Simulation of Aerosol Flow in a Nose-only Inhalation Exposure System using Ansys Computational Fluid Dynamics (CFD) Software

Seonggi Min[1], Dong-Jin Yang[1], Jae-Hyun Kim[1], Jinghai Yi[1], Gregory Pellar[1], Susan Chemerynski[2], Steven B. Yee[2], Reema Goel[2], Pamela Roque[2], and Prabha Kc[2]

[1] National Center for Toxicological Research, U.S. Food and Drug Administration, Jefferson, AR
[2] Center for Tobacco Products, U.S. Food and Drug Administration, Silver Spring, MD

Abstract

Inhalation chambers are widely used for evaluating the toxicity of chemicals in aerosols, including particulate matter. Ensuring consistent and uniform spatial distribution of aerosols within the inhalation chamber is crucial for accurately assessing toxicity. The CTP/NCTR Inhalation Toxicology Core Facility uses a 5-tier (10 ports/tier) nose-only inhalation exposure system in animal studies. Previous studies have investigated the air flow dynamics within the inhalation chamber. However, the impact of the flow on the concentration and distribution of aerosols is not fully understood. In this study, we used the Ansys CFX 17.2 computational fluid dynamics software to simulate the trajectories and distribution of aerosols across all tiers and ports of the inhalation chamber. A cylindrical rod (crown shaped at the top to minimize air resistance) was inserted into the inhalation chamber. A tier without any output ports was added on the top of the 5th tier of the inhalation chamber to help equilibrate the pressure distribution.

Simulation of aerosol flow (75% propylene glycol/25% water) was performed with 25 rods of varying sizes using k-ω shear stress transport turbulence and discrete phase models. The 5 rods with the smallest relative standard deviation of aerosol flow in the simulation were selected for experimental testing. The aerosol spatial distributions were compared from 8 ports across all 5-tiers of the inhalation chamber simultaneously. Aerosols were generated using a collision nebulizer at 25 LPM of air flow. The rod sizes selected were 40x35, 40x40, 40x45, 40x50, and 45x45 mm.

The difference of aerosol flow between the simulation and experimental results ranged between 0.7-10.44% for all the 5 selected rods. Aerosol concentration throughout the study was within 90-110% of the average value. Overall, this work supports the utilization of simulations in the development of homogenous aerosol flow for uniform dosing in animal inhalation exposures.

Inhalation Exposure System

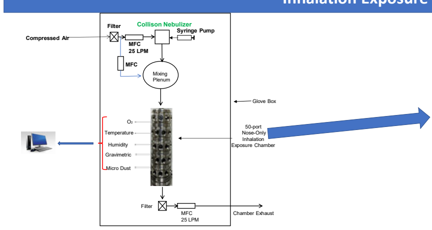


Figure 1. Diagram of the nose-only inhalation (NOI) exposure system. Six 5-tier NOI exposure chambers are used. Each NOI exposure system consisted of (1) an aerosol generation system, (2) a 50-port NOI exposure chamber (10 ports per tier), and (3) a test atmosphere control and monitor system.

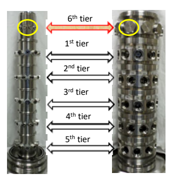


Figure 2. 6-tier NOI exposure tower [inner shell (left) and outer shell (right)]. A 5-tier system produced inhomogeneous aerosol flow at each tier. An insertion of a rod in the inner space and addition of a sixth tier (with all ports closed) were hypothesized to create homogenous aerosol flow throughout the NOI exposure system.

Simulation

1. Software : Ansys CFD 17.2 (Ansys Inc., San Jose, CA)
2. Simulation model : k-w SST, Discrete phase model (DPM)
3. Mesh number : 17,573,004 (30x30 mm rod) – 11,974,245 (50x50 mm rod)
4. 25 size rods (eMachineshop, Mahwah, NJ)

Top Diameter (mm)	30	35	40	45	50
Bottom diameter (mm)	30	30	30	30	30
	35	35	35	35	35
	40	40	40	40	40
	45	45	45	45	45
	50	50	50	50	50

Table. 1. Simulation using Ansys CFD 17.2 software and 25 different rod sizes.

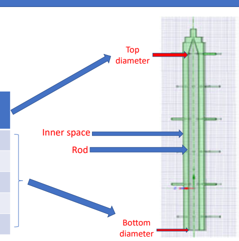


Figure 3. Diagram of aerosol flow space within the simulation.

Measurement

1. Liquid : Propylene glycol (PG) 75% + Water 25 %
2. 25 LPM of input air flow + collision nebulizer
3. Collecting aerosol from 8 ports (2 ports at 1st tier, 2 ports at 2nd tier, 1 port at 3rd tier, 1 port at 4th tier, and 2 ports at 5th tier) simultaneously. The weight of aerosol was measured, then the aerosol concentration was calculated.

Results

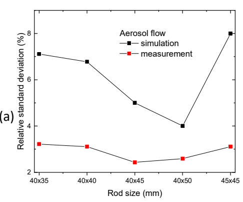
Bottom Diameter	Top Diameter : 30 mm Average Aerosol Concentration (mg/L)	Standard Deviation (STD)	Relative STD (%)	Top Diameter : 35 mm Average Aerosol Concentration (mg/L)	Standard Deviation (STD)	Relative STD (%)
30 mm	9.31	1.63	16.21	9.72	1.49	15.28
35 mm	9.96	1.41	14.21	9.64	1.33	13.81
40 mm	10.04	1.41	14.02	9.71	1.22	12.54
45 mm	10.11	1.44	14.23	10.53	2.97	28.17
50 mm	10.11	1.51	14.91	9.64	1.20	12.47

Bottom Diameter	Top Diameter : 40 mm Average Aerosol Concentration (mg/L)	Standard Deviation (STD)	Relative STD (%)	Top Diameter : 45 mm Average Aerosol Concentration (mg/L)	Standard Deviation (STD)	Relative STD (%)
30 mm	10.18	0.97	9.55	10.28	1.05	10.23
35 mm	10.16	0.72	7.11	10.51	1.08	10.29
40 mm	10.14	0.69	6.77	10.52	0.98	9.27
45 mm	10.19	0.51	5.00	10.30	0.82	7.96
50 mm	10.18	0.41	4.04	10.21	0.86	8.41

Bottom Diameter	Top Diameter : 50 mm Average Aerosol Concentration (mg/L)	Standard Deviation (STD)	Relative STD (%)
30 mm	10.67	1.78	16.67
35 mm	10.68	1.71	15.97
40 mm	10.65	1.53	14.32
45 mm	10.63	1.27	11.96
50 mm	10.29	1.52	14.80

Table 2. Average simulation aerosol concentration results, with standard deviation (STD) and relative standard deviation (RSD), for the 25 rods.

(a)



Rods	Relative STD (%) Simulation	Measurement
40x35 mm	7.11	3.22
40x40 mm	6.77	3.11
40x45 mm	5.00	2.43
40x50 mm	4.04	2.59
45x45 mm	7.96	3.11

Figure 4 (Left) and Table 3 (Right). The relative standard deviation with 25 size rods. From these results, the 5 rods (40x35, 40x40, 40x45, 40x50, and 45x45) that show the smallest standard deviation were selected.

Rod 40x35 mm	Relative Aerosol Concentration (%) Simulation	Measurement
1st	99.21	102.32
2nd	90.65	98.06
3rd	96.49	92.98
4th	108.58	98.14
5th	105.07	101.40

Rod 40x40 mm	Relative Aerosol Concentration (%) Simulation	Measurement
1st	100.21	100.93
2nd	92.18	97.52
3rd	94.94	92.78
4th	108.72	99.79
5th	103.95	102.43

Rod 40x45 mm	Relative Aerosol Concentration (%) Simulation	Measurement
1st	100.93	102.02
2nd	94.96	96.15
3rd	97.66	94.85
4th	104.82	100.76
5th	101.64	100.30

Rod 40x50 mm	Relative Aerosol Concentration (%) Simulation	Measurement
1st	103.51	98.78
2nd	98.13	97.05
3rd	99.06	105.95
4th	102.83	100.23
5th	96.48	99.83

Rod 45x45 mm	Relative Aerosol Concentration (%) Simulation	Measurement
1st	94.01	99.29
2nd	97.92	94.27
3rd	106.85	102.98
4th	109.67	102.54
5th	91.55	100.67

Table 4. Relative aerosol concentration of simulation and measurement results at each tier for (a) 40x35 mm, (b) 40x40 mm, (c) 40x45 mm, (d) 40x50 mm, and (e) 45x45 mm rods.

Conclusions

1. The simulation was successfully completed using 25 different size rods.
2. The 40x35 mm, 40x40 mm, 40x45 mm, 40x50 mm, and 45x45 mm rods were selected to measure the aerosol flow.
3. Simulation results and measurement results are very similar (trend) but are not exactly the same.
4. The difference of aerosol flow between the simulation and experimental results ranged between 0.7-10.44 % for all the 5 selected rods.
5. Aerosol concentration throughout the study was within 90-110 % of the average value.
6. Overall, this work supports the development of homogenous aerosol flow for uniform dosing in animal inhalation exposure.