Multi-fidelity Computational Fluid Dynamics of Aerosolized Viral Load Dispersion in the context of the COVID-19 Pandemic

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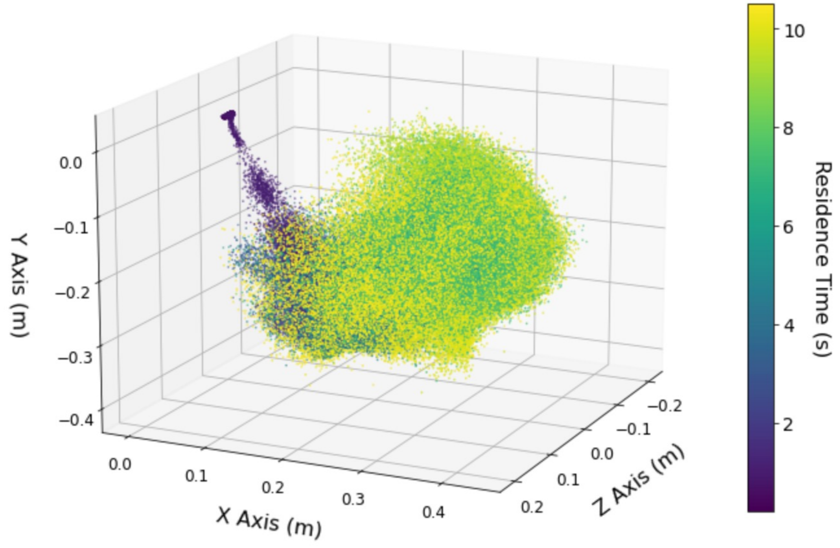

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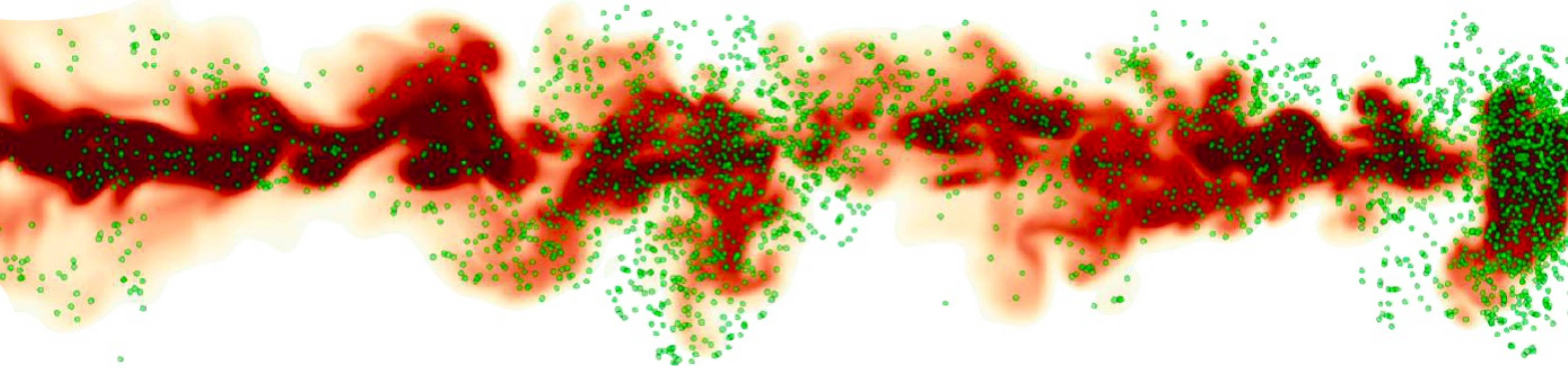


Figure 1

Objective

- COVID-19 spreads predominantly through aerosols and droplets via the air
  - Ease of access to lower fidelity software has left CFD center stage
- **Demonstrate the future potential merits of "multi-fidelity" CFD with regards to the COVID-19 pandemic and future**
  - **Is low fidelity CFD software designed for higher velocity flows able to be utilized in modeling lower velocity respiratory events?**
  - **Ability to streamline decision-making process regarding safety guidelines in urgent times, when the ability to wait for higher fidelity results is not an option**

Figure 1: "Turbulent Gas Clouds and Respiratory Pathogen Emissions: Potential Implications for Reducing Transmission of COVID-19 | Infectious Diseases | JAMA | JAMA Network." https://jamanetwork.com/journals/jama/fullarticle/2763852 (accessed Jan. 15, 2021).
[1] G. Pascarella et al., "COVID-19 diagnosis and management: a comprehensive review," Journal of Internal Medicine, vol. 288, no. 2, pp. 192–206, 2020, doi: 10.1111/joim.13091.

Background: Transmission, Structure and Behavior

- Airborne transmission - two infection mechanisms:
  - ‘Close’ infection due to large droplets
  - ‘Distant’ infection due to small droplets
- Most droplets expelled evaporate within a few seconds to form droplet nuclei **(aerosols)**
  - Suspended in air for hours
  - Half-life of airborne virions/viral load necessary for contraction is still under debate

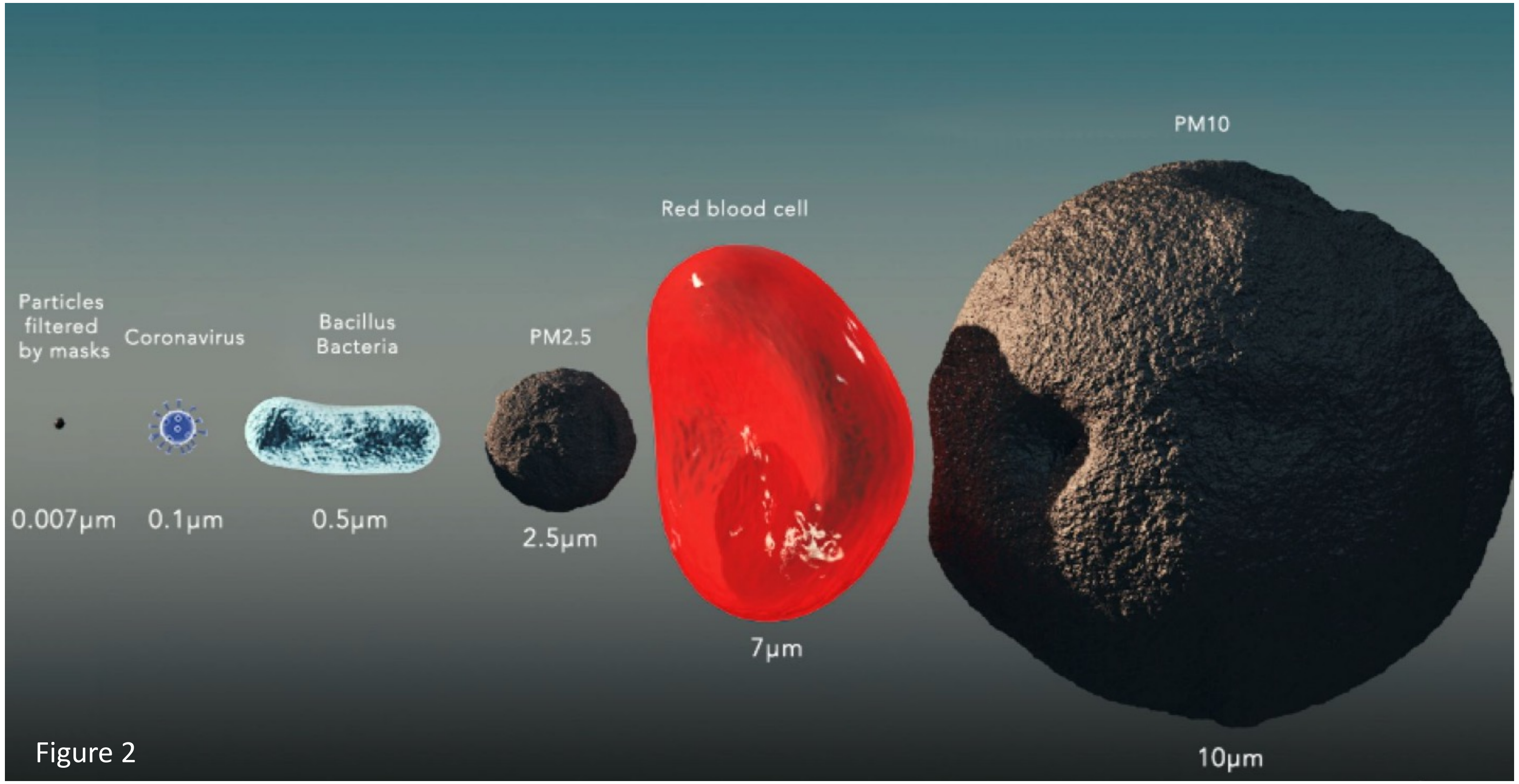


Figure 2

Figure 2: N. Zhu *et al.*, “A Novel Coronavirus from Patients with Pneumonia in China, 2019,” *N Engl J Med*, vol. 382, no. 8, pp. 727–733, Feb. 2020, doi: 10.1056/NEJMoa2001017.
[2] G. Seminara, B. Carli, G. Forni, S. Fuzzi, A. Mazzino, and A. Rinaldo, “Biological fluiddynamics of airborne COVID-19 infection,” Rend Lincei Sci Fis Nat, pp. 1–33, Aug. 2020,52 doi: 10.1007/s12210-020-00938-2.

Computational Fluid Dynamic Methods

- **Computational fluid dynamics (CFD)** is a division of fluid mechanics that utilizes numerical analysis and data structures to evaluate and resolve problems involving fluid flows
    - Reynolds-Averaging Navier Stokes (RANS)
    - Large Eddy Simulation (LES)
    - Direct Numerical Simulation (DNS)
- Low Fidelity vs. High Fidelity
    - RANS: ~ 13 hours
    - DNS: ~ 200+hours
    - For only 11.4s of flow time!

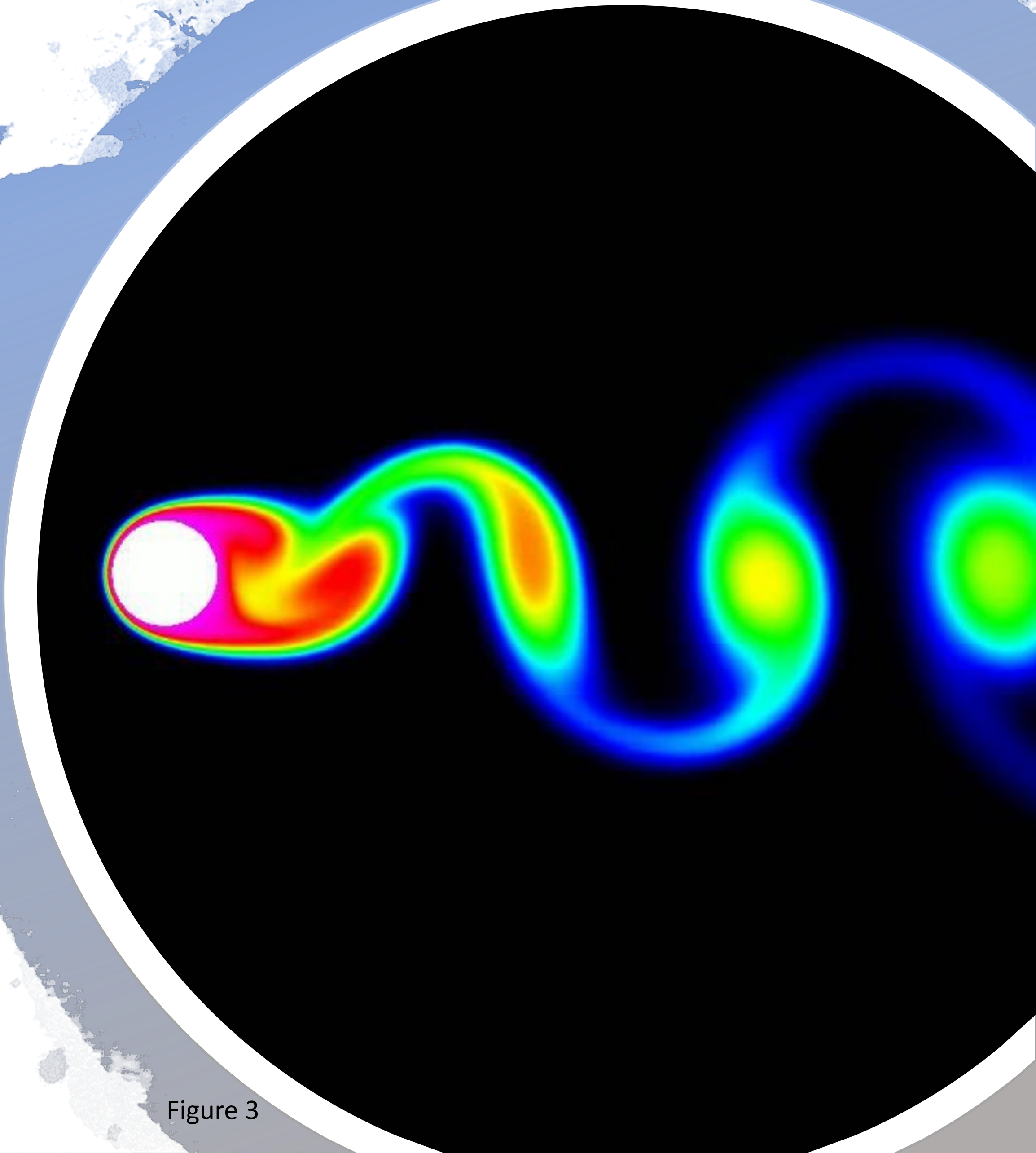
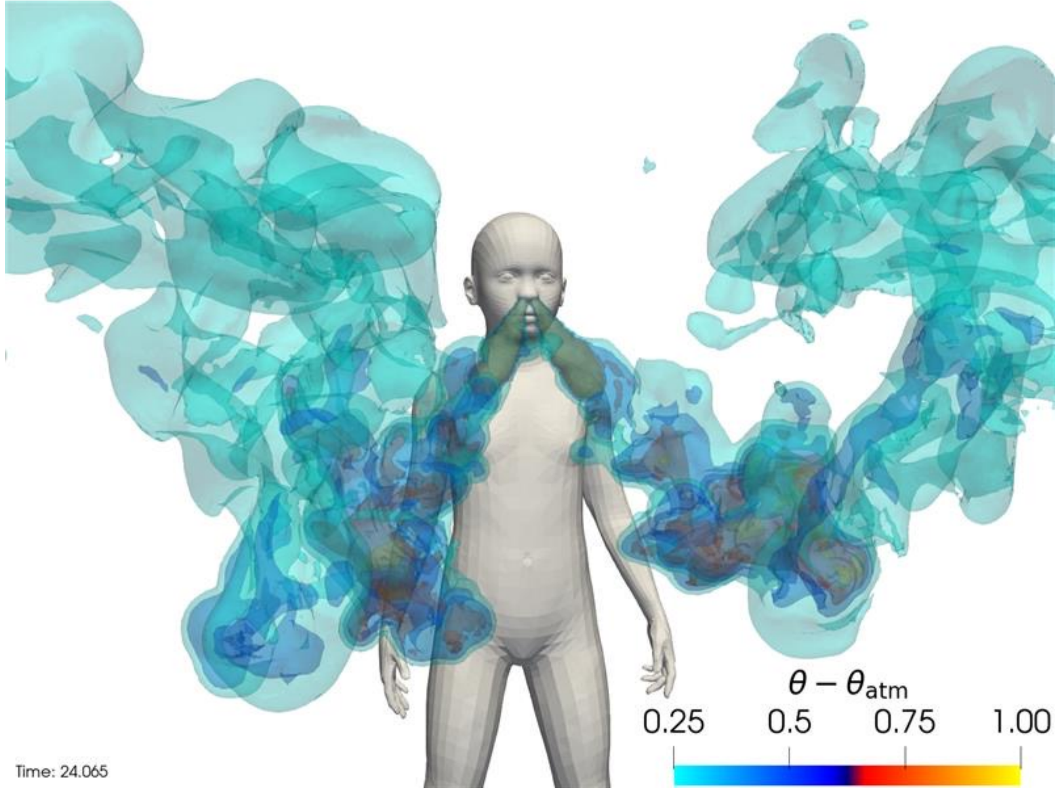


Figure 3

Figure 3: DolfynNet, *Von Karman vortex street (laminar, temperature), Re = 250*. 2010.

High Fidelity Further Explained

- Yales2 is a High Fidelity Large Eddy Simulation (HFLES)
    - Essentially simulates the larger eddies that contribute to most to the energy of turbulence
    - The contribution of smaller scales is also modeled
- Higher demands…
    - Conservation of energy
    - Multiphysics
    - Scaling



[3] High Fidelity CFD against COVID-19, Y. Dubief, et al

RANS Further Explained

- Reynolds Stress arises from Reynolds averaging process
  - RANS - EQ: (1)
  - Must be solved to close the equations
- Two most common methods
  1. Boussinesq Hypothesis (EQ: 2)
     - Calculate dynamic eddy viscosity (μ_t)
  2. Reynolds Stress Model (RSM)
     - Solves transport equations, greater CPU cost

$$\frac{\partial(\rho U)}{\partial t} + \nabla\cdot(\rho U U) = -\nabla p + \nabla\cdot[\mu(\nabla U + (\nabla U)^T)] + \rho g - \nabla\left(\frac{2}{3}\mu(\nabla\cdot U)\right) \underbrace{-\nabla\cdot(\rho\bar{U}'\bar{U}')}_{\text{Reynolds-Stress}} \qquad (1)$$

$$\underbrace{-\rho\bar{U}'\bar{U}'}_{\text{Reynolds-Stress}} = \overbrace{\mu_t}^{\text{Turbulent Dynamic Viscosity}} \underbrace{(\nabla U + (\nabla U)^T)}_{\text{Mean Velocity Gradient}} - \frac{2}{3}\rho k I - \frac{2}{3}(\nabla\cdot U) I \qquad (2)$$

Simulation Methodology

- Simulate nose-breathing as closely as possible
- 8 breath cycles, exhalation only
  - 0s - 1.8s exhalation
  - 1.8s – 2.7s 0 velocity (inhalation)
  - 2.7s – 2.85s 0 velocity (rest)
- Aerosols injected for first four breaths
  - Four breaths each given 11.4s to evolve
- Parameters of interest
  - XYZ Position
  - XYZ Velocity
- Species Transport: Air and Steam
  - Nose Jet: 308.15 K, 0.012 mass fraction H_2O

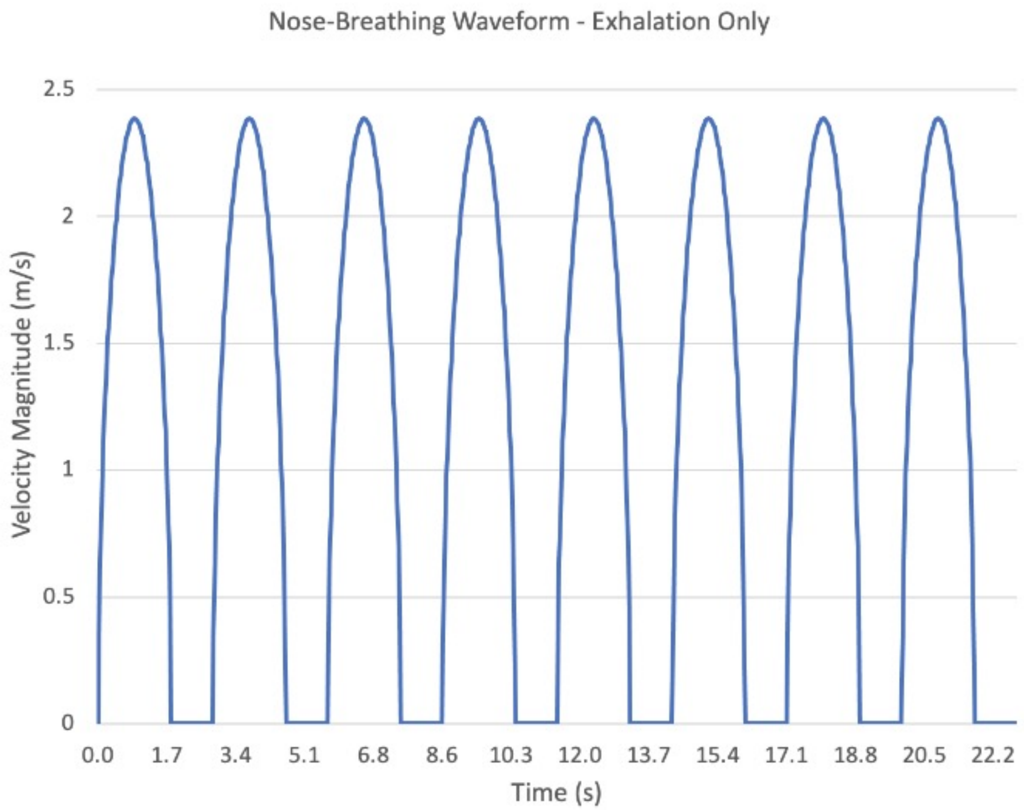
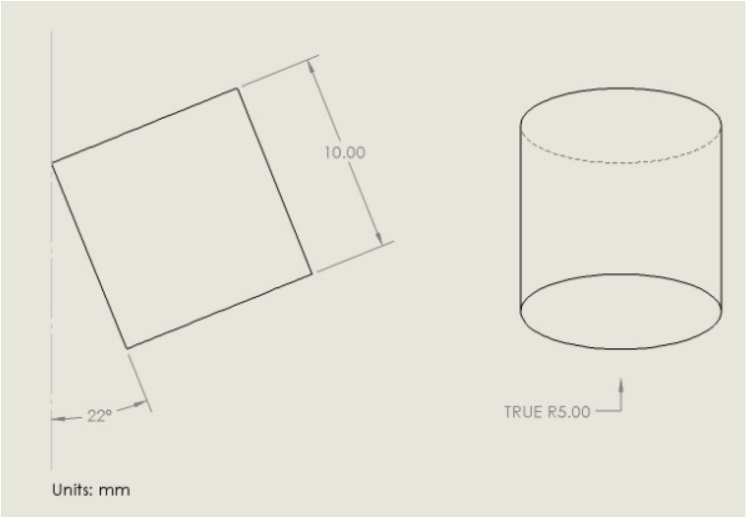


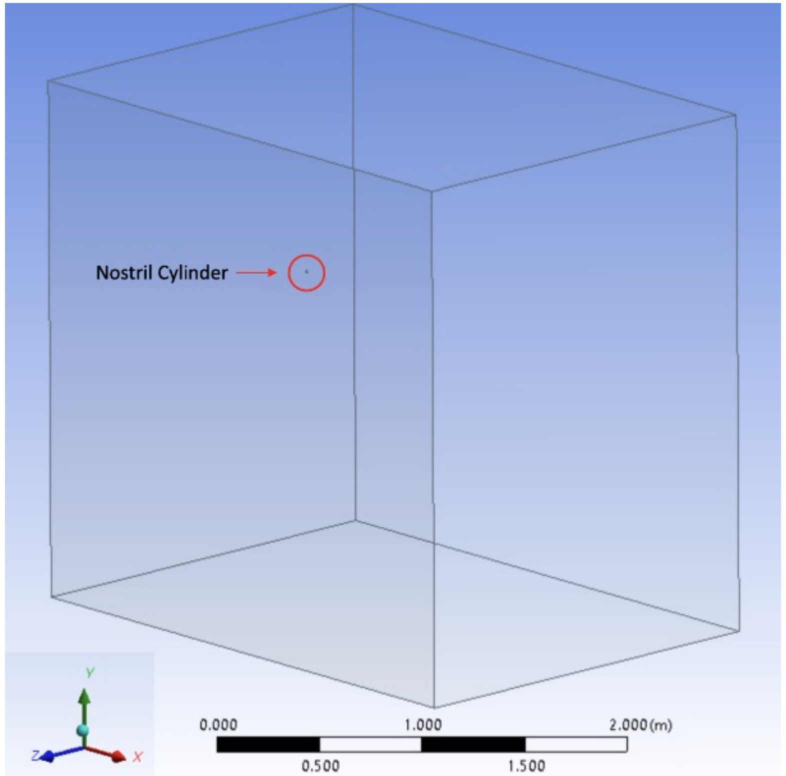
Figure 8: Nose-Breathing Waveform

[5] Zhang, G. Guo, C. Zhu, Z. Ji, and C.-H. Lin, "Transport and trajectory of cough-induced bimodal aerosol in an air-conditioned space," Indoor and Built Environment, p. 1420326X20941166, Jul. 2020, doi: 10.1177/1420326X20941166.

Physical Model

- Single cylinder sized and oriented to represent a human nostril
  - Height: 1.6m
- Enclosure that allows for full dispersion
  - 14.512 m^3

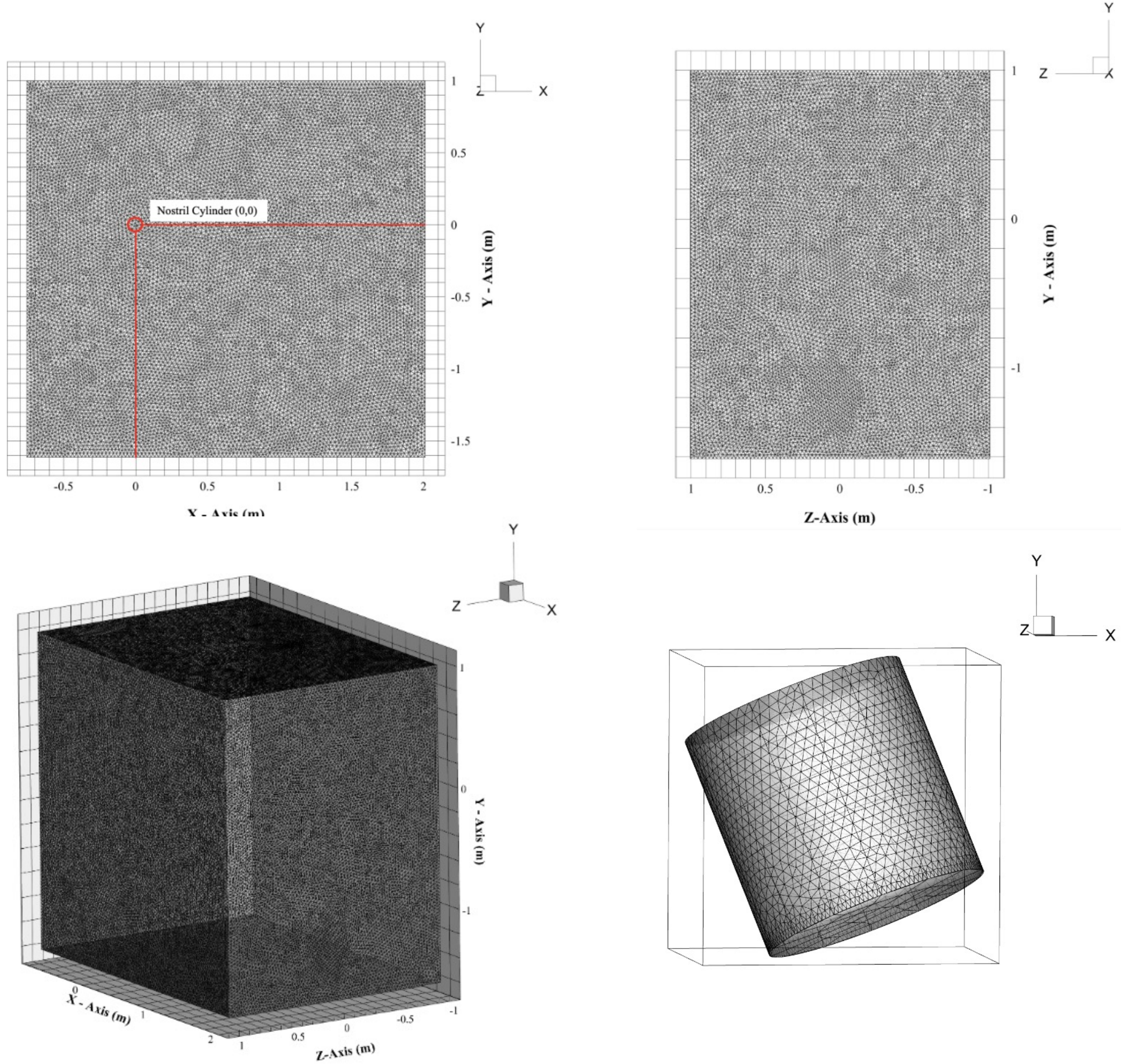




[3] Schriever, Valentin & Hummel, Thomas & Lundström, Johan & Freiherr, Jessica. (2012). Size of nostril opening as a measure of intranasal volume. Physiology & behavior. 110-111. 10.1016/j.physbeh.2012.12.007.

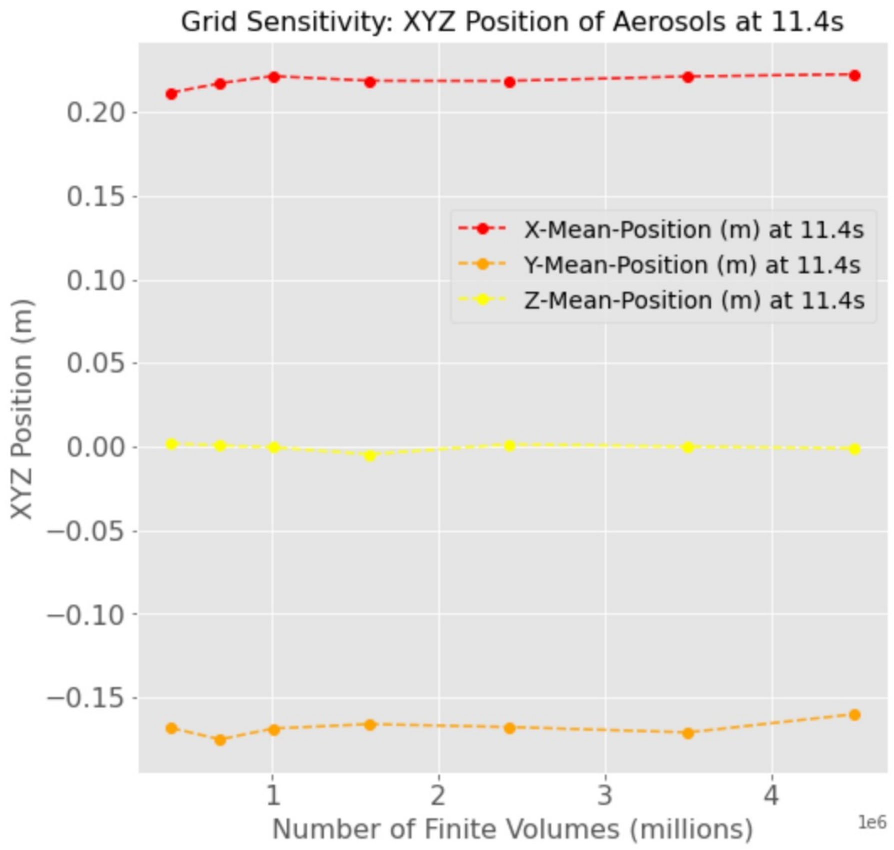
Computational Domain

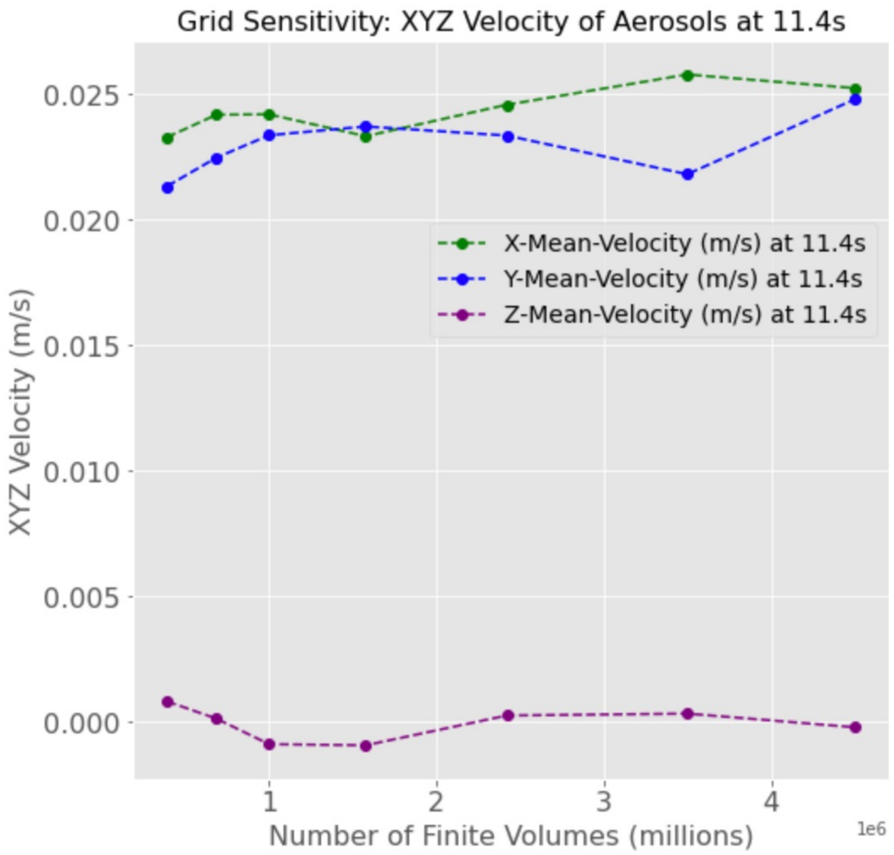
- Unstructured 3D mesh
- Approximately 1.5 million elements
- Finer mesh controls implemented on cylinder
- Coarser mesh sizing surrounding domain



Grid Sensitivity and Timestep Check

- Grid sensitivity performed to ensure effectiveness of mesh
- Timestep comparison of 0.0001 and 0.1 was also performed to check for major differences between time step sizes





Numerical Methods

- Solver: Pressure Based
- Velocity Formation: Absolute
- Time: Transient
- Gravity: ON -9.8 m/s^2
- Species Transport Model: ON
- Discrete Phase Model: ON
- Pressure-Velocity Coupling: Coupled
- Spatial Discretization:
  - Gradient: Least Squares Cell Based
  - Pressure: PRESTO!
- Transient Formulation: 1st Order Implicit
- Time Step Size: 0.0285
- Time Step Number: 700
- Max Iterations per Time Step: 75
- Flow Courant Number: 200

Numerical Methods Cont.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\epsilon - Y_M + S_k \qquad (3)$$

Time — Convection — Diffusion — Sources and Sinks

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_i}(\rho u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial \epsilon}{\partial x_j}\right] + C_{1\epsilon}\frac{\epsilon}{k}(G_k + C_{3\epsilon}G_b) - C_{2\epsilon}\rho\frac{\epsilon^2}{k} + S_\epsilon \qquad (4)$$

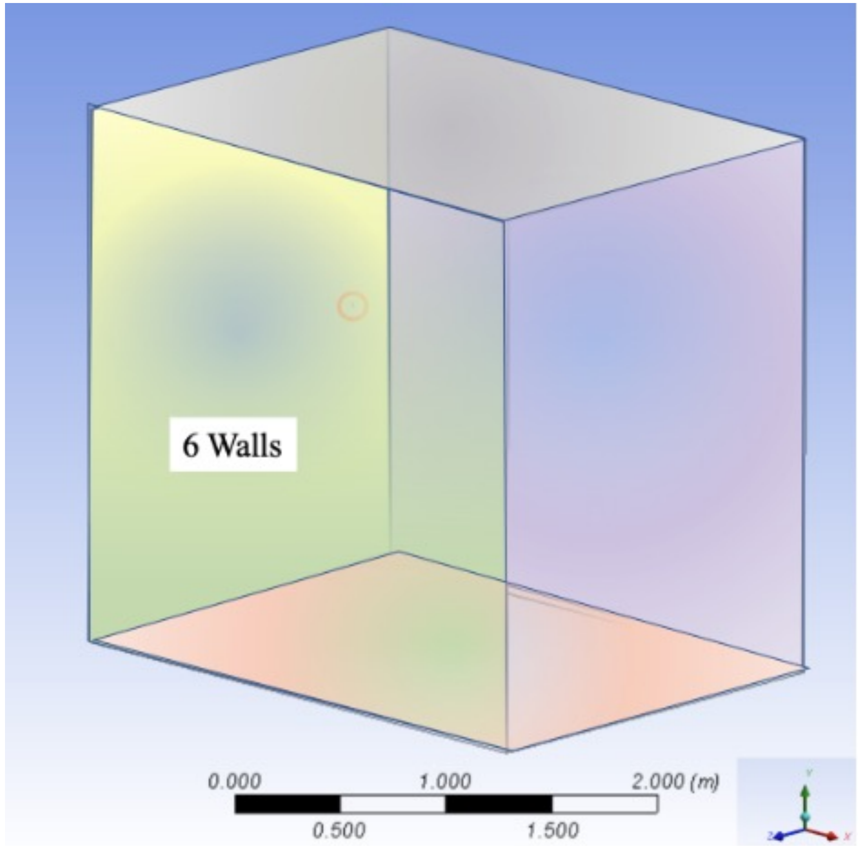
Time — Convection — Diffusion — Sources and Sinks

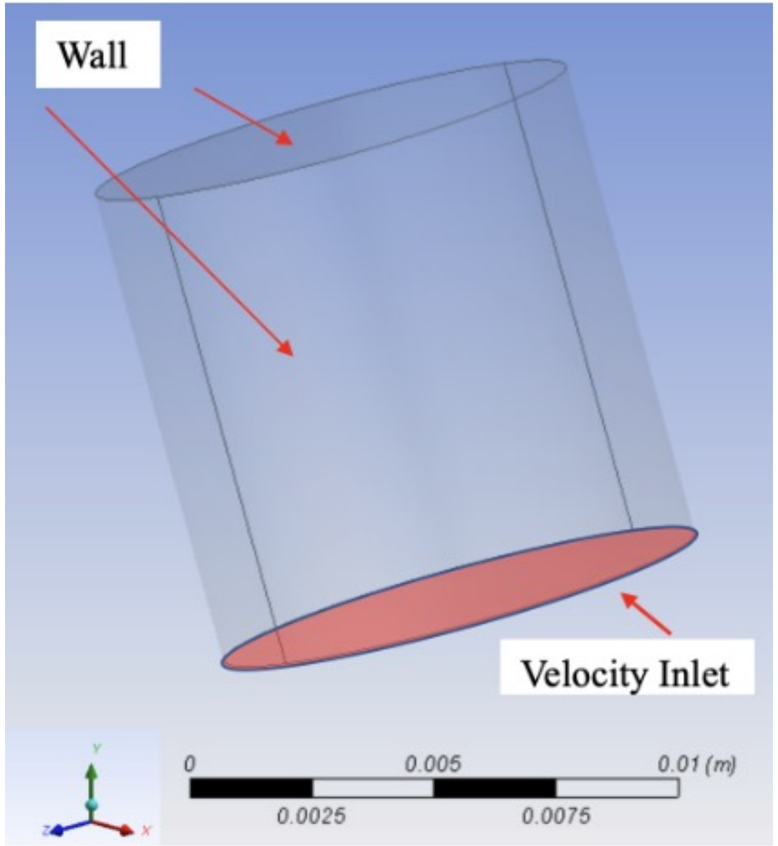
- Turbulence model: Standard K-Epsilon
  - Free shear flows, small pressure gradients, wall action not of concern
  - Transport EQs for kinetic energy (3) and turbulent dissipation rate (4)

[4] "ANSYS FLUENT 12.0 Theory Guide - 4.5.1 Standard - Model."
https://www.afs.enea.it/project/neptunius/docs/fluent/html/th/node66.htm (accessed Dec. 02, 2020).

Initial Conditions

- Walls
  - Adiabatic
  - No Slip
  - Trap DPM condition
- Velocity Inlet:
  - Bottom of cylinder
  - Escape DPM condition
  - UDF Profile
- Injection Surface
  - Bottom of cylinder
- Ambient Temp: 293.15K

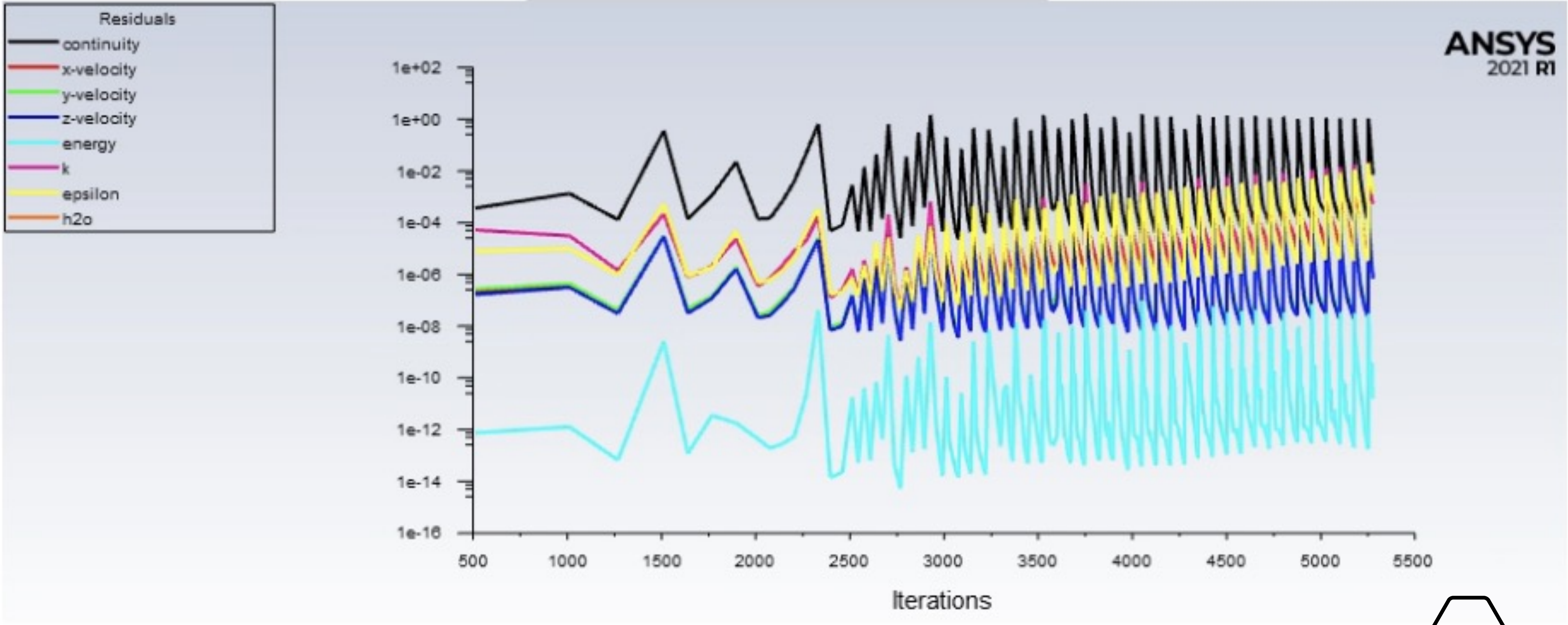




Droplet Tracking Model

- ANSYS Fluent Discrete Phase Model (DPM)
- One-Way Coupling
- Aerosol Properties
  - Diameter: 0.1 micron
  - Inert H_2O particles
  - Mass Flow Rate: 9.40e-15 kg/s
  - Temperature: 300K
  - Follow velocity profile for timing
- Spherical Drag Law
- Discrete Random Walk Model

Breath Number	Duration of Total Breath Cycle (s)	Particles Injected?
1	0s - 2.85s	Yes (0s -1.8s)
2	2.8785s - 5.7s	Yes (2.8785s - 4.6455s)
3	5.7285s - 8.55s	Yes (5.7285s - 7.4955s)
4	8.5785s - 11.4s	Yes (8.5785s - 10.3455s)
5	11.4285s - 14.25s	No
6	14.2785s - 17.1s	No
7	17.1285s - 19.95 s	No
8	19.9785s - 22.8s	No



Convergence (RANS)

Aerosol Dispersion – 11.4s - RANS

- Nostril located at (0,0,0)
- **Residence Time:** Time passed since the particle was released
- Initial downward trajectory until y-velocity dissipates and buoyant forces prevail

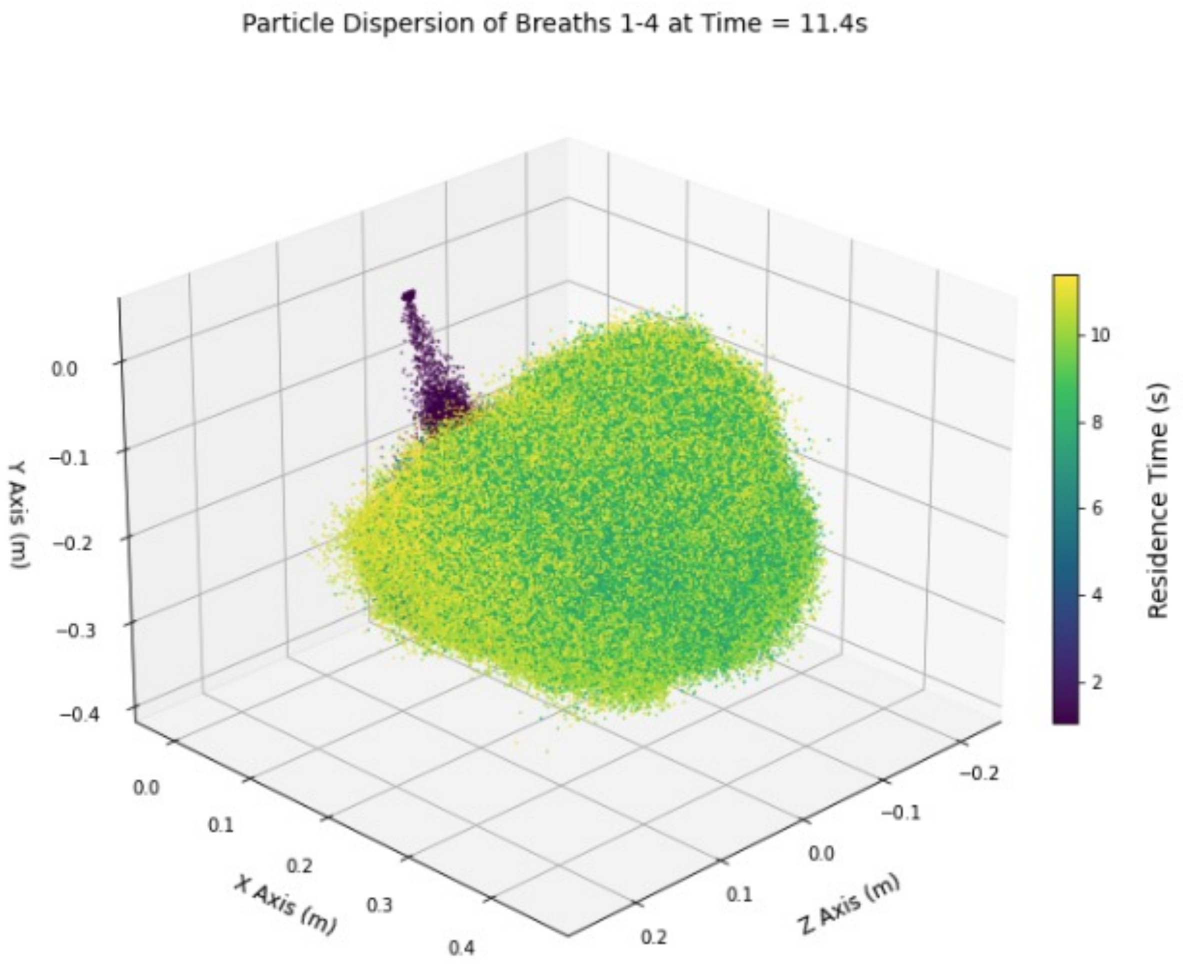
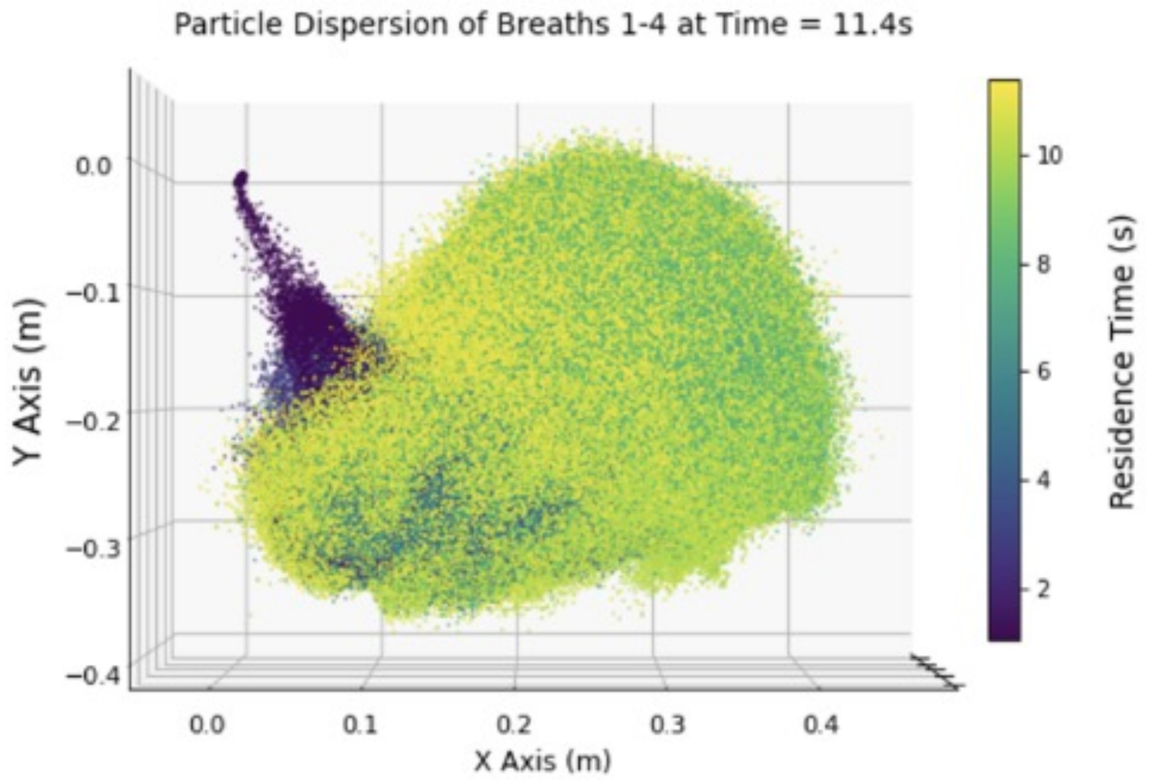
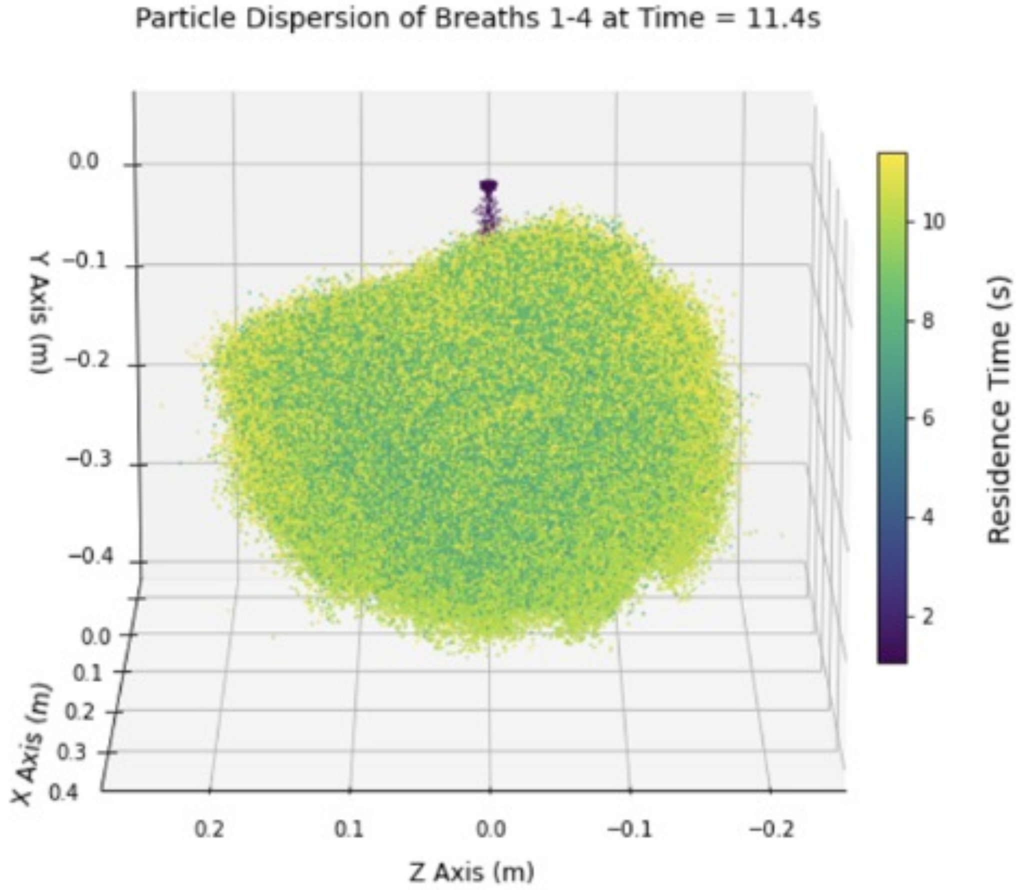


Figure 9: XYZ Position of Aerosols at 11.4s

Qualitative Observations – 11.4s Cont.

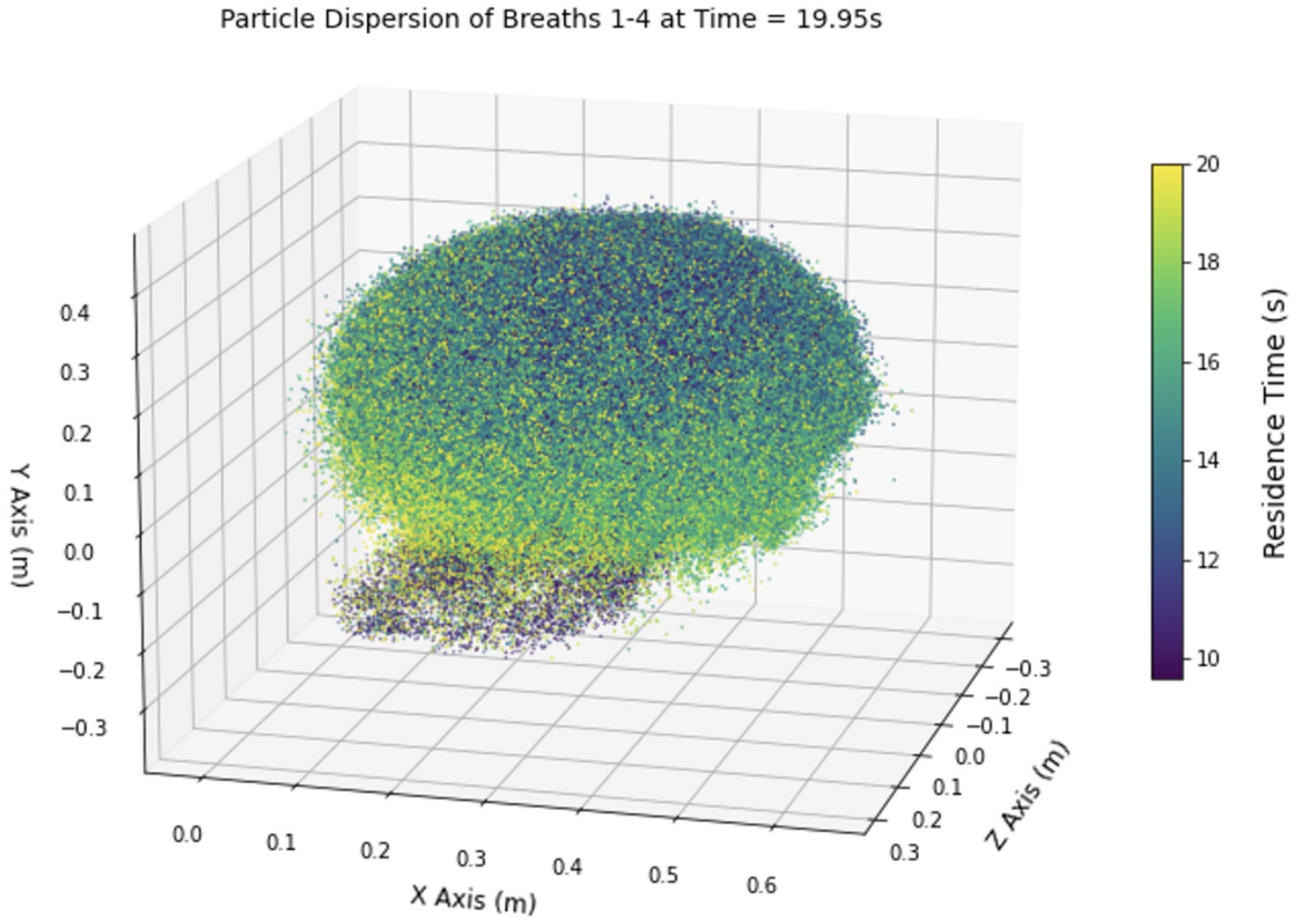




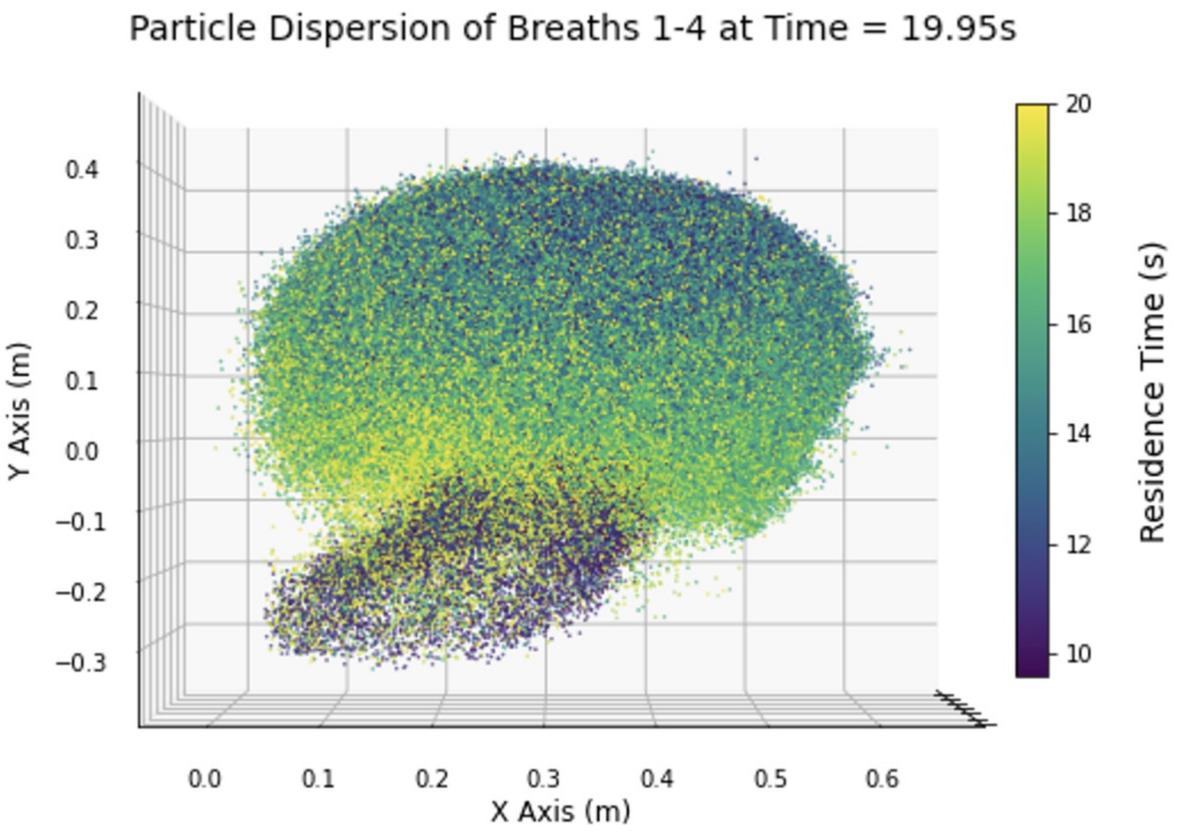
- Y Displacement Range: - 0.4 m to 0.05 m
- X Displacement Range: 0 m to 0.4 m
- Z Displacement Range: -0.2 m to 0.2 m

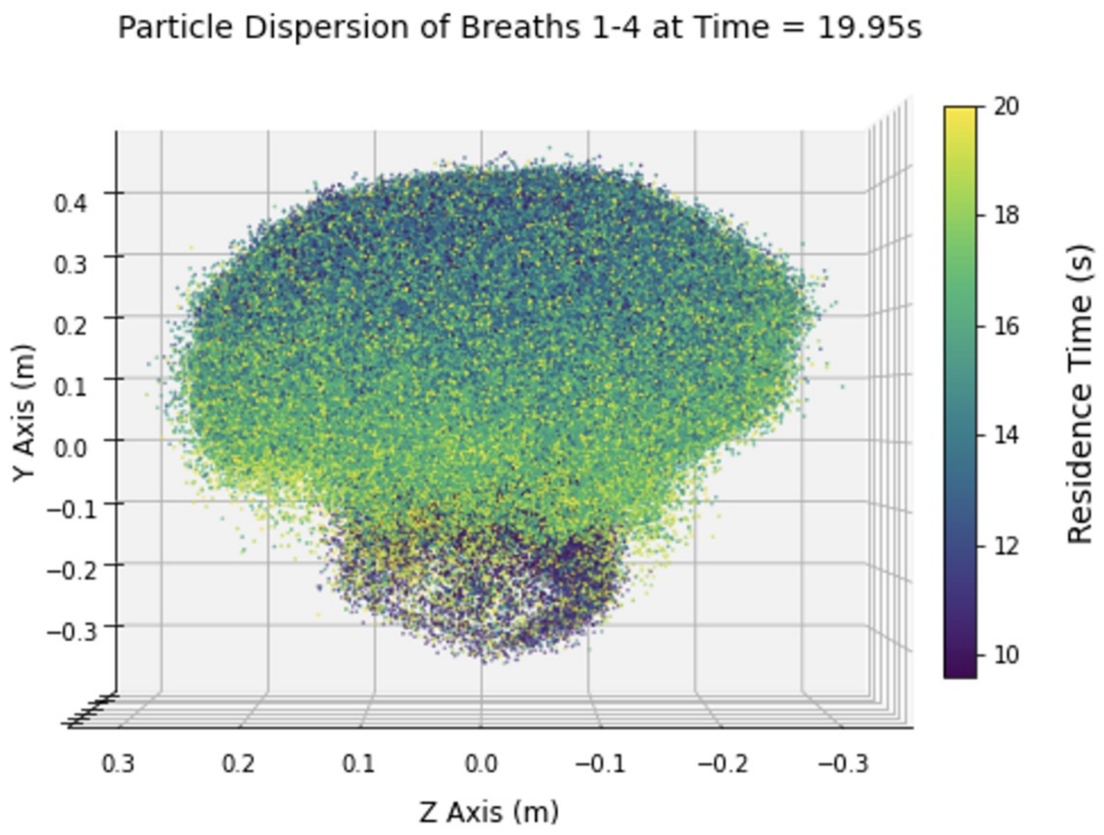
Qualitative Observations – 19.95s - RANS

- Rise of particles significant distance above (0,0,0)
- Aerosols are not residing near the nostril, but are continuing to rise



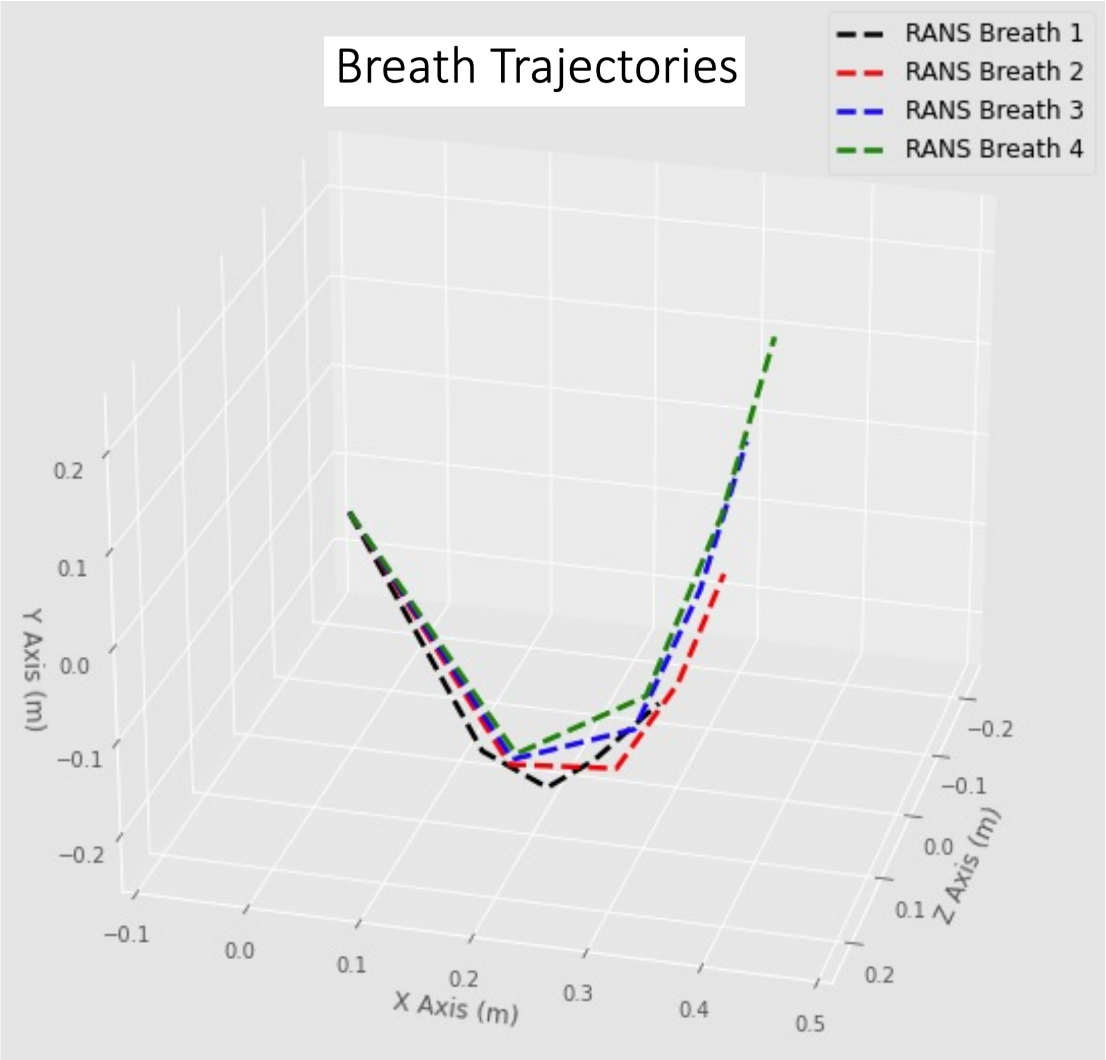
Qualitative Observations – 19.95s Cont.





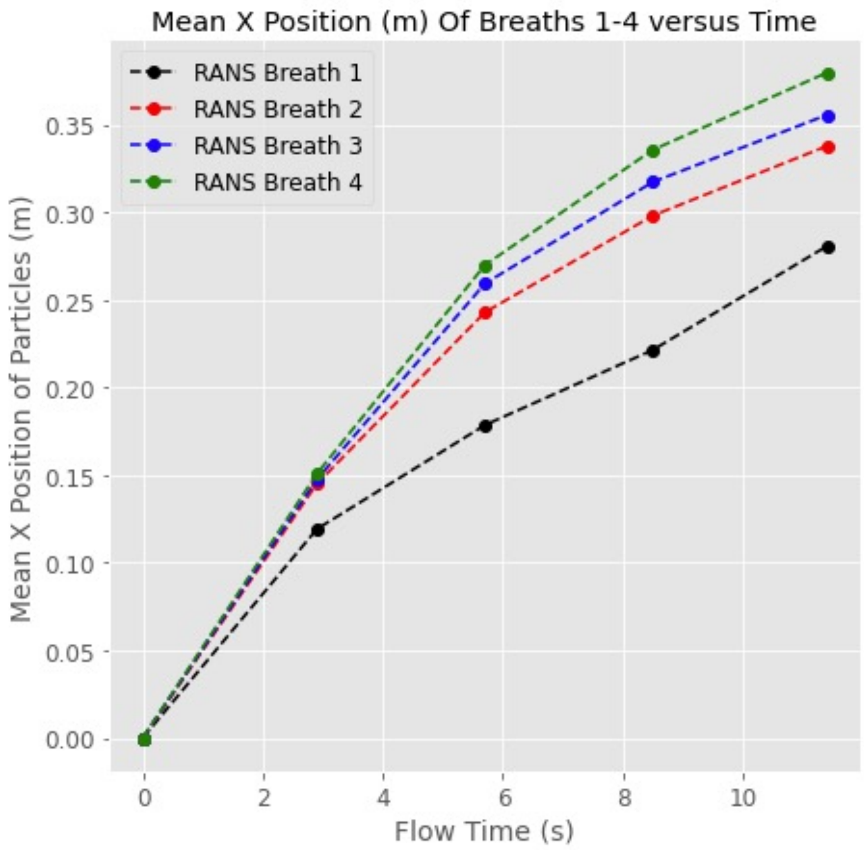
Breath Trajectories

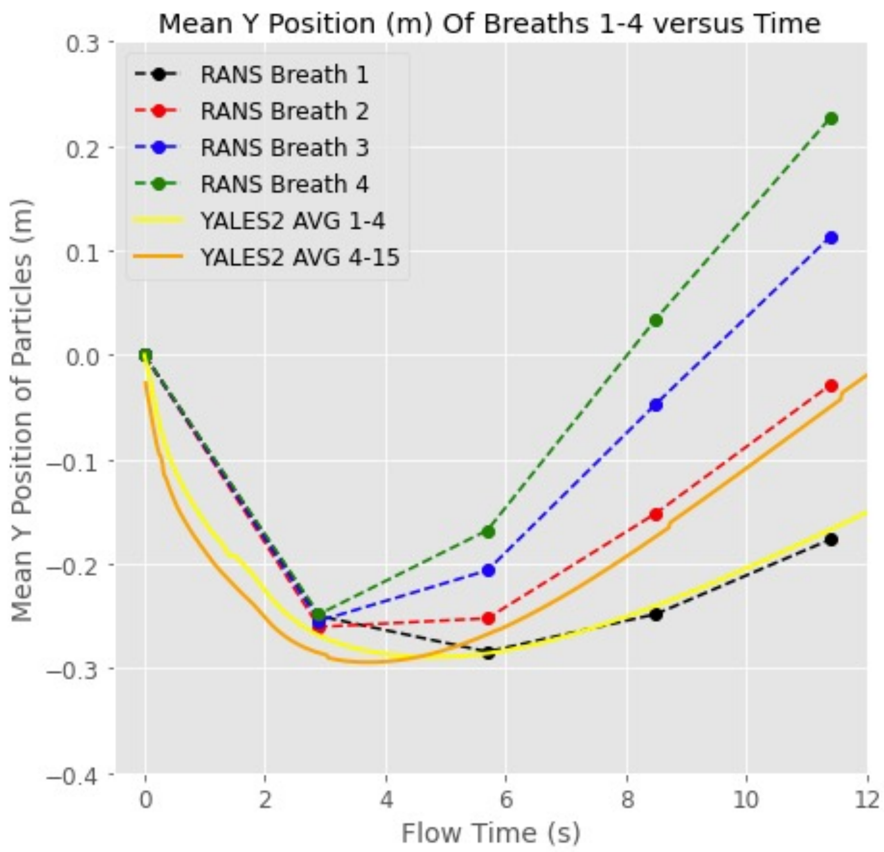
- 3D plot showing trajectories of mean XYZ positions for breaths 1-4
- The figure to the right and figures that will follow this slide were all calculated using the mean of ϕ, where ϕ is the variable of interest.
- The mean of ϕ was taken for all the particles of each breath at a specific point in time.



Mean X and Y Position

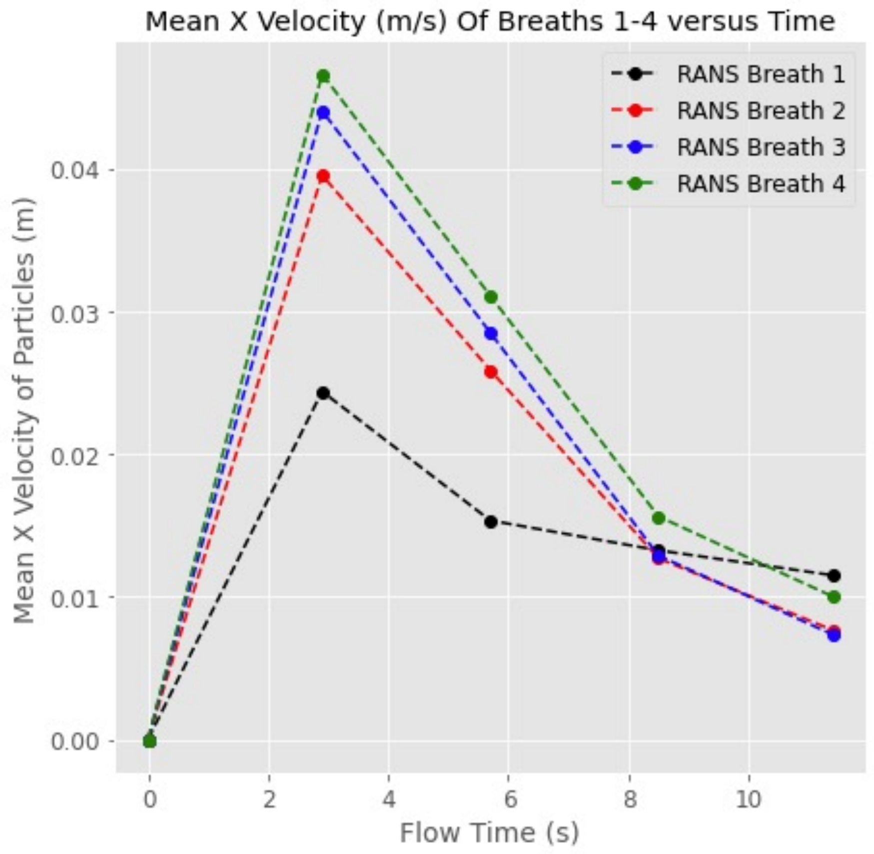
YALES2 Comparison



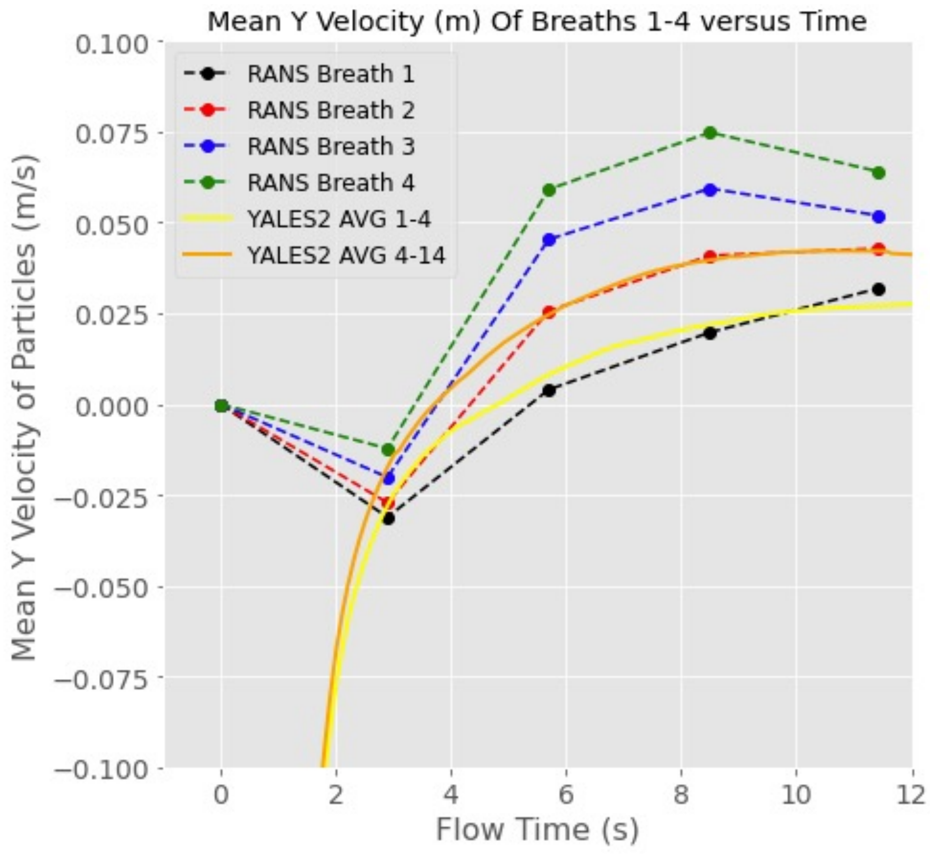


- Mean X Position: First breath does not travel as far as 2,3,4 but alludes to equilibrium
- Mean Y Position: Same trend as X-position but greater difference in values
- ANSYS to Yales2: Slightly greater -Y distance traveled,

Mean X and Y Velocity



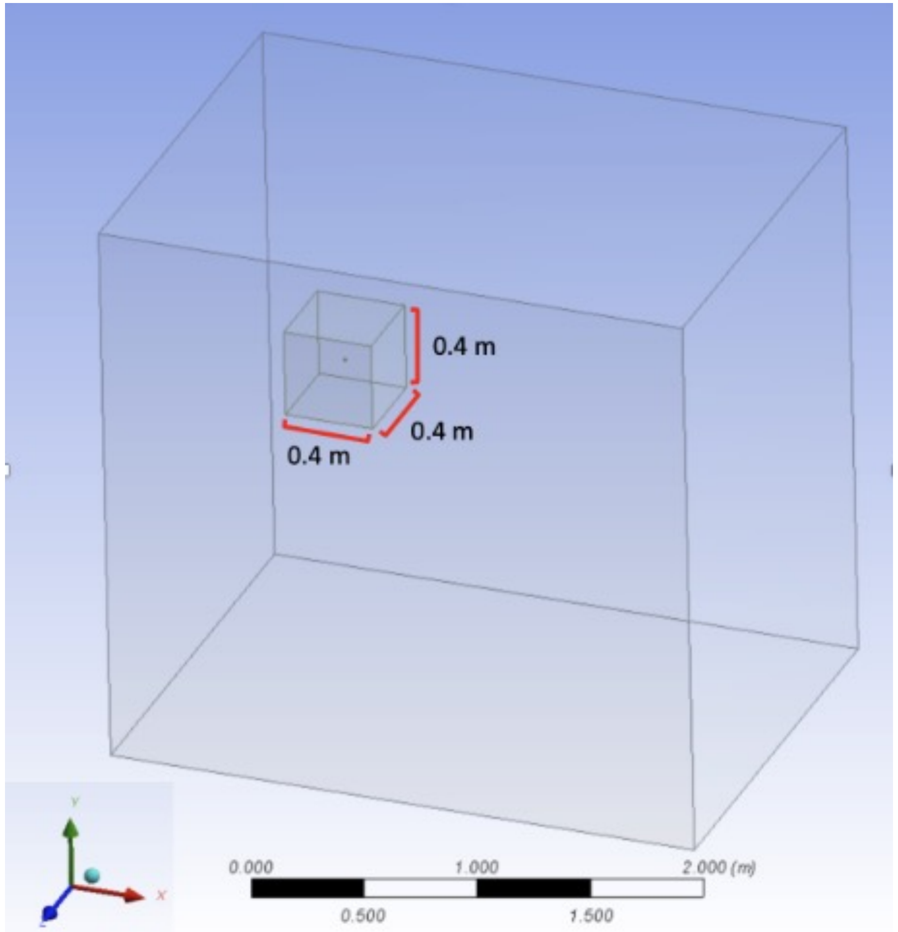
YALES2 Comparison



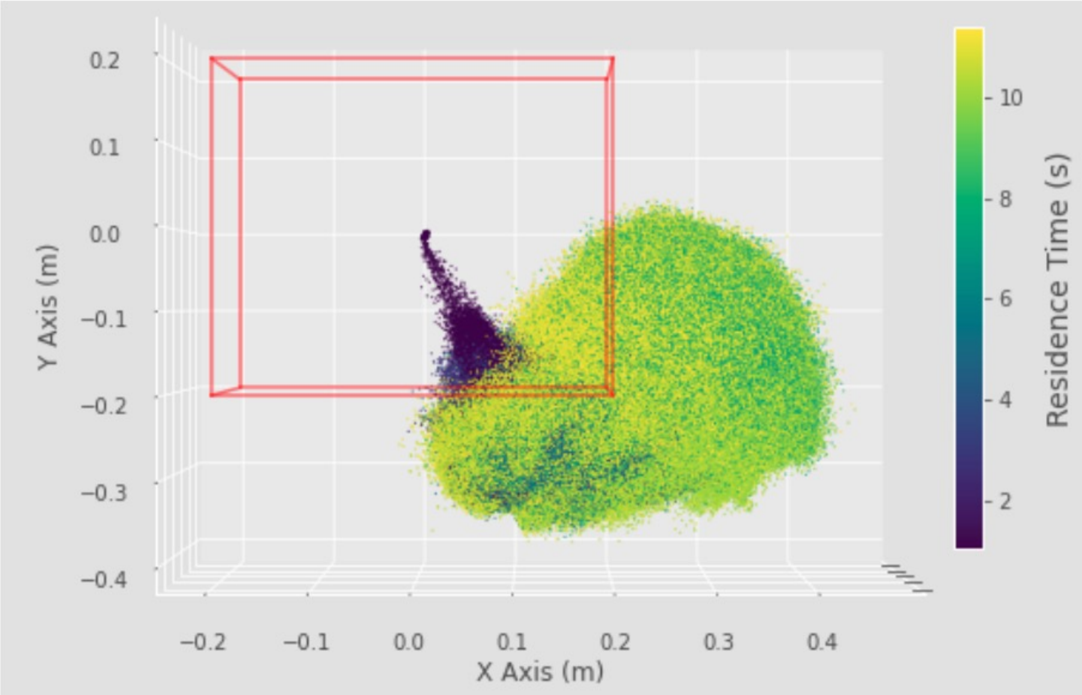
- Mean X Velocity: Steep decrease matches with Y vel increase (rising motion)
- Mean Y Velocity: Increases until leveling out at constant vertical velocity
- ANSYS to Yales2: Lower plateau velocity from Yales2

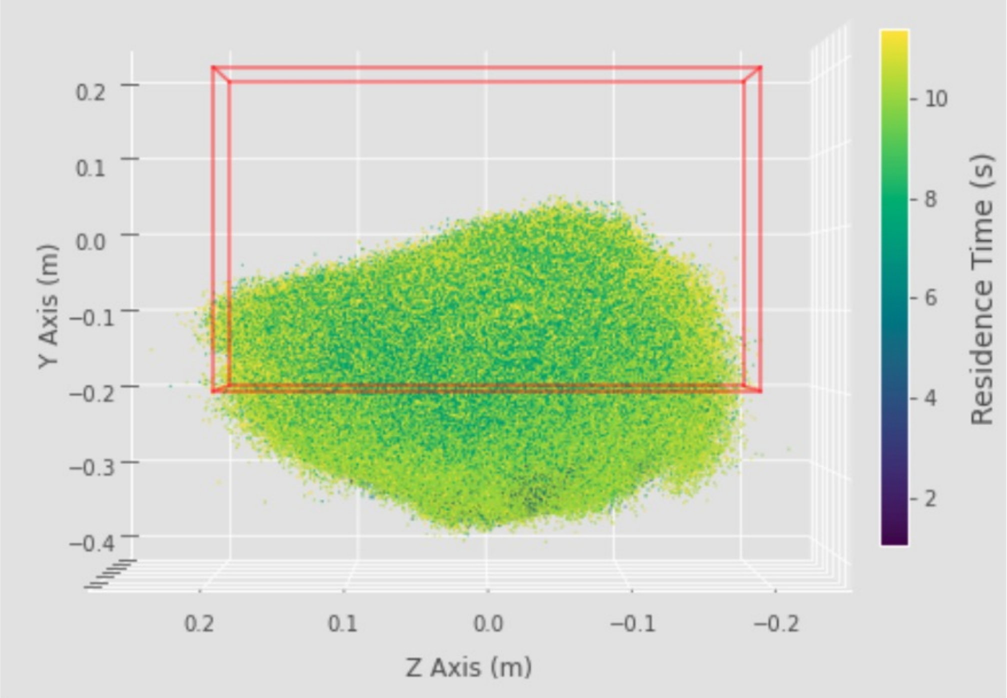
Inhalation Risk Zone: 3D Binned Aerosols

- Aerosol behavior directly affects transmission
- Concentration closest to nose and mouth can be considered highest inhalation risk area
- At 11.4s: 83,397 of 1,006,188 aerosols, or **8.288 %** lay within the region
- At 19.95s: 73,044 of 1,006,184 aerosols, or **7.260%** lay within the region

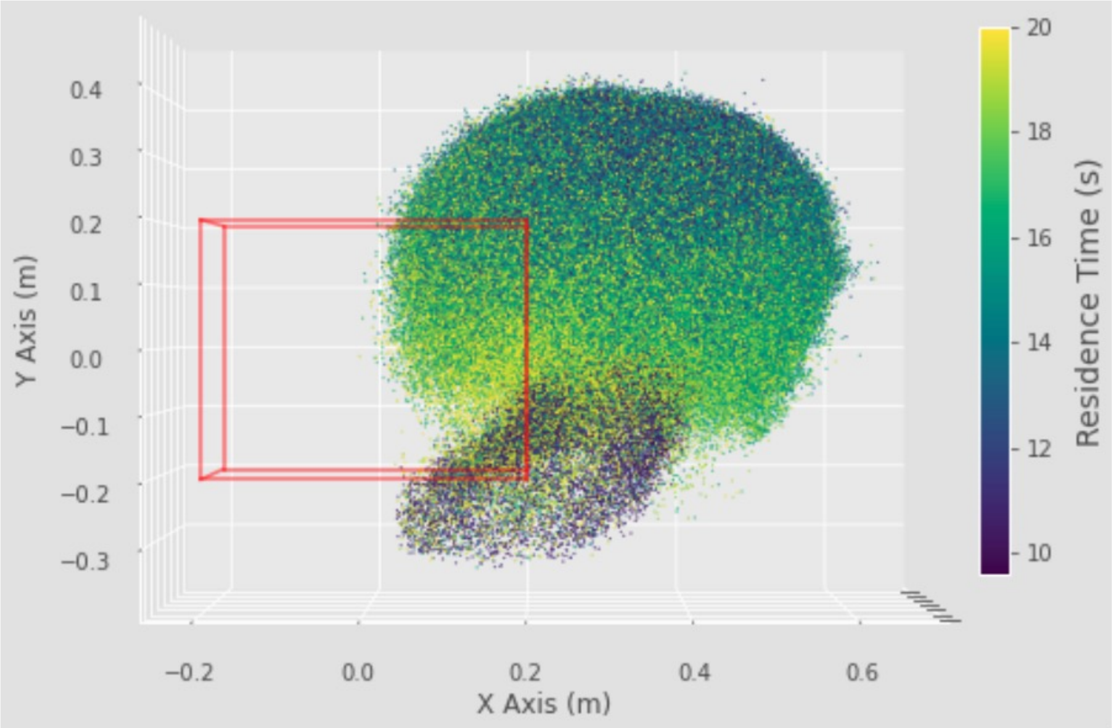


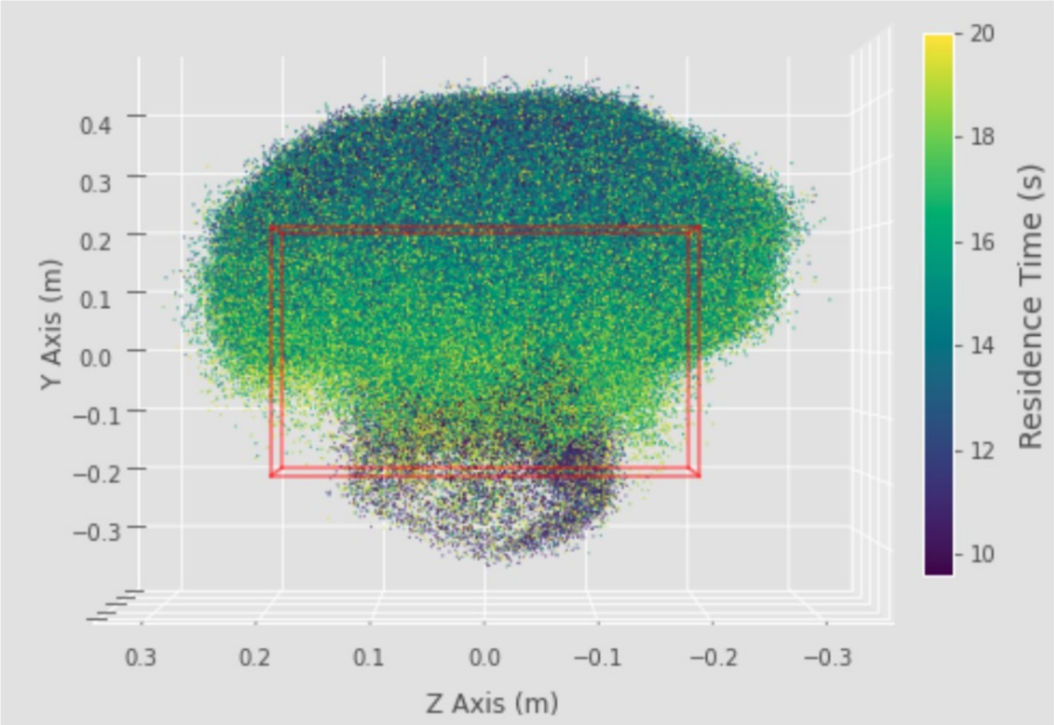
Inhalation Zone: 11.4s - RANS





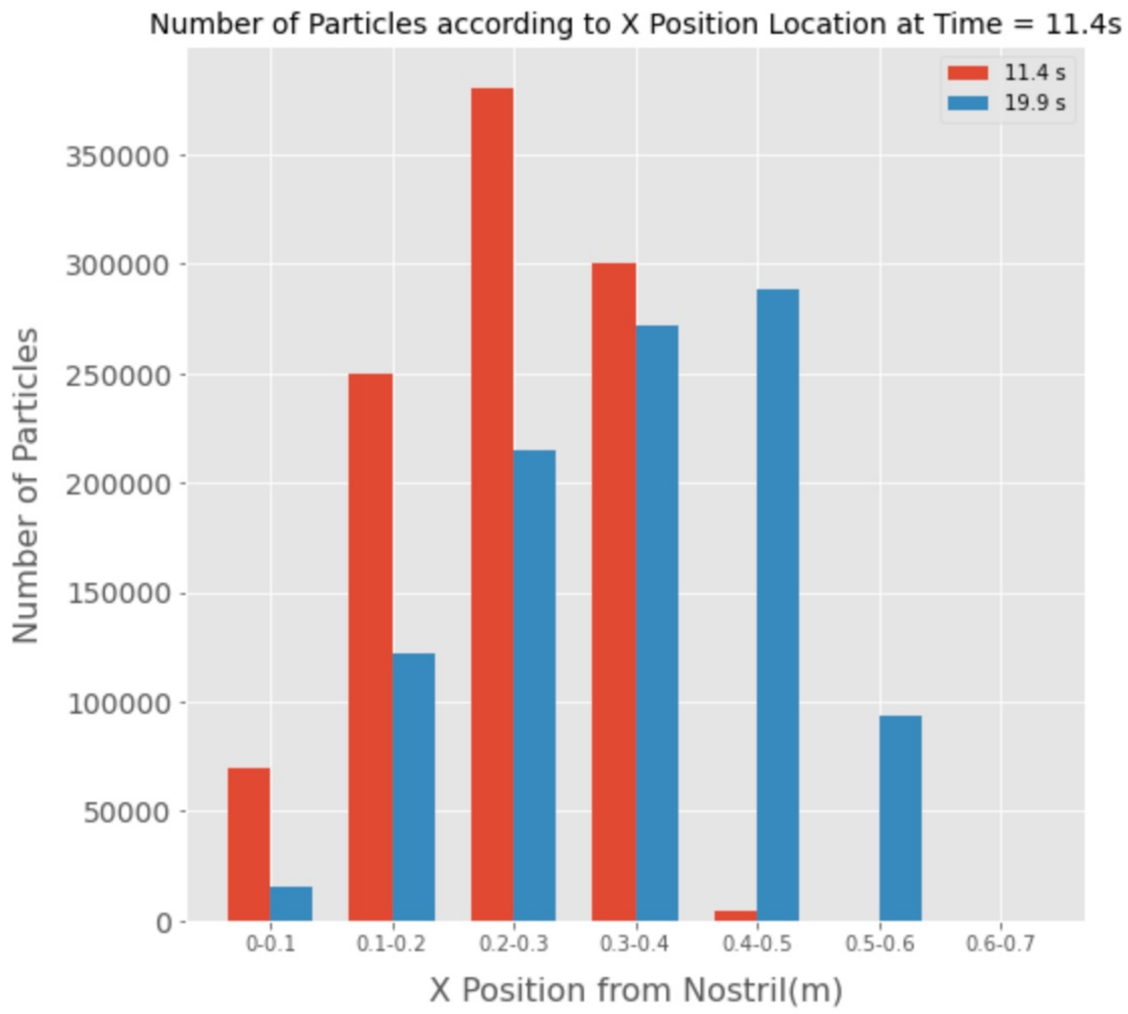
Inhalation Zone: 19.95s - RANS





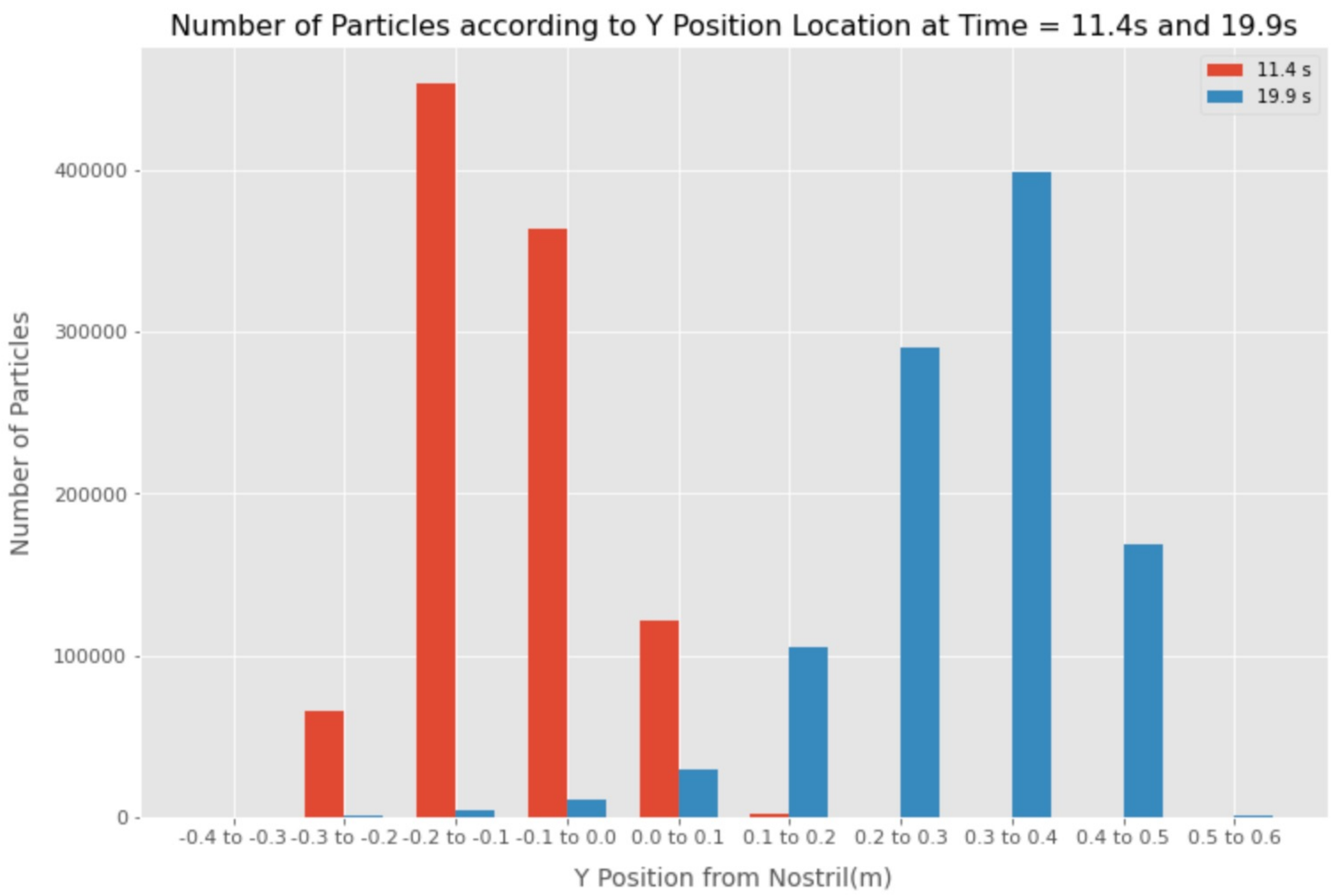
X, Y and Z Axis - Binned Aerosols - RANS

- Split up by axis allows for deeper analysis of binned aerosols
- Aerosols show that they continue to travel in x-direction past 19.95 seconds



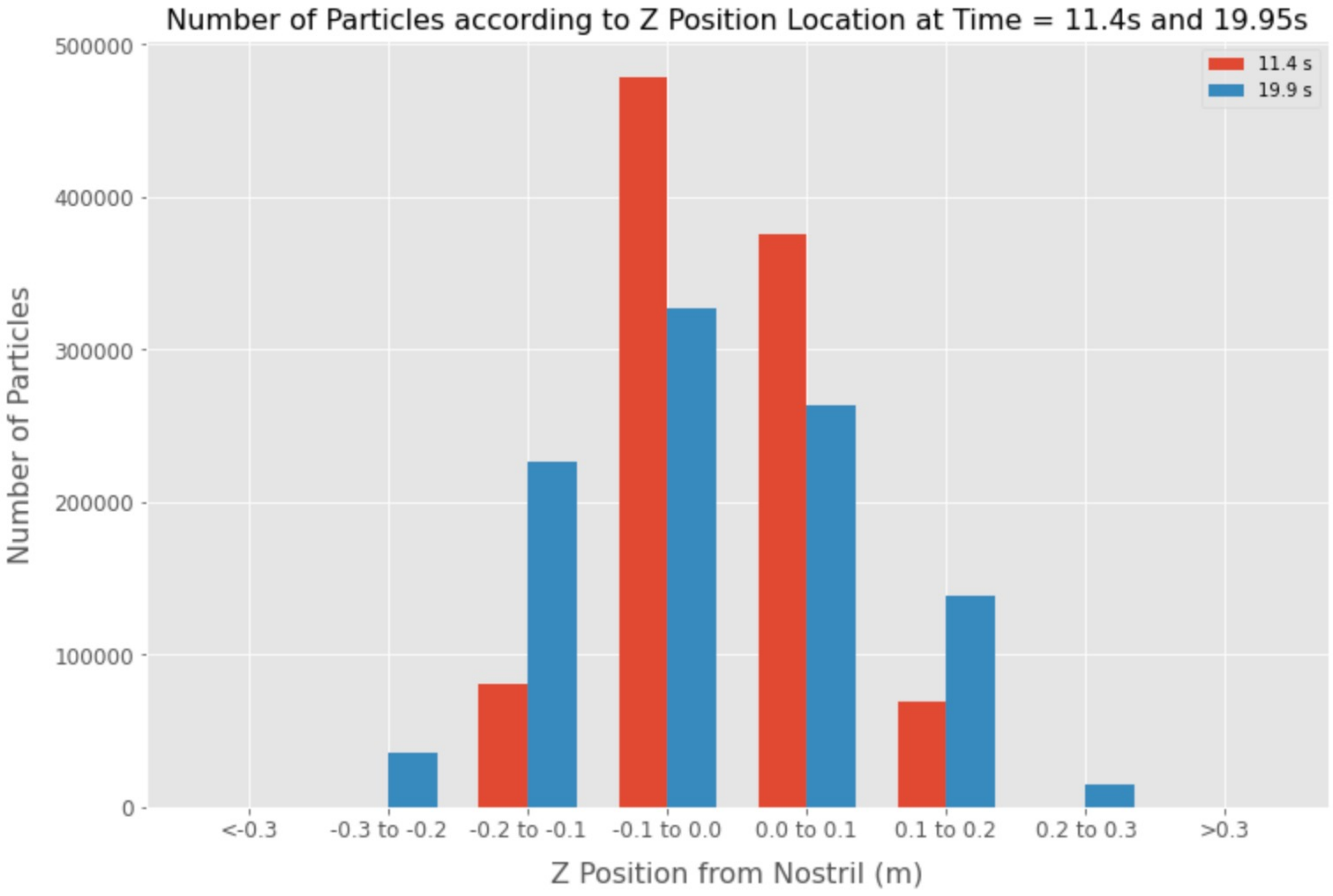
X, Y and Z Axis - Binned Aerosols - RANS

- Aerosols have clearly risen at 11.4s (red) as they do not remain at the lower elevations
- At 19.95s (blue) the aerosols have continued to rise up to 0.6m above the release point



X, Y and Z Axis - Binned Aerosols - RANS

- Aerosols remain evenly distributed along z-axis as expected as no angle is applied to the nostril with respect to the z-axis



Conclusions

- The COVID-19 pandemic stands as an example where early and accurate characterization of dispersion behavior could help define effective safety guidelines.
- The role of CFD in risk evaluation
  - Define areas of increased aerosol density which can be correlated to locations of higher risk
- The results show that continued breathing affects the behavior of aerosols as their behavior adjusts breath to breath
  - Numerous breaths must be simulated for greater accuracy
- Quantitative differences of meaningful magnitude present themselves between the ANSYS RANS and YALES2 comparison
- RANS ability to reproduce similar qualitative results to the high-fidelity simulation suggests value in continuing to pursue the use of multi-fidelity CFD with regards to low velocity flow situations

Future Work

- **Overall:**
  - Simulate a greater number of breaths
  - Compare ANSYS and Yales2 with identical mesh/setup
  - Fine-tune RANS controls
- **Physical Domain:**
  - Include a human body and head to account for any possible effects on the flow
  - Adaptive mesh refinement
- **Methodology:**
  - Allow nose breath to develop within a geometry that represents a nostril before entering the domain
  - Introduce small amounts of turbulence to see how the aerosol dispersion is affected
  - Introduce other disruptive factors: heat commonly found indoors that may have convective effects, such as humans or light sources

Acknowledgements

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KNOWLEDGE BASE