# Simulation of Hygroscopic Particle Motion and Deposition under Oral-Pharyngeal Boundary Heat Transfer: Postprint

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## Abstract

This study developed an oral-throat respiratory tract model incorporating the mucus layer and tissues surrounding the respiratory tract, enabling simulation of water vapor species transport and convective heat transfer on the mucus layer, latent heat of vaporization within the mucus layer, and heat conduction within the mucus layer and surrounding respiratory tissues. Under inlet air conditions of 27.60°C and 34.7% relative humidity, the transport and deposition of multicomponent hygroscopic particles were simulated in an idealized oral-throat model under two boundary conditions: 1) accounting for heat conduction, convection, and latent heat of vaporization in the respiratory tract, mucus layer, and tissues, and 2) a constant respiratory wall temperature of 37°C. The results indicate that Condition 1 yielded an average relative humidity 2.3% higher than Condition 2, yet the particle deposition rate was lower than that of Condition 2, with a maximum difference of up to 9%. The particle deposition patterns were similar, but the average diameter of deposited particles under Condition 1 was 40.7% smaller than that under Condition 2, and the average diameter of escaped particles was 14.3% smaller.

## Full Text

### Numerical Study of the Transport and Deposition of Hygroscopic Particles in a Mouth-Throat Airway with Heat-Transfer Boundary Conditions

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## Abstract

This study constructs a mouth-throat (MT) airway model incorporating the surrounding airway tissue and mucus layer, enabling simulation of water vapor transport above the mucus layer, convective heat transfer, latent heat from mucus evaporation, and heat conduction within the airway tissue. The transport and deposition of multi-component hygroscopic particles are simulated under inlet air conditions of 27.6ºC and 34.7% relative humidity (RH) for two boundary conditions: (1) considering heat conduction, convection, and latent heat generation in the airway, mucus layer, and tissue; and (2) a constant airway wall temperature of 37ºC. Results show that while the average RH in condition 1 is 2.3% higher than in condition 2, the particle deposition efficiency (DE) is lower, with a maximum difference of approximately 9%. Although deposition patterns are similar between the two conditions, the average diameter of deposited particles in condition 1 is 40.7% smaller than in condition 2, and the average diameter of escaped particles is 14.3% smaller.

**Key words:** heat-transfer boundary; airway; inhalable particle; hygroscopicity; multi-component

## Introduction

In recent years, with deepening research on inhalable particles in the respiratory tract, investigators have increasingly focused on utilizing transport and deposition patterns to achieve targeted drug delivery in the respiratory system. Among these, hygroscopic particle research has attracted considerable attention. Studies have shown that by controlling the initial diameter of hygroscopic particles to minimize deposition in the upper respiratory tract, significant hygroscopic growth occurs after entering the lungs due to substantially higher humidity, leading to increased particle diameter and inertia that enables efficient deposition in the lung[1-3].

Since the hygroscopic growth process is highly sensitive to ambient temperature and humidity[4], accurate simulation of temperature and humidity conditions in the respiratory tract is a prerequisite for predicting the transport and deposition of hygroscopic inhalable particles. However, previous studies have typically employed boundary conditions of constant respiratory wall temperature at 37ºC and relative humidity (RH) of 99.5% or 100%[5,6]. Additionally, current experiments generally use 3D printing and rapid prototyping to fabricate respiratory models from materials such as plastics and resins, making it difficult to replicate mucus transport on respiratory surfaces and tissue heat transfer processes[3,7]. In reality, ambient temperature and RH are generally lower than physiological respiratory conditions, so during breathing, the mucus layer on the respiratory wall and surrounding tissue exchange heat with inhaled air through convective heat transfer, latent heat loss from water evaporation, and conduction within the tissue[8].

This study constructs an idealized mouth-throat model incorporating the mucus layer and surrounding human tissue, and simulates the transport and deposition of hygroscopic inhalable particles under different heat transfer boundary conditions. Specifically, under inlet air conditions of T = 27.6ºC and RH = 34.7%, we compare temperature and RH distributions as well as deposition efficiency and patterns of multi-component particles for two boundary conditions: (1) considering heat conduction, convection, and latent heat from water vapor evaporation in the tissue, mucus layer, and airway; and (2) a constant respiratory wall temperature of 37ºC.

### 1.1 Gas Phase

Due to the gradually contracting cross-section in the mouth-throat model, flow velocity increases progressively, leading to laminar-to-turbulent transition and turbulent flow. Therefore, the Transition SST model is employed for gas-phase flow simulation. For brevity, the governing equations are not listed here; details can be found in previous studies[9,10], and applications in respiratory airways are described in the work of Zhang and Kleinstreuer (2011)[11]. To analyze water vapor distribution in the respiratory tract, two species—dry air and water vapor—are adopted. The species transport model is given by[12]: $e_{surf} v_e^{sat}$

The corresponding energy equation is[12]: $\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (k \nabla T)$

### 1.2 Particle Phase

The particle-phase governing equations consist of two main aspects. One is the motion equation. Assuming inhalable particles form a dilute phase and inter-particle collisions are neglected, their motion can be determined by Newton' s second law[13,14]: $\rho_p \frac{d\mathbf{u}_p}{dt} = \mathbf{F}_{drag} + \mathbf{F}_{other}$

The other is the interaction equation between particles and vapor in the surrounding fluid. This model assumes a thin layer of negligible thickness on the particle surface, where the gaseous component concentration is determined by the surface composition of the particle (droplet). During the mass transfer process between vapor components in this thin layer and those in the surrounding fluid, the average mass flux of the evaporable component e is[15,16]: $Sh D_e \frac{C_{e,\infty} - C_{e,surf}}{\delta}$

From this, the hygroscopic growth/evaporation of particles can be determined[6,15,16]. In Equation (4), the mass fraction of component e at the particle surface, $Y_{e,surf}$, is obtained from the modified Raoult' s law[4,15,16]: $Y_{e,surf} = \alpha_{ve} X_e \gamma_e p_{sat}$

### 1.3 Solid Phase

Only heat conduction occurs in the solid phase, with the governing equation: $\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + S_h$, where the heat source term $S_h$, representing the heat absorbed by water vapor evaporation in the mucus layer, exists only in grid cells representing the mucus layer.

The water vapor flux on the mucus layer can be obtained from the following equation: $J_{wv} = h_m(C_{wv,surf} - C_{wv,\infty})$. From this, combined with the latent heat of vaporization of water, $S_h$ can be determined.

## 2 Simulation Object and Conditions

The cavity structure of the idealized mouth-throat model follows that proposed by Zhang et al. (2006)[17], with an oral inlet diameter of 30 mm and a throat outlet of 8.5 mm. Wu et al. (2014) reported that the thickness of respiratory tissue affected by heat transfer is approximately 0.5 mm[8]; therefore, a mucus layer-tissue region with a total thickness of 1 mm was added outside the model used by Zhang et al. (2006). The schematic diagram of the idealized mouth-throat model and mesh generation is shown in Figure 1 [Figure 1: see original paper]. The fluid domain employs an O-grid topology with boundary layer refinement to ensure the first grid y+ value is less than 1. A similar refinement method is used for the mucus layer-tissue region, where the first layer adjacent to the fluid has a thickness of 10  m, representing the mucus layer, while the remaining nine layers gradually increase in thickness to occupy 990  m, representing the surrounding respiratory tissue. Three grids with 616,000, 2.893 million, and 9.885 million cells were generated. After grid independence verification, the grid with 2.893 million cells was selected, comprising 2.287 million cells in the fluid domain and 606,000 cells in the mucus layer-tissue region.

The simulation assumes a steady inhalation flow rate of 23.6 L/min (Reynolds number Re = 832.6 at the inlet and Re = 2938.7 at the outlet), with a parabolic velocity profile for laminar flow at the inlet. The wall RH is assumed to be 99.5%, while the inlet air conditions are T = 27.6ºC and RH = 34.7%. Flow simulations are first conducted for two-component gas (dry air and water vapor) under two conditions: (1) considering heat conduction, convection, and latent heat, and (2) constant respiratory wall temperature of 37ºC.

After flow simulation convergence (residual $< 10^{-4}$), transport and deposition of hygroscopic multi-component particles are simulated in the steady flow field. The particles initially consist of water, alcohol, NaCl, and fluorescent agent with a mass ratio of 400:100:100:2.5. Under low RH conditions, particles evaporate water and alcohol components to form solid particles (containing only NaCl and fluorescent agent, with a diameter of 44.3% of the initial diameter). When particles enter high RH regions near the wall, hygroscopic growth may occur. As shown in Table 1 , eight groups of simulations with different particle initial diameters are performed for each boundary condition to obtain the relationship between particle deposition efficiency and Stokes number.

In each particle transport and deposition simulation, 10,000 particles are released at the inlet. The particle distribution probability density at the inlet is proportional to the local velocity, resulting in a parabolic profile, and the initial particle velocity equals the flow velocity. To ensure stability of the hygroscopic/evaporation simulation, the particle motion time step is set to $10^{-7}$

s. Additionally, particle fluctuating velocity[18] and near-wall correction for turbulent fluctuations[19] are implemented through self-developed UDFs.

## 3 Results and Discussion

### 3.1 Temperature and RH Distribution

Due to space limitations, the flow field distribution in the idealized mouth-throat model is not detailed here; specifics can be found in previous studies[17]. Figure 2 [Figure 2: see original paper] presents the temperature distributions on the mid-plane, outlet, and within the mucus layer for both the heat-transfer boundary (condition 1) and constant wall temperature (condition 2). Overall, the temperature distributions on the mid-plane and outlet (Figure 2(a)) exhibit patterns similar to the velocity field but with opposite trends, as the inlet air temperature is lower than the respiratory boundary, and the faster-moving air in the pipe center cannot fully exchange heat with the respiratory surface. When considering heat conduction, convection, and latent heat effects on the respiratory surface (Figure 2(b)), non-uniform temperature distribution in the mucus layer is clearly observed, with lower temperatures in the curved pharyngeal region due to enhanced convective heat transfer and water vapor evaporation from airflow scouring. Under constant wall temperature conditions, temperatures near the wall are higher than in condition 1 (Figure 2(c)), and no temperature gradient exists in the mucus layer-tissue region at the outlet.

Figure 3 [Figure 3: see original paper] shows the RH distributions on the mid-plane and outlet of the idealized mouth-throat model under different conditions. The two distributions are similar, but the high RH region in condition 1 extends more deeply into the central flow area at the pharynx and outlet. Comparing the average RH in the fluid domain reveals that condition 1 is 2.3% higher than condition 2. Previous studies have found that the hygroscopic growth process of particles is highly sensitive to RH[6]; if extended to the entire respiratory system, this could lead to significant differences in hygroscopic particle deposition.

### 3.2 Deposition Rate

Figure 4 [Figure 4: see original paper] shows the relationship between hygroscopic particle deposition efficiency and Stokes number under both conditions. It can be observed that despite the relatively higher average RH in the fluid domain in condition 1 (see Figure 3(a)), its deposition efficiency remains lower than that of condition 2 (the maximum deposition efficiency difference is approximately 9% at St = 0.025). This differs from the positive correlation between particle hygroscopic capacity and RH under constant temperature conditions, suggesting that the hygroscopic growth/evaporation process of particles may depend not only on RH but also on temperature. Therefore, the simplified constant wall temperature condition may overestimate hygroscopic particle deposition efficiency. Meanwhile, under this condition, the RH in most regions of the respiratory tract remains below the threshold for NaCl hygroscopic growth[20,21].

### 3.3 Deposition Distribution

Figure 5 [Figure 5: see original paper] shows the deposition and exit distributions as well as final particle diameters for hygroscopic particles with an initial diameter of 11.25 m under both conditions. Since the differences between the two conditions primarily lie in temperature, the flow field and particle trajectories are essentially similar. It can be observed that deposited particles concentrate mainly in the curved throat region, while particles are relatively uniformly deposited around the entire throat circumference, indicating that particles follow secondary flow motion to some extent rather than being directly controlled by inertia to collide with the posterior wall. This is likely related to particle shrinkage due to evaporation of water and alcohol components in the low RH region at the inlet section. Meanwhile, observing the particle distribution at the outlet reveals that large particles concentrate mainly near the wall, i.e., in high RH regions, with some large particles entrained into the central airway by secondary flow. Particles in regions with RH $< 70\%$ (refer to Figure 3) remain essentially dry (shown in blue in Figure 5). Statistical analysis of particle diameters in Figure 5 shows that the average diameter of deposited particles is 6.20 m in condition 1 and 10.45 m in condition 2, while the average diameter of escaped particles is 6.15 m in condition 1 and 7.18 m in condition 2. This difference may become more pronounced in more complex flow fields (such as the nasal cavity) or larger respiratory tract regions.

## Conclusions

This study constructed an idealized mouth-throat model incorporating the mucus layer and surrounding human tissue, and simulated the transport and deposition of multi-component hygroscopic inhalable particles under inlet air conditions of 27.6ºC and 34.7% RH. Two boundary conditions were compared: (1) considering heat conduction, convection, and latent heat in the airway, mucus layer, and tissue; and (2) constant respiratory wall temperature of 37ºC. The temperature and RH distributions in the idealized mouth-throat model as well as particle deposition efficiency and patterns were analyzed. The main conclusions are:

1) When considering heat conduction, convection, and latent heat, non-uniform temperature distribution in the mucus layer below 37ºC can be clearly observed.

2) Under condition 1, the average RH is about 2% higher than in condition 2, yet particle deposition efficiency is lower, with a maximum difference of up to 9%, indicating that particle hygroscopic growth depends not only on RH but also on temperature distribution.

3) Particle deposition patterns are similar under both conditions, but the average diameters of deposited and escaped particles in condition 2 are 40.7% and 14.3% larger than in condition 1, respectively. This difference may become more significant in complex flow fields (such as the nasal

cavity) and larger respiratory tract regions, though this remains to be investigated.

## Nomenclature

$c_p, T$: Specific heat at constant pressure
$D_{wv}$: Water vapor thermal diffusion coefficient
Mass diffusion coefficient of component e
Turbulent thermal conductivity
Kelvin effect correction factor for component e
$v_e^{sat}, p_T$: Saturation pressure at temperature T
Schmidt number
Sherwood number
Mole fraction of component e in solution
Gas mass fraction
Activity coefficient of component e in solution
Turbulent dynamic viscosity

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