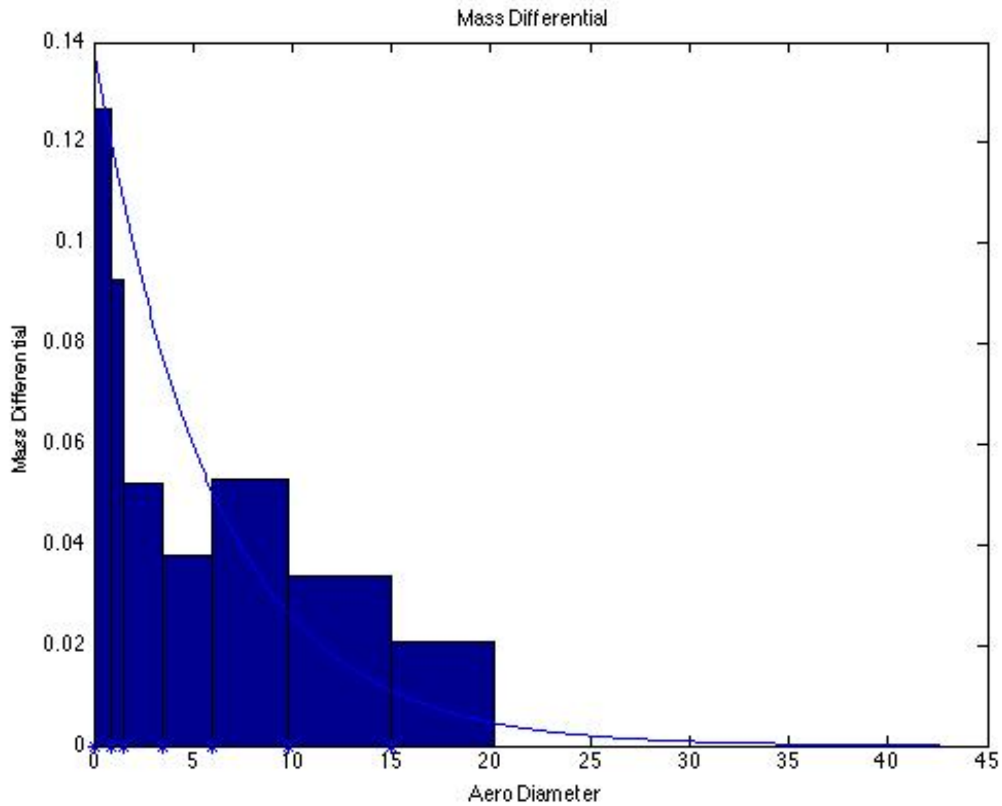

Figure 3.3.1

An exponential curve fit of the current data was placed over the mass differential histogram in Figure 3.3.1. However, the curve was hand-plotted and the parameters were estimated, so this is only an estimated curve-fit, not an analytical solution.

3.4.0 Cumulative Mass

Another way to look at mass distribution is cumulative mass. A cumulative mass plot shows how the mass accumulates from zero to the total mass. Figure 3.4.1 shows the cumulative mass for the given data. Because of the abundance of smaller particles, and how they are distributed, 80% of the mass is particles smaller than 20 micrometers.

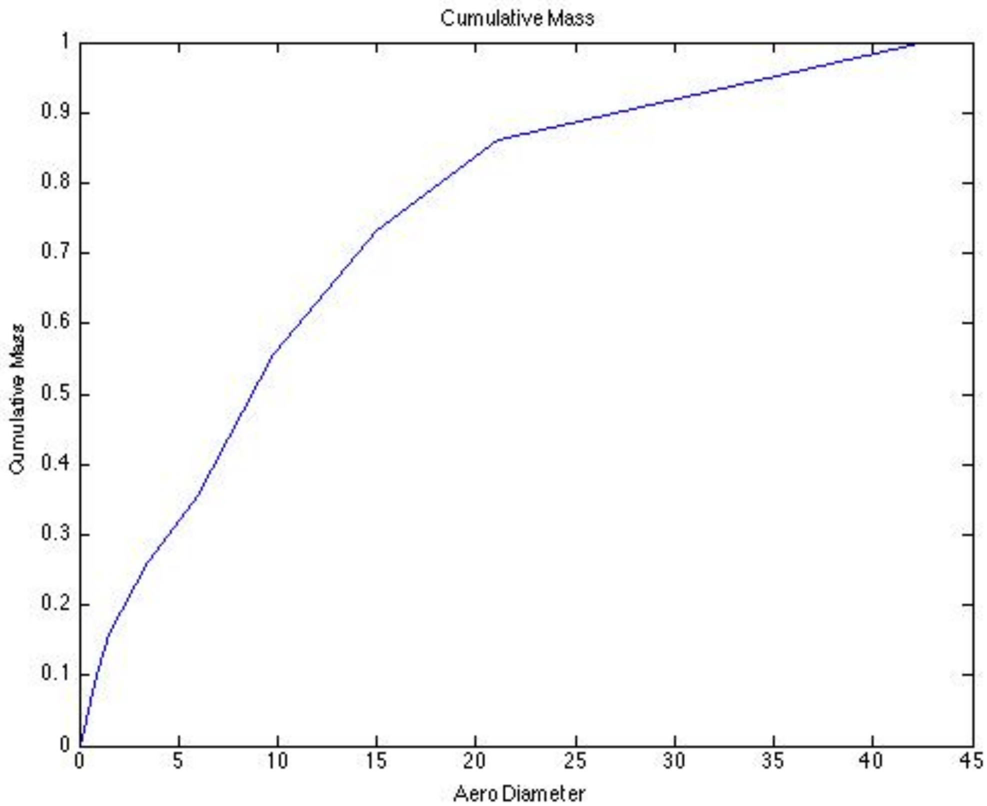

Figure 3.4.1

3.5.0 Count Distribution

Another type of distribution is the count distribution. Many applications of aerosol data require knowledge of the number of particles in different sizes, rather than just the total mass for each size range. Especially when looking at small particles, the number of particles needed to create the mass in the first couple bins is enormous.

If the mass density function is defined as g(x), then it is equal to the count function f(x) times the volume and the density of the particles. This is shown in Eq. 3.5.02.

$$g(x) = f(x)\rho_p \frac{\pi}{6} {d_p}^3 \qquad \text{(Eq. 3.5.01)}$$

Substitute aerodynamic diameter for physical diameter from Eq. 3.1.01.

$$g(x) = f(x)\rho_p \frac{\pi}{6} {d_a}^3 \left(\frac{\rho_0 x}{\rho_p}\right)^{3/2} \qquad \text{(Eq. 3.5.02)}$$

Then simplify and pull x^3 out of constants.

$$g(x) = \rho_p \left(\frac{\rho_0 x}{\rho_p}\right)^{3/2} \frac{\pi}{6} x^3 f(x) \quad \text{(Eq. 3.5.03)}$$

Combine constants into one symbol, C.

$$g(x) = Cx^3 f(x) \quad \text{(Eq. 3.5.04)}$$

Therefore the count distribution as a function of the mass distribution is shown by Eq. 3.5.05.

$$f(x) = \frac{g(x)}{Cx^3} \quad \text{(Eq. 3.5.05)}$$

The count distribution has a different shape than that of the mass distribution because of the higher number of smaller particles. Both graphs plotted in log scale are shown in Figure 3.5.1.

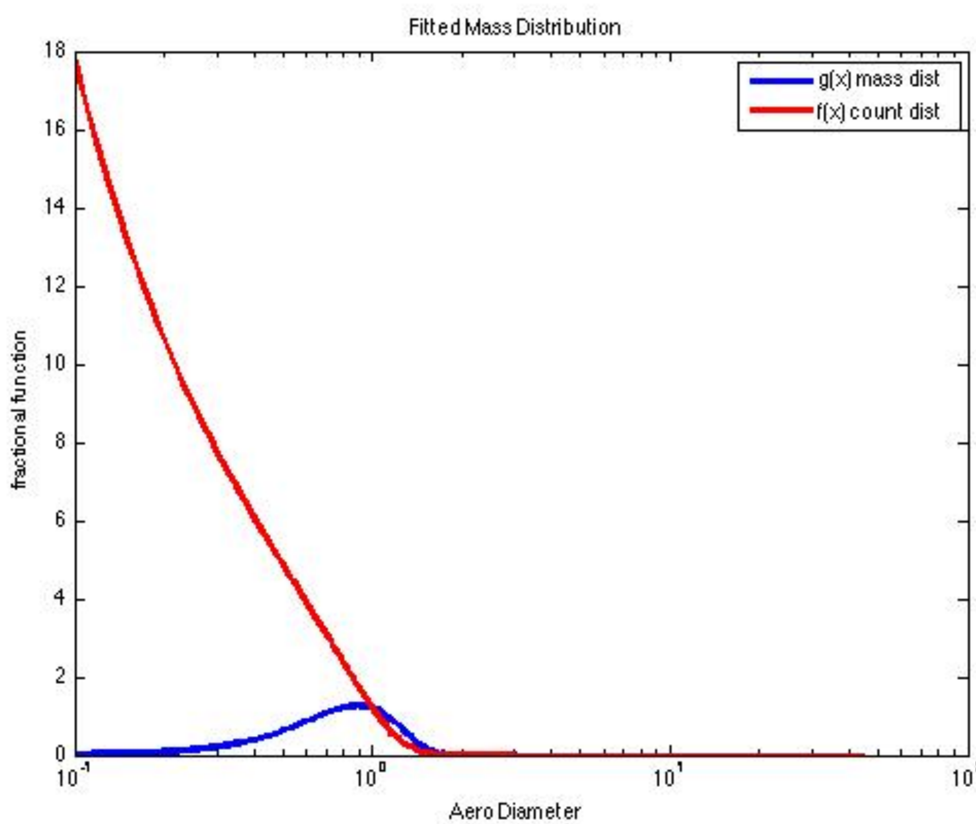

Figure 3.5.1

As is shown in Figure 3.5.1, the count distribution is an order of magnitude different than the mass distribution. Depending on the requirements for ANSYS Fluent, one will be used over the other.

4.0 INTERFACE WITH FLUENT

ANSYS Fluent is a computational fluid dynamics (CFD) program that allows the user to analyze fluid flows. Fluent uses injections to create particles in the model space. Built into Fluent is a Rosin-Rammler particle distribution, which requires a number of parameters. A Rosin-Rammler distribution is a form of the Weibull distribution function. When creating an injection, Fluent requires the initial velocity, temperature, and total flow rate (mass flow rate). If an injection with a Rosin-Rammler distribution is created, Fluent calls for for a few more parameters: minimum diameter, maximum diameter, mean diameter, spread parameter, and number of diameters.

The diameter parameters can easily be determined from the data, but the spread parameter has to be analytically computed. The formula for the spread parameter is given by,

$$n = \frac{\ln\left(-\ln[Y_d]\right)}{\ln\left(d/\bar{d}\right)} \qquad \text{(Eq. 4.01)}$$

where Y_d is the mass distribution function. The Rosin-Rammler distribution function used by Fluent is shown in Eq. 4.02.

$$Y_d = e^{\left[-\left(d/\bar{d}\right)^n\right]} \qquad \text{(Eq. 4.02)}$$

From the description of the Rosin-Rammler function in the *ANSYS FLUENT User's Guide*, *"Using The Rosin-Rammler Distribution Method",* it can be said that Fluent is computing the mass distribution and not the count distribution from the given inputs.

4.1.0 Injections

Fluent uses multiple streams of monodisperse particles to model polydisperse injections. This means that each stream has one diameter size. According to a distribution function, the different streams inject particles at different rates. The Number of Diameters parameter for the Rosin-Rammler injection defines how many monodisperse streams are present. For a Rosin-Rammler injection, Fluent adjusts the rate for each stream to obtain the Rosin-Rammler distribution of particles. This is one method of producing the particles into the system. There may be other methods that involve writing custom injection files.

4.2.0 Testing injection in Tube

Custom injection files were not used in further experimentation. Before testing injections in complex-geometry meshes, different injection types were tested in a simple-geometry environment to verify particle size distributions. A tube was created and particles injected into the flow on one end and recoded at the other.

The surface injections used in the tube application allowed for many particles to be created using relatively few tries or number of diameters. For comparison purposes, the same parameters that were used in later injections were used in the simple-case experiment. The purpose of using the tube to verify particle distributions was to become familiar with the process of using Fluent to create distribution graphs and creating injections. Because of the extremely simple geometry, very little steps were needed to produce calculations with none, if not relatively few, incomplete particles. Number of particles produced using the initial conditions for the sphere are shown in Table 4.2.0.1. The number of particles produced using the initial conditions for the wheel release are shown in Table 4.2.0.2.

Table 4.2.0.1

Tries	Diameters	Steps	Total Particles	Incomplete Particles
120	40	1300	447200	0
150	40	1200	543000	0
200	50	1100	890000	5
250	60	1000	1335000	88

Table 4.2.0.2

Tries	Diameters	Steps	Total Particles	Incomplete Particles
150	40	1000	543000	32
200	50	1000	890000	70
225	50	1000	1001250	74
250	50	1000	1112500	80
250	60	1000	1335000	88
275	60	1000	1468500	113

In both cases, the same combination of number of tries and number of diameters produced the same amount of particles. The things that changed between each type of injection were the min and max diameters, as well as the spread parameter. Increasing the number of diameters provided better resolution on histograms for the distributions. The intent of using the same initial conditions as subsequent test was to transfer the numbers to future test to replicate the results. However, this was not the case because of differences in how the injections were handled.

4.3.0 Box cases

After the two types of injections were tested in the simple-geometry tube, they were applied to full-mesh turbulent environments. Two similar box environments were used, with different flow types to simulated different conditions. The first is a sphere release, with particles released outward from a point. The second type was a wheel release, with particles released in a circle tangentially. Early on, it was discovered that how the particles were released and the size of the surface injecting the particles was much smaller than in the tube test case. This led to a discrepancy in the number of particles produced, which was corrected by increasing the number of tries or the number of streams, depending on the release type.

To save time and test for a certain number of particles, the number of steps was set to 5, and tries to 1 to see how many particles that particular configuration would produce, was used. Subsequent tests were produced after inferring the number of particles desired from the baseline test.

The purpose of these simulations is to predict particle distributions flowing out of industrial glove boxes to improve worker safety. If particles being released from a glove box are within the 'respirable range' (0.1 to 10 microns) then a leak in an air system could be hazardous. If it is known how particles coming out of a glove box are distributed, then that air can be better managed.

Particles that have fallen to the floor, called the deposition, was also measured and charted. Charts presented are mass by unit area in a logarithmic scale.

4.3.1 Sphere release

In the Sphere case, particles were released outward from a spherical surface near the center of the glove box. The inlet is quite large, moving a large volume of fluid into the box, and the outlet is small and located on the top of the box, as shown in Figure 4.3.1.1.

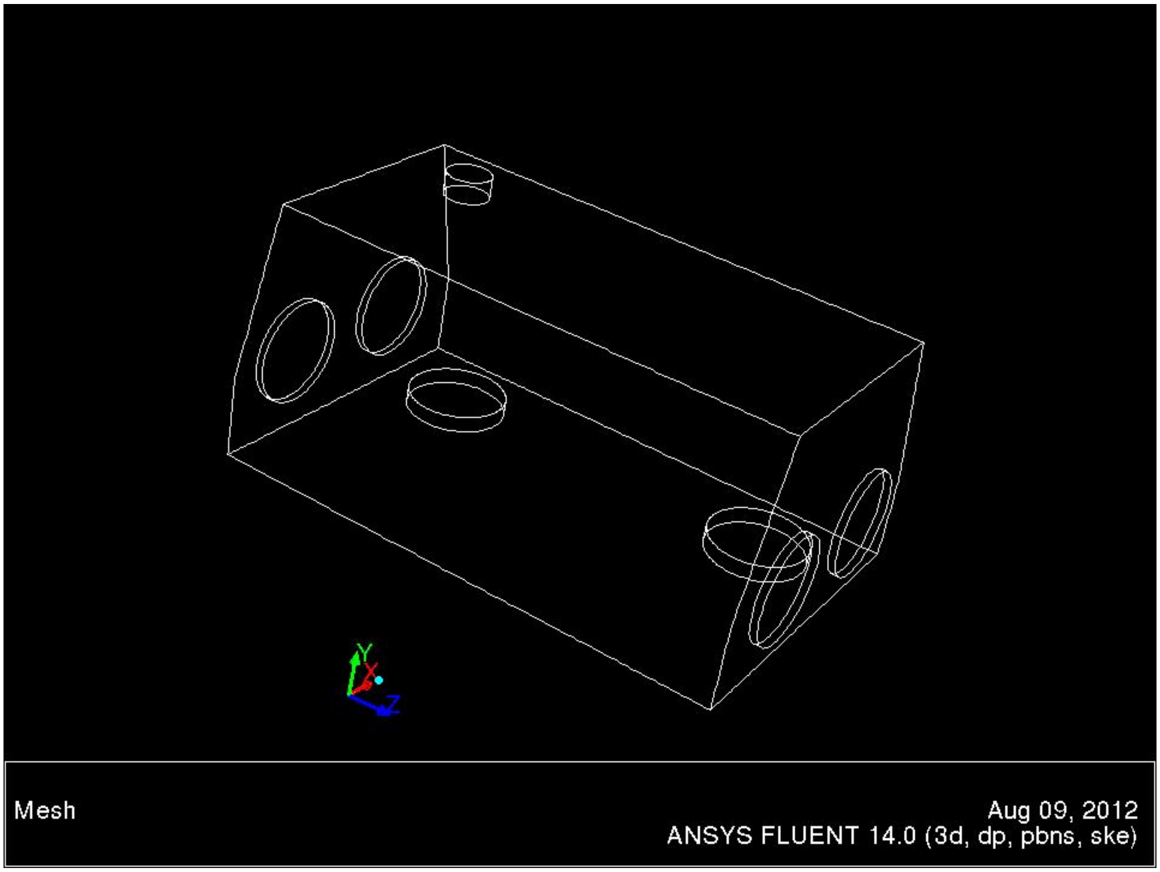

Figure 4.3.1.1

The initial baseline test, as shown in the first row of Table 4.3.1.1, the number of particles for one try was 54720. This meant that to get around 500,000 particles, 9 tries were needed, as shown in the second row of Table 4.3.1.1

Table 4.3.1.1

Trial	Steps	Diameters	Tries	Total Particles	Trapped Particles	Incomplete Particles	Escaped Particles
1	5	40	1	54720	0	54720	0
2	20000	40	9	492480	428561	555	63364
3	5	50	1	68400	0	68400	0
4	20000	50	15	1026000	859345	1512	165143
5	5	60	1	82080	0	82080	0
6	20000	60	18	1477440	1238452	2189	236799

After the desired number of particles was achieved, a plot of the deposition was created for each iteration with trapped particles. Figure 4.3.1.2 details how the particles settled on the floor of the glove box for 1 million particles.

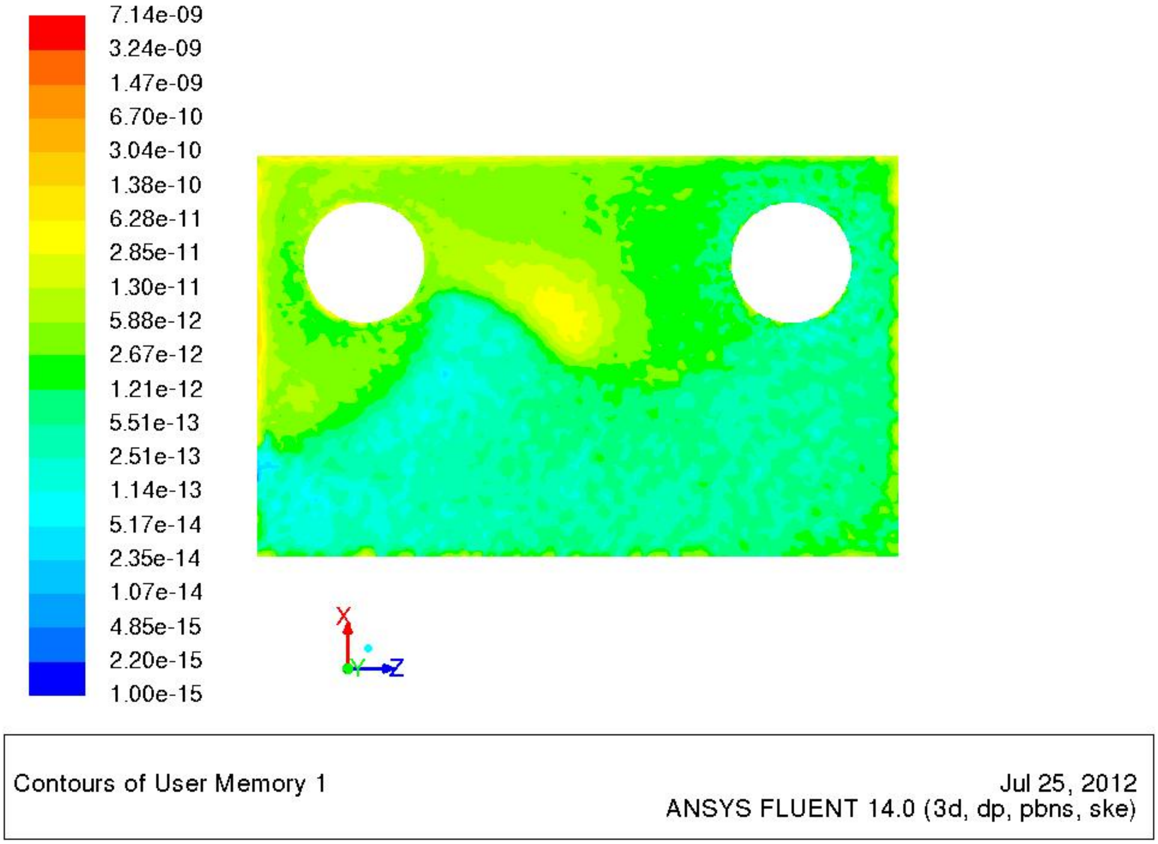

Figure 4.3.1.2

The scale in Figure 4.3.1.2 is in mass per unit area (g/m^2), and increasing the number of particles did not appreciably change the shape and concentration of particles on the floor.

The size of the particles trapped on the floor was also recorded in a histogram for each case with escaped particles. Figures 4.3.1.3, 4.3.1.4, and 4.3.1.5 show the size distribution from the floor of 500,000, 1 million, and 1.5 million particles respectively.

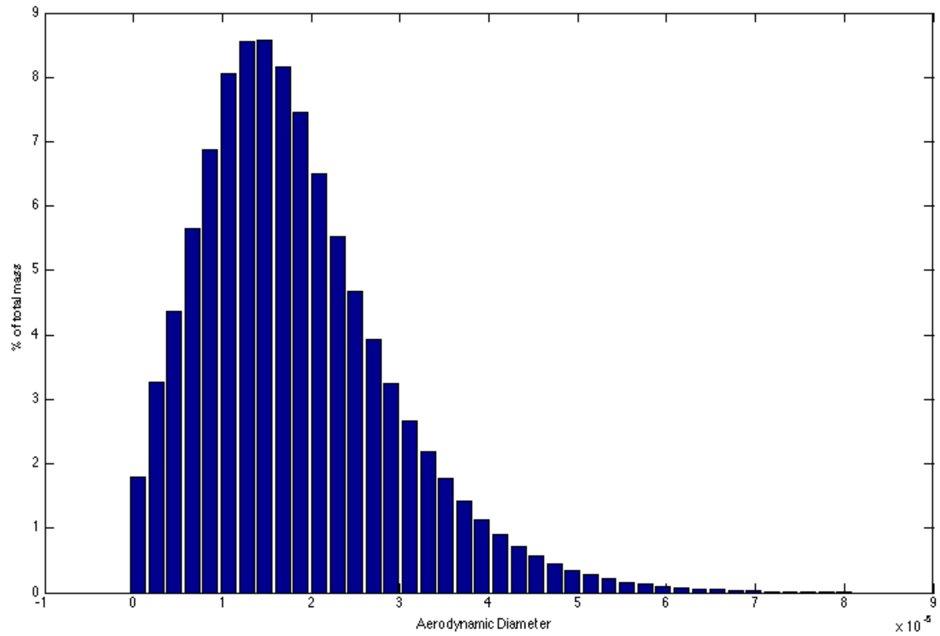

Figure 4.3.1.3, 500,000 particles

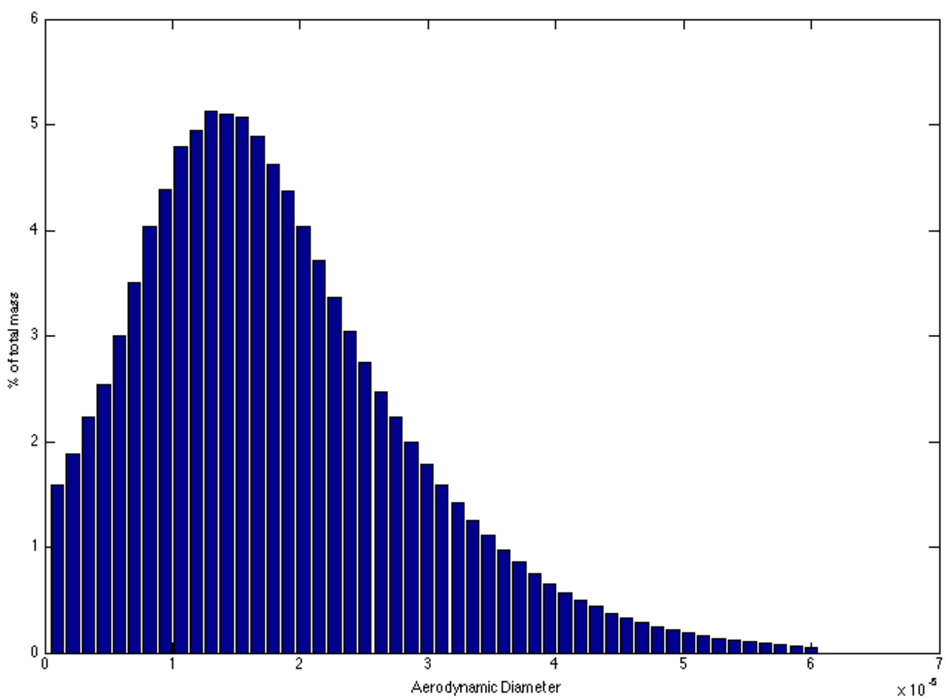

Figure 4.3.1.4, 1 million particles

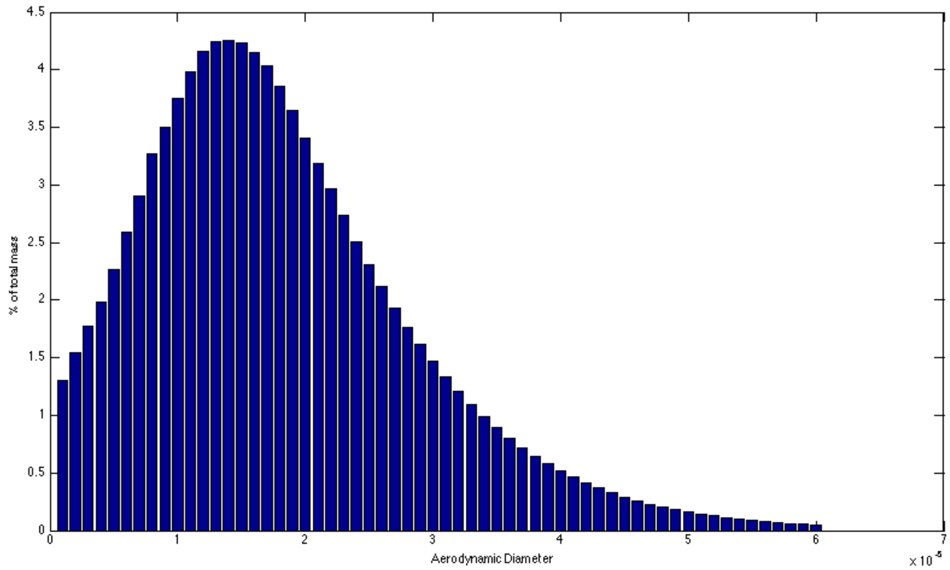

Figure 4.3.1.5, 1.5 million particles

Comparing the different plots of diameters it can be shown that the shape of the distribution does not change appreciably, however, the total distribution changes more between 500,000 particles and 1 million particles. After 1 million particles, there is a noticeably smaller change when compared to the 1.5 million particles distribution. 97% of particles released are trapped on the floor, and only smaller particles escape the box.

The distribution of particles leaving the glove box for 1 million particles is shown in Figure 4.3.1.6. In order to produce a sufficient amount of particles at the outlet, at least 1 million particles should be released.

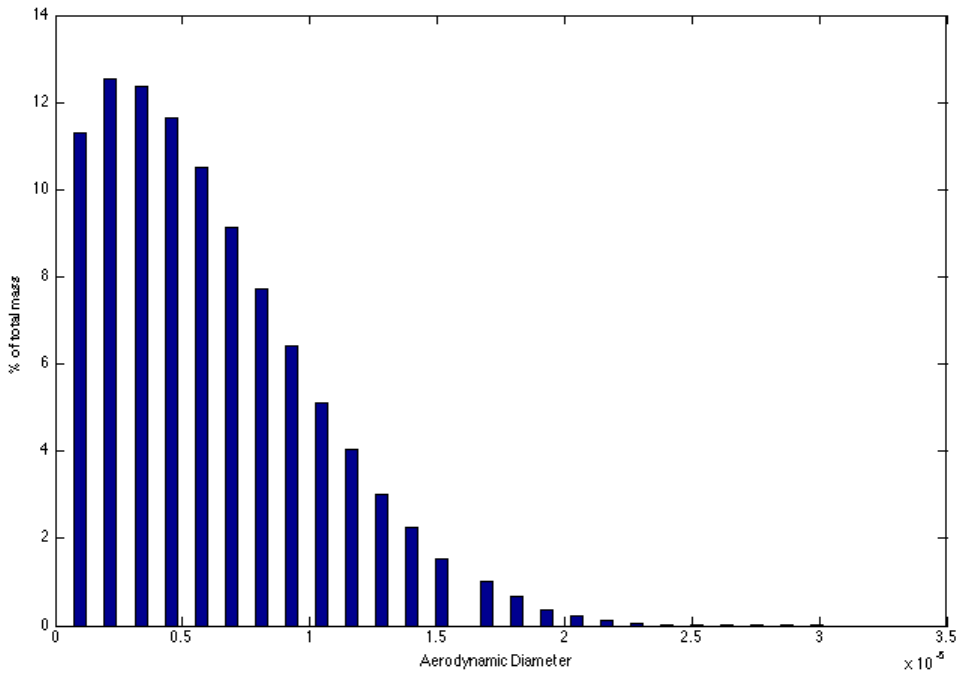

Figure 4.3.1.6, 1 million particles outlet.

The distributions for 500,000 particles and 1.5 million particles are similar to the distribution of the 1 million particles case. There was less resolution for the 500,000 particles case, and adding another 500,000 particles did not change the distribution.

Compared to the particles released from the source, the few particles that escape the glove box are smaller particles that were not heavy enough to settle out of the flow.

The majority of particles settle and deposit on the floor, and a User Defined Function (UDF) was implemented to capture data about the mass concentration of particles on the floor of the box. Functions within Fluent were used to plot the deposition data visually. The mass concentration for the 1 million particles release is detailed in Figure 4.3.1.7 below.

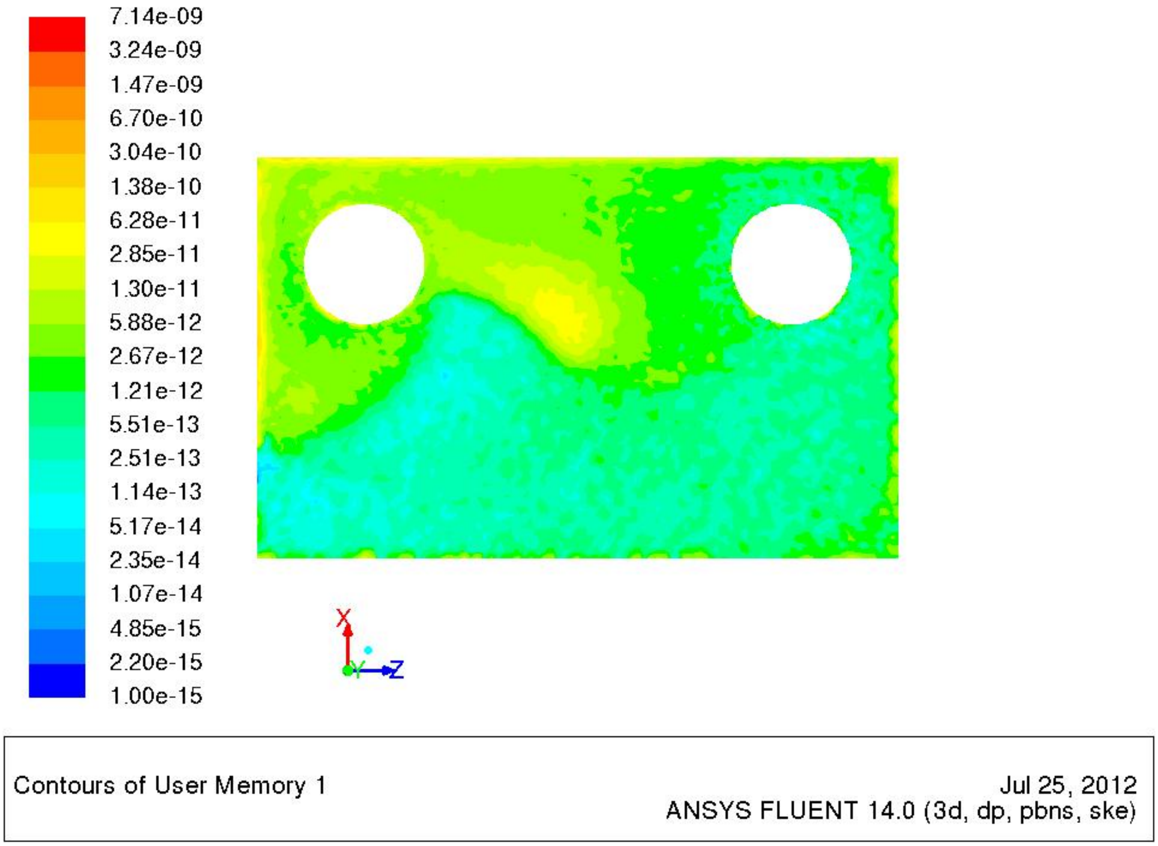

Figure 4.3.1.7, deposition of 1 Million particles

After comparing plots of particles from all three test cases, it was determined that the relative concentration of particles did not change between each case. The total concentration increased the scale for the deposition when more particles were released, but did not affect the shape or area of concentration.

4.3.2 Wheel release

For the Wheel release, particles were released on a plane in a disk, as if there was an object spinning and releasing particles. The release was a cone release, with many streams that released particles tangentially. In contrast to the sphere release, the wheel release uses a number of streams to release particles. The number of streams was varied to attempt to detect differences in particle distributions after the release. The inlet was small and in the lower corner of the box, and the outlet was on the top of the box, producing a swirling flow. The box used in the wheel release is shown in Figure 4.3.2.1.

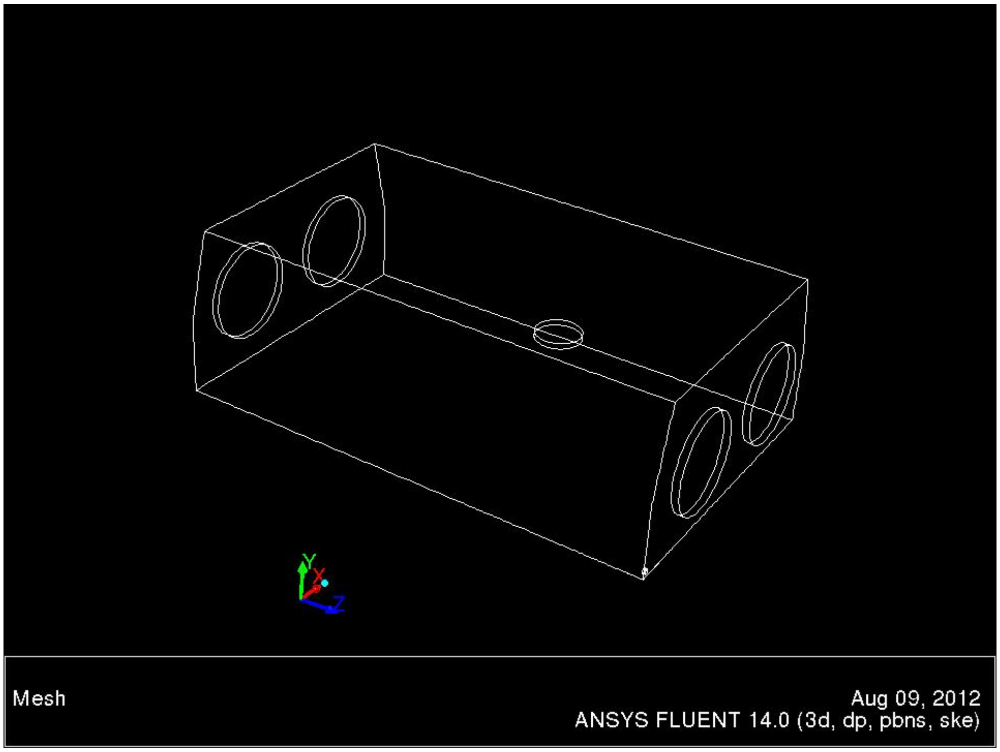

Figure 4.3.2.1

Histograms were studied to detect differences in the particle distributions because of different injection methods. A number of trials were conducted to produce results of 500,000 particles, 1 million particles and 1.5 million particles with three different numbers of streams, as shown in Table 4.3.2.1.

Table 4.3.2.1

Trial	Steps	Diameters	Streams	Tries	Particles	Trapped	Incomplete	Escaped
1	5	40	20	1	800	0	800	0
2	20000	40	20	625	500000	483262	10807	5931
3	5	50	20	1	1000	0	1000	0
4	20000	50	20	1000	1000000	968296	20667	11037
5	5	60	20	1	1200	0	1200	0
6	20000	60	20	1250	1500000	1453889	29948	16163
7	5	60	50	1	3000	0	3000	0
8	20000	60	50	167	501000	485665	9941	5347
9	20000	60	50	333	999000	968384	20012	10604
10	20000	60	50	500	1500000	1453771	30242	15987
11	5	60	75	1	4500	0	4500	0
12	20000	60	75	111	499500	484103	10050	5347
13	20000	60	75	222	999000	968153	20065	10782
14	20000	60	75	333	1498500	1452957	29358	16185

For all trials, a plot of the deposition and histograms of particles on the floor and particles that escaped the outlet were created in Fluent. Trends in outlet and deposition distributions were studied to determine a sufficient sample size. The difference in size distribution due to changes in the set up was studied. Three different methods were used to create test cases for 500,000 particles, 1 million, and 1.5 million particles with the wheel release.

The first test case was with 20 streams of particles, which required many tries to achieve the desired number of particles. The deposition for the 1 million particles with 20, 50, and 75 streams test cases are shown in Figure 4.3.2.2, Figure 4.3.2.3, and Figure 4.3.2.4 respectively.

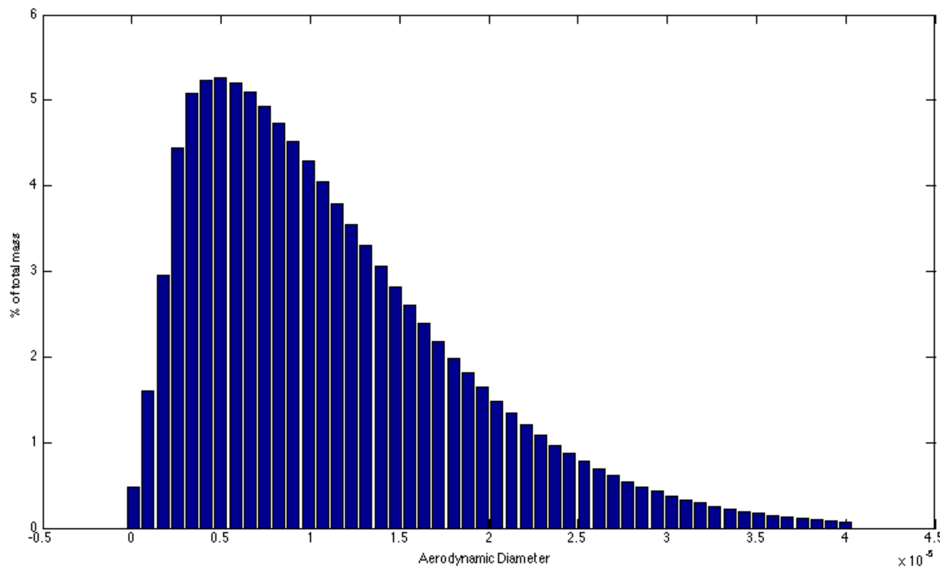

Figure 4.3.2.2, 20 streams, 1 million particles.

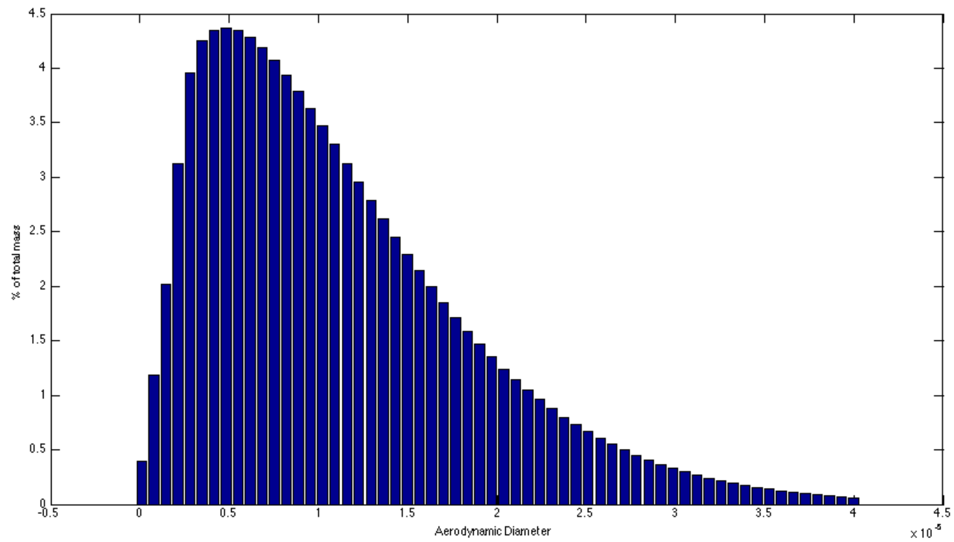

Figure 4.3.2.3, 50 streams, 1 million particles

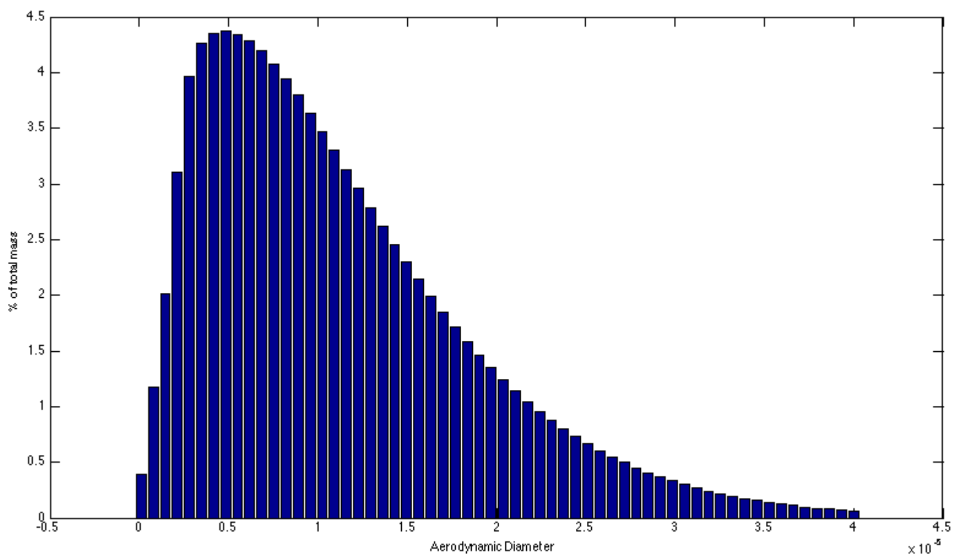

Figure 4.3.2.4, 75 streams, 1 million particles

The difference in heights of the first two histograms is due to the fact that the number of diameters changed between trials. More diameters mean that each bin has less of the total mass. The difference in the histograms between 50 streams and 75 streams is negligible; there is no noticeable difference in particle production methods. The time required to complete the computation is less when more streams are used.

Also studied were the particles leaving the outlet of the glove box. Because the majority of particles, around ninety-seven percent, settle to the floor, and the production of particles is limited to around 50 or 60 sizes, the size of the distributions leaving the glove box is limited, as shown in Figure 4.3.2.5.

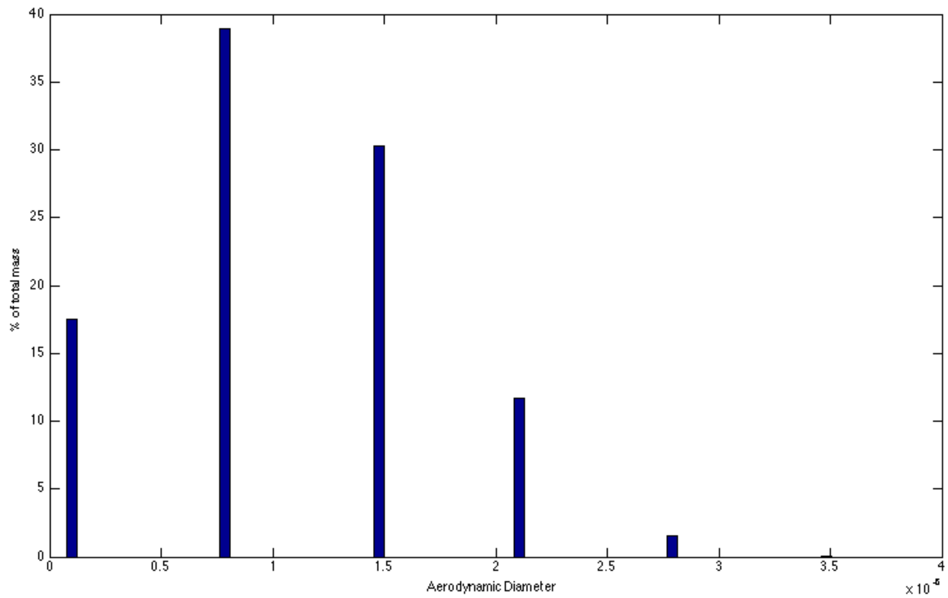

Figure 4.3.2.5, 75 streams, 1 million particles outlet.

Most of the larger particles have settled to the floor, and only smaller particles remain to leave the glove box system. There are only a few histogram bins shown here because of the limits of the production of particles in Fluent. Particles in the respirable range (<10 microns) still remain here and are a hazard if a leak were to occur.

5.0 Conclusion

The production of particles in ANSYS Fluent can be facilitated in a number of different ways, and the method of that production wide and varied. For the modeling of Aerosol particles in Fluent, the Rosin-Rammler distribution is an in-exact but close estimate of popular particle distributions. Rosin-Rammler distributions are built into Fluent and no UDF attachment is available, therefore it is the only distribution model available.

When modeling particles in a glove box-sized environment, about a million particles is necessary to provide statistically relevant data for analysis. Using fewer particles will produce variations in results because of the resolution of the data. One should also be aware of the use of the number of diameters for the Rosin-Rammler distribution. A sufficient number of diameters for particle capture was shown to be 50 or 60; fewer than that and graphs become further apart and difficult to analyze. Using more particles may be prudent in a more complicated environment, however, for this model it was unnecessary.

It is still not completely understood how Fluent handles the particle data, but a better understanding has been achieved through a careful study. All evidence points to the use of a mass distribution within Fluent, which does not account for the large number of particles present in the lower-regions of distributions.

Overall, a method for aerosol data sampling and modeling has been produced. Fluent can be made to accept values for distributions for many types of aerosols to be modeled. An amount of around 1 million particles should be used to model the particle behavior without much computational time, with good resolution of the results. With a combination of MATLAB and Fluent, a predictive model of a glove box environment for health-physics applications can be produced.

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