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

Part 6: Simplifications and Future Work

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Simplifications in this Case Study

In this case study, several simplifications have been made to facilitate the learning process and reduce computational complexity:

1. **Truncated Airway Geometry:** The airway geometry used is a truncated version of the human respiratory system, without mouth/nose-to-trachea upper airway and G9 to alveoli geometry. This reduces the computational domain size and complexity but also neglects the influence of those anatomical features on aerosol transport dynamics.
2. **Static Airway:** The airway geometry is assumed to be static without physiologically realistic expansion and contraction motion.
3. **Laminar Flow Assumption:** The inhalation flow rate is set at 6 L/min, representing a laminar flow regime. This assumption simplifies the flow calculations and avoids the complexities of transitional or turbulent flow simulations, which is needed for other human inhalation activities with higher flow rates.
4. **One-Way Coupled DPM:** In the Discrete Phase Model (DPM) simulations, one-way coupling is used. This assumes that the particle motion is influenced by the airflow, but the airflow is not affected by the particles, simplifying the computational model.
5. **Dirichlet Boundary Condition for Nicotine Absorption:** The nicotine absorption at the airway wall is modeled using a Dirichlet boundary condition, assuming an infinitely fast absorption rate. This avoids the need for more complex boundary conditions representing a finite absorption rate that would require calibration.
6. **Constant Properties:** The physical properties of air, particles, and nicotine vapor are assumed constant throughout the simulation. Temperature variations and their effects on properties like density and viscosity are not considered.
7. **Neglect of Secondary Forces:** In the DPM simulations, secondary forces such as the Saffman lift force, virtual mass force, and Brownian motion are neglected for simplicity. Only the primary forces, such as drag and gravity, are considered.

Future Work: Physiologically Realistic Digital Twin for Human Respiratory System

Future work aims to develop a physiologically realistic digital twin of the human respiratory system to enhance the accuracy and applicability of CFD simulations in biomedical research. To resolve the simplifications outlined in the current case study, future work should address each limitation by incorporating more complex and realistic modeling approaches. Below is a detailed plan for future work to tackle each simplification:

1. **Truncated Airway Geometry:**
   - *Inclusion of Upper Airway and G9 to Alveoli Geometry:* Future studies should extend the computational domain to include the entire airway, from the mouth/nose to the alveoli. This will provide a more accurate representation of aerosol transport dynamics throughout the respiratory system.
   - *High-Resolution Imaging and Segmentation:* Utilize high-resolution imaging techniques, such as CT or MRI, to obtain detailed anatomical data. Advanced segmentation algorithms can then be employed to reconstruct a complete and accurate airway geometry.

2. **Static Airway:**
   » *Dynamic Airway Modeling:* Implement models that account for the physiological expansion and contraction of the airways during respiration. This can be achieved using fluid-structure interaction (FSI) techniques to couple airflow simulations with the mechanical properties of the airway tissues.
   » *Validation with Experimental Data:* Use experimental data from respiratory physiology studies to validate the dynamic airway models, ensuring they accurately reflect real-life breathing patterns.
3. **Laminar Flow Assumption:**
   » *Turbulent Flow Modeling:* Incorporate turbulence models, such as k-ε, k-ω, or large eddy simulation (LES), to capture the complexities of airflow at higher inhalation rates. This will be particularly important for modeling activities involving deep or rapid breaths.
   » *Flow Regime Analysis:* Perform a thorough analysis of different inhalation scenarios to determine the appropriate flow regimes and ensure the selected turbulence models are accurately capturing the transitional and turbulent flow characteristics.
4. **One-Way Coupled DPM:**
   » *Two-Way Coupling:* Implement two-way coupling in the Discrete Phase Model (DPM) simulations to account for the interaction between particles and airflow. This will involve solving the coupled equations of motion for both phases and will provide a more realistic representation of aerosol transport.
   » *Particle-Flow Interaction Studies:* Conduct studies to understand the impact of particles on airflow, particularly in regions of high particle concentration or where particle deposition significantly alters flow characteristics.
5. **Dirichlet Boundary Condition for Nicotine Absorption:**
   » *Finite Absorption Rate Modeling:* Develop boundary conditions that represent finite absorption rates of nicotine at the airway walls. This can be achieved by incorporating reaction kinetics or using empirical data to calibrate the absorption rates.
   » *Multiphase Mass Transfer Models:* Implement multiphase mass transfer models to capture the complex interactions between nicotine vapor, particles, and the airway lining fluid.
6. **Constant Properties:**
   » *Variable Properties with Temperature Effects:* Introduce temperature-dependent properties for air, particles, and nicotine vapor. This will require solving the energy equation and incorporating temperature effects on density, viscosity, and other relevant properties.
   » *Thermal Analysis:* Perform thermal analysis to understand the impact of temperature variations on aerosol transport and deposition, particularly in scenarios involving heated aerosols or variable ambient temperatures.
7. **Neglect of Secondary Forces:**
   » *Inclusion of Secondary Forces:* Integrate secondary forces such as the Saffman lift force, virtual mass force, and Brownian motion into the DPM simulations. This will provide a more comprehensive understanding of particle dynamics, especially for small particles or those in complex flow regions
   » *Force Interaction Studies:* Conduct detailed studies on the relative importance of different forces under various conditions to prioritize their inclusion in the simulations and ensure computational efficiency without sacrificing accuracy.

By addressing these simplifications, future research can provide a more accurate and comprehensive understanding of aerosol transport and deposition in the human respiratory system. Accordingly, the future digital twin will be a powerful tool for advancing pulmonary healthcare, optimizing inhalation therapies, and assessing occupational exposure risks, ultimately contributing to improved respiratory health and safety.

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