Exploring inhaled air-particle-vapor mixtures in the Human Respiratory System with Ansys Fluent® simulations

Part 1: Problem Specifications

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Ansys Software Used

This tutorial uses Ansys Fluent®, the fluid simulation software.

Learning Goals

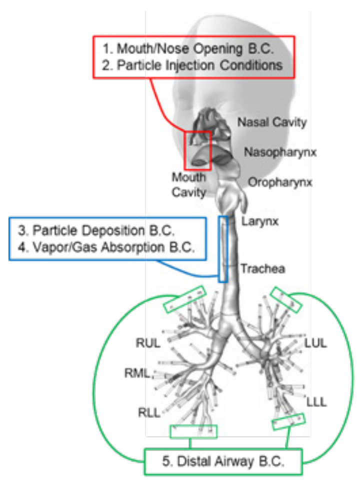
In this tutorial series, you will learn to:

- Generate a mesh for a subject-specific trachea to generation 6 (G6) using the Ansys Fluent Meshing tool.
- Set up and run air-particle and air-vapor flow dynamics in the upper airway using the Discrete Phase Model (DPM) and specific transport models enabled by User-Defined Scalars (UDS) (e.g., the advection-diffusion equation) in Ansys Fluent.
- Visualize the air-particle and air-vapor flow dynamics using Ansys CFD-Post and Ansys EnSight.

Background

Computational Fluid Dynamics (CFD) simulations of pulmonary air-particle-vapor flow are crucial for advancing both pulmonary healthcare and occupational exposure risk assessment. In pulmonary healthcare, these simulations enable a detailed understanding of how inhaled particles and vapors interact with the complex structures of the respiratory system (see Fig. 1). This insight is essential for developing targeted drug delivery systems, optimizing inhalation therapies, and improving the overall effectiveness of treatments for respiratory diseases. In the context of occupational exposure, CFD simulations help assess the risk of inhaling harmful particles and vapors in various work environments. By predicting the behavior and deposition patterns of these substances in the lungs, safety measures can be better designed to protect workers from respiratory hazards, ensuring safer working conditions and reducing the incidence of occupational lung diseases.

Fig.1. Representative human respiratory system (mouth/nose to generation 6)



Tools and Software

In this tutorial, we will employ a trachea-to-bronchi 3D airway geometry as a subject-specific but less complex computational domain than a tracheobronchial tree, which is usually used in silico pulmonary research nowadays as a quick example for tutorial purposes. The geometry can be constructed using from subject-specific CT chest scan images (see Fig. 2). The Trachea inlet hydraulic diameter is 6.93 mm. The diameters of the outlets are 6.30 mm (Outlet 1) and 3.85 mm (Outlet 2), respectively.

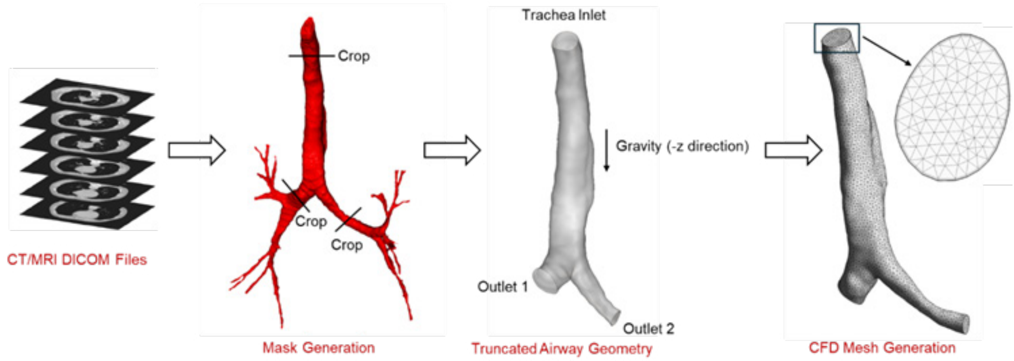


Figure 2: CFD geometry construction and mesh generation from CT/MRI medical images[1]

For CFD simulations, Ansys Fluent software[2] was chosen to provide a more research-level geometry (see Fig. 3). The diameter of the circular trachea inlet is 16 mm. The density of the air is 1.225 kg/m3. The spherical particles will be simulated with a monodispersed aerodynamic diameter of 5 µm. Using the aerodynamic diameter, we can assume the particle density equals water density, which is 1000 kg/m3. Breathing flow rate is at 6 L/min, representing adult male breathing condition at rest. This leads to a Reynolds number of around 600, which is laminar. We will also simulate nicotine transport and absorption in the airway mixed with a great excess of air. The binary diffusivity of nicotine in great excess of the air at body temperature (i.e., 37 oC or 310.15 K) can then be given as 0.695e-5 m2/s (Sperry et al., 2023). More details on initial and boundary conditions will be provided in Lesson 2.

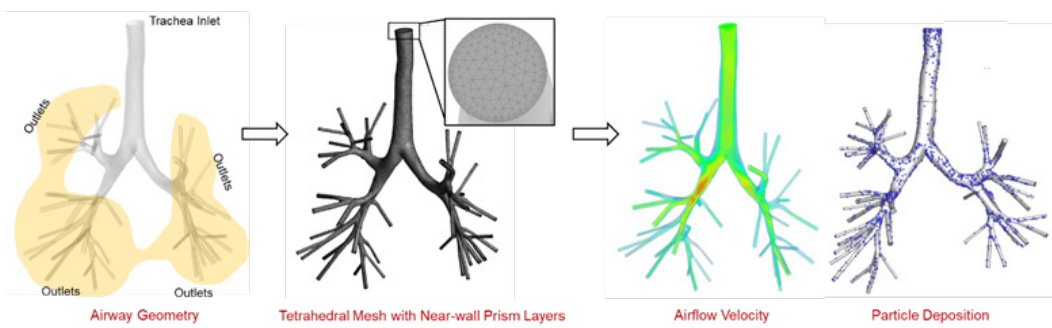


Figure 3: Geometry, mesh, and CFD simulation result examples using a subject-specific trachea-to-G6 airway geometry

Note: It is worth noting that the breathing conditions for humans can be much higher than 6 L/min, which will lead to transitional flow or turbulence in the computational domain. Therefore, selecting appropriate turbulence models in CFD simulations will be necessary. Details can be found in (Feng et al., 2021)

Reference:

Feng, Y., Zhao, J., Hayati, H., Sperry, T., Yi, H. (2021). Tutorial: Understanding the transport, deposition, and translocation of particles in human respiratory systems using Computational Fluid-Particle Dynamics and Physiologically Based Toxicokinetic models. Journal of Aerosol Science, 151, 105672

Sperry, T., Feng, Y. , Zhao, J., Song, C., Shi, Z. (2023). Prediction of the transport, deposition, and absorption of multicomponent E-cigarette aerosols in a subject-specific mouth-to-G10 human respiratory system. Journal of Aerosol Science. 170, 106157

1 These images were made using v ScanIP software

2 This tutorial was made using Ansys Fluent 2023R2 release. The interface may look different, depending on which release you use.

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Document Information

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