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

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

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Ansys Software Used

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

Learning Goals

In the Pre-Analysis step, we'll review the following:

- **Governing Equations:** The governing equations for airflow, particle transport, and vapor species will be reviewed, solving this problem.
- **Boundary Conditions:** We will review the boundary conditions applied in this problem, such as the no-slip boundary condition, velocity inlet, pressure outlet, trapped wall, and species flux/value boundary conditions.

Flow Regime

As clarified in Part 1, to simplify this tutorial, the inhalation flow rate is set at 6 L/min, representing the breathing rate of an adult human at rest. Accordingly, the flow regime in this tutorial is laminar. For transitional and turbulent airflow simulations in the human respiratory system, please refer to Feng *et al.* (2021) for guidance on turbulence model choices and numerical setup.

Governing Equations

Primary Phase: Airflow

The airflow dynamics in the respiratory tract are usually unsteady, driven by ventilation and the cyclic breathing processes. To accurately predict airflow fields containing both laminar and turbulence regimes, the incompressible Navier-Stokes (N-S) equation is employed to characterize airflow in the human respiratory tract, accompanied by continuity equation, energy equation, and constitutive equations, *i.e.*,

Continuity Equation

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

in which u_j represents the air velocity, and ρ is the air density.

Navier-Stokes (N-S) Equation

$$\rho\left(\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j}\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \tag{2}$$

where p is the pressure, g_i is the gravitational acceleration vector. The viscous stress tensor τ_{ij} in Eq. (2) is given by:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{3}$$

where μ is the air viscosity.

Energy Equation

$$\rho \frac{\partial (c_p T)}{\partial t} + \rho \frac{\partial (c_p u_j T)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[k \frac{\partial T}{\partial x_j}\right] + \Phi + S_T \tag{4}$$

where T is the temperature, k is thermal conductivity and c_p is specific heat capacity. Furthermore, S_T is the thermal sink or source term due to the heat exchange of phase change induced by condensation or evaporation, *etc*. Φ is the dissipation function, which can be given as:

$$\Phi = \tau_{ij} \frac{\partial u_i}{\partial x_j} \tag{5}$$

Secondary Lagrangian Phase (Discrete Phase Model): Particulate Matter

To track discrete particulate matter using the Euler-Lagrange method (Feng et al., 2021), the kinematics of a particle in the airflow must be accurately predicted. This prediction depends on precisely describing the external forces exerted on the particle by the suspending medium or carrier fluid. The Euler-Lagrange method, also known as the discrete phase model (DPM), provides a direct description of particulate flow by tracking the motion of individual particles. The continuous phase, i.e., fluid flow, is governed by continuum equations, which can be solved as the Eulerian phase (see Eqs. (1) to (5)). For spherical particles, their motions are governed by Newton's second law, which employs empirical correlations for hydraulic forces acting on the particles. For dilute particle suspensions, the one-way coupled method is applied, indicating that the particle motion is influenced by the flow field, while the flow field is not disturbed by the particles. Specifically, for an individual particle, the trajectory can be obtained by solving the particle motion equation, *i.e.*, Newton's second law.

$$\frac{d}{dt}(m_p \vec{u}^{\mathrm{p}}) = \sum \vec{F}_{body} + \sum \vec{F}_{surface} + \sum \vec{F}_{interaction} \tag{6}$$

In Eq. (6), forces acting on the particles are categorized into three terms:

(1) $\sum \vec{F}_{body}$ are body forces which are proportional to the particle mass,

(2) $\sum \vec{F}_{surface}$ are surface forces of which the magnitudes are proportional to the particle surface area and related to the surrounding fluid stress

(3) $\sum \vec{F}_{interaction}$ are particle-particle and particle-wall interactions.

Forces may be considered in Eq. (6) are listed as follows:

$$\sum \vec{F}_{body} = \vec{F}_G + \vec{F}_{buoyancy} + \vec{F}_{VM} + \vec{F}_{BM} \tag{7}$$

$$\sum \vec{F}_{surface} = \vec{F}_D + \vec{F}_{pressure} + \vec{F}_{Saffman} \tag{8}$$

$$\sum \vec{F}_{interaction} = \vec{F}_{particle-particle} + \vec{F}_{particle-wall} \tag{9}$$

where F_G is the gravity, $F_{buoyancy}$ is the buoyancy force , F_{VM} is the virtual mass force, F_{BM} is the Brownian motion induced force, F_D is the Stokes drag force, $F_{pressure}$ is the pressure gradient force, $F_{Saffman}$ is the Saffman lift force, $F_{particle\text{-}particle}$ is the summation of adhesive and repulsive forces between particles, and $F_{particle\text{-}wall}$ is the summation of adhesive and repulsive forces between particles and wall boundaries. It should be emphasized that F_{BM} is included in Eq. (7), only because the Brownian motion induced force is numerically treated as an additional body force as an approximation (Feng et al., 2021).

Not all forces in Eqs. (7) to (9) are necessary to be considered, since some of them may be negligible compared with other forces in magnitude. The relative order of magnitude analysis (ROMA) (Kleinstreuer, 2003) should be done to determine the forces that need to be considered in Eq. (6), to guarantee the accuracy and computational efficiency of employed models. Usually, the relative importance of forces is determined based on the comparison with F_D.

It is worth mentioning that most existing CFPD models for pulmonary air-particle flow dynamics assume that particles are spherical and treat them as mass points. Equation (6) can be complex as it includes a wide range of length scales and time scales as well as issues concerning turbulence, convection, settling, two-way coupling, collisions, aggregation, etc. For instance, most airborne particles are non-spherical, and some of them are highly anisotropic in shape, such as fiber-like particles, whose rotational motions should be accurately predicted. Furthermore, particles or droplets may also change in size during transport due to condensation and evaporation effects, which need to be accurately captured since the size change of particles can significantly influence their trajectories and deposition locations. Therefore, supplementary equations must be included. Details for modeling advanced particles can be found in the references listed in Feng et al. (2021).

Secondary Eulerian Phase: Vapor/Gas

Gases and vapors can be harmful to the pulmonary tract via inhalation. Their transport phenomena can be predicted by solving species transport equations (*i.e.*, advection-diffusion equations) with or without turbulence dispersion (J. Zhao et al., 2019a), *i.e.*,

$$\frac{\partial(\rho_{a-g}Y_s)}{\partial t} + \frac{\partial(\rho_{a-g}u_jY_s)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\rho_{a-g}\widetilde{D}_{a-g,s} + \frac{\mu_t}{\sigma_Y}\right)\frac{\partial Y_s}{\partial x_j}\right] + S_{v-d}^{(Y_s)} \tag{10}$$

where Y_s is the mass fraction of the s-th gas/vapor species, σ_Y is the turbulent Schmidt number, μ_t is the turbulence viscosity, which will be equal to zero for laminar flow, ρ_{a-g} is the mixture density, and $D_{a-g,s}$ is the molecular diffusivity of the s-th gas species in the air, which can be either estimated using the Stokes-Einstein equation or directly obtained from experimental measurements and discrete particle trajectory simulations. $S_{v-d}^{(Ys)}$ is the source term for describing phase changes between vapor and liquid, specifically those caused by evaporation and condensation. $S_{v-d}^{(Ys)}$ can be given by:

$$S_{v-d,s}^{(Y)} = \frac{\sum_{i=1}^{N_{d,cell}}(\overline{J_s}A_d)_i}{V_{cell}} \tag{11}$$

where j_s is the average evaporation/condensation mass flux normal to the droplet surface of s[th] component (*i.e.*, $j_s>0$ for evaporation and $j_s<0$ for condensation). A_d is the droplet surface area. For solid particle simulations with constant particle diameters, $S_{v-d}^{(Ys)}=0$. It is worth mentioning that Y_s can be modeled as a user-defined scalar (UDS).

Boundary Conditions

Inlet Boundary Conditions

In this tutorial, the velocity inlet condition will be applied. Other inlet conditions can also be employed, such as mass flow inlet conditions. We can use user-defined functions (UDFs) or customized expressions in the Ansys Fluent solver to define a transient velocity inlet condition.

Distal Airway Boundary Conditions

Since most of the human respiratory system geometries used in CFD simulations are incomplete and truncated at certain generations. Therefore, it is hard to obtain physiologically realistic values of airflow velocities or pressures at the truncated distal airway openings (see Fig. 1 in Lesson 1). With simplifications, commonly accepted distal airway boundary conditions (B.C.s) include uniform pressure/velocity outlets and mass flow rate distributions supported by experimental measurements. It has been claimed that using uniform pressure/velocity outlets may not be physiologically realistic and will lead to noticeable differences in the airflow field predictions in human respiratory systems. Accordingly, utilizing experimental data, including 4D medical images, methods to estimate more physiologically realistic pressure or volumetric flow rate B.C.s are developed. Specifically, the radiological characteristics and volumetric changes of each lobe shown in 4D CT images can be used to estimate the regional ventilation conditions of the distal airways of different lobes.

Airway Wall Boundary Conditions

Airflow

No-slip boundary conditions will be applied for airflow wall B.C.s.

Discrete Particulate Matter

The internal walls of the human respiratory system are covered by mucus layers. Mucus layers trap particulate matter (PM) in the inspired air and thereby perform a filtration function. Based on this fact, 100% trapping wall B.C.s are widely used as particle deposition B.C. Specifically, if the distance between the spherical particle center and the airway wall is less than the particle radius, the particle is considered deposited.

Vapor/Gas

For vapor/gas absorption rate calculation at the airway wall, both Dirichlet and Robin boundary conditions have been applied in existing research efforts. Specifically, the Dirichlet boundary condition (species value B.C. for UDS) can be given by:

$$Y_s|_{wall} = 0 \tag{12}$$

which implies the fast removal of vapor/gas with an infinite absorption rate.
However, the infinite absorption rate is not always realistic. In contrast, the Robin B.C. is more realistic since it represents a limited absorption rate (specific flux B.C. for UDS), but it needs calibration based on experiments. The Robin B.C. for gas/vapor absorption can be given as:

$$\frac{\partial Y_s}{\partial n}|_{wall} + \Gamma_{S,W} \cdot Y_s|_{wall} = 0 \tag{13}$$

where n represents the normal direction of the airway surface, $\Gamma_{s,w}$ is the wall absorption coefficient, which can be given by:

$$\Gamma_{S,W} = \frac{\tilde{D}_{m,s}}{\tilde{D}_{a-v,s}\, k_{H,s,a-m} H_m} \tag{14}$$

in which $D_{a\text{-}v,s}$ and $D_{m,s}$ are the vapor diffusivity in the air and the liquid mucus phase, respectively. H_m is the mucus thickness, which can vary from 8.3 µm in the trachea to 1.8 µm in the lower bronchioles. $k_{H,s,a\text{-}m}$ is the equilibrium partition coefficient for a given contaminant molecule, which can be determined by Henry's law. Derivation of Eq. (25) can be found in Keyhani et al. (1997).

Initial Conditions

For accurate and realistic temporal variations of variables, reasonable initial conditions (I.C.s) must be given for CFD simulations. Unless the simulation result of interest is steady-state, I.C.s must accurately reflect the conditions at time *t=0*, *e.g.*, the initial distributions of velocity, temperature, and pressure in the pulmonary airflow fields.

References:

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Kleinstreuer, C. (2003). Two-phase flow: theory and applications: CRC Press.

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