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

# Facilitator's Guide

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## Ansys Software Used

This tutorial uses Ansys Fluent®, the fluid simulation software and Ansys EnSight™, the simulation data visualization software.

## Tutorial Summary

Unlock the potential of CFD with this comprehensive tutorial on simulating inhaled air-particle-vapor mixtures in the human respiratory system using Ansys Fluent software, as well as post-processing simulation results using Ansys CFD-Post and EnSight tools. This guide details the step-by-step process of generating research-level meshes for subject-specific airway geometry and setting up advanced simulations to analyze airflow, particle transport, and vapor distribution in the respiratory tract.

Explore the intricacies of airflow dynamics, particle interactions using the Discrete Phase Model (DPM), and species transport via User-Defined Scalars (UDS). Detailed instructions ensure learners grasp the essentials of pre-processing, solver configuration, and post-processing, providing a thorough understanding of the CFD workflow for computational lung aerosol dynamics.

Ideal for researchers, engineers, and healthcare professionals, this tutorial not only enhances CFD simulation skills but also contributes to advancing pulmonary healthcare and occupational safety. Mastering these simulations equips learners to develop targeted drug delivery systems, optimize inhalation therapies, and assess occupational exposure risks.

## Tutorial Content Breakdown

This tutorial contains six separate PDF documents, allowing for parts to be used in separate lab/ homework sections, depending on the needs of the instructor.

### Part 1: Introduction

- Learning Goals: Outline the goals of the case study, focusing on airflow, gas, and particle dynamics in the human respiratory system.
- Background: Overview of the human respiratory system and the importance of modeling airflow and particles.
- Tools and Software: Brief on the tools and software will be used in this tutorial, i.e., Simpleware ScanIP, Ansys Fluent Meshing, Ansys Fluent Solver, Ansys CFD-Post, and Ansys Ensight.

### Part 2: Pre-Processing: Flow Regime, Governing Equations, and Initial/Boundary Conditions

- Governing Equations: Introduce the governing equations to model the pulmonary air-particle-vapor multiphase flow.
- Boundary Conditions: This section briefly discusses the popular inlet, outlet, and wall boundary conditions employed in the CFD simulations of air-particle-vapor flow dynamics in the human respiratory system.
- Initial Conditions: Overview of the overall rules for initial condition setup for steady-state and transient pulmonary airflow simulations.

## Part 3: Pre-Processing: Geometry Import and Mesh Generation using Ansys Fluent Meshing

- Geometry Import: Import the airway geometry into Ansys Fluent in Meshing Mode using an ASCII format STL file and visualize it.
- Mesh Size Determination: Measure geometric dimensions to determine the appropriate mesh size for surface mesh generation.
- Surface Mesh Generation: Set up scope sizing rules and generate the surface mesh for the airway geometry.
- Mesh Quality Check: Diagnose and improve surface mesh quality by reducing free-faces, multi-faces, and skewness.
- Material Point Creation and Volumetric Region Creation: Create a material point within the computational domain to help the software identify the fluid domain.
- Volume Mesh Generation: Generate a tetrahedral volume mesh with near-wall prism layers.
- Volume Mesh Quality Check and Improvement: Improve the volume mesh quality by adjusting quality limits and performing auto-corrections.
- Export Mesh: Export the mesh as a .msh.h5 file for use in Ansys Fluent Meshing and ensure it meets element count requirements for student license usage.

## Part 4: Ansys Fluent Solver Setup (Single Phase Flow, DPM, and Species Transport)

- Physics and Solver Settings in Ansys Fluent Solver
    - Material Properties
        - Defining properties of air, gas, and particles.
        - Assigning material properties in Ansys Fluent Solver.
    - Boundary Conditions
        - Inlet and outlet conditions.
        - Wall boundary conditions.
- Solver Settings
    - Choosing the appropriate flow model (i.e., laminar in this tutorial)
    - Multiphase flow setup: Eulerian, Lagrangian, or other suitable models.
    - Setting up species transport for gas simulation with user-defined scalar (UDS).
- Simulation Setup
    - Time-step size, convergence criteria, and iteration settings.

## Part 5: Post-Processing: Results Visualization in Ansys CFD-Post and Ansys Ensight

- Contours of spatiotemporal distributions of variables
- 3D distributions of variables using volume rendering
- Particle tracking and residence time analysis.
- Gas concentration profiles.

## Part 6: Summary

- Simplifications in this Case Study: Discuss the simplifications made in this CFD tutorial, emphasizing how the case study differs from a physiologically realistic human respiratory system.
- Future Work: Explore opportunities for further research and improvements to develop a more physiologically realistic digital twin of the human respiratory system.

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**Document Information**
This case study is part of a set of teaching resources to help introduce students to topics related to fluids and how to visualize data.

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