Medical Spray Dynamics in an Innovative Hood-Shaped Inhaler

D. Katoshevski¹*, T. Shakked¹, D. M. Broday² and I. Amirav³
¹Department of Biotechnology and Environmental Engineering
Ben-Gurion University of the Negev
Beer-Sheva, Israel
²Faculty of Civil and Environmental Engineering
Technion – Israel Institute of Technology
Haifa, Israel
³Pediatric Department, Sieff Hospital, Safed, Israel

Abstract
Using a hood for aerosol therapy to infants was found to be effective and friendly to handle over the commonly used face-mask. The currently available hood design has yet a greater potential in terms of efficiency, and a numerical simulation can serve as a tool for its optimization. The present study describes the development and utilization of a numerical simulation for studying the transport and fate of the aerosol particles and the carrier gas within a 3-D realistic representation of the hood and the infant's head. The study further incorporates realistic breathing patterns, with longer expiration phase than the inspiration one. Both nose and mouth breathing are simulated. While the base case assumes that the funnel that delivers the aerosol within the hood is perpendicular to the infant's face, more realistic scenarios include a funnel that is slanted with respect to the infant face, the infant's head taking a general position with respect to the funnel, and the funnel and the head being both tilted. In addition, the assessment of the amount of aerosol that reaches the eyes of the patient when administering medications with such a device was studied. A good agreement is found between computation and experimental results. As expected, the most efficient drug delivery, 18%, is achieved when the funnel is normal to the infant's face. The quantitative evaluation of different scenarios presented in this work increases the knowledge of physicians, nurses and parents regarding the efficacy of the treatment, in terms of the actual amount of drug inhaled under various modes of function of the device.

*Corresponding author
Introduction

A major drawback of delivering aerosol medication with a face mask is the difficulty of achieving a good mask-face seal when the infant is screaming and crying [1]. Moreover, nebulizer treatments take about 10 minutes, much longer than most infants readily tolerate when using a mask. The infant's impatience further reduces the efficiency of drug delivery to the lungs [2,3]. It was found that the hood is preferred by parents and better tolerated by infants and has the same drug delivery efficiency as the conventional face mask [4]. This has led to the development of a hood-shaped device in the form shown in Fig. 1. A realistic and representative configuration with realistic nasal breathing that is practiced 80% of the time by infants are considered. Specifically, this work considers a detailed 3-D configuration of the hood and the infant's head, including the chin, shoulders, mouth, nose and nostrils, with all dimensions based on data from a real 5-month-old infant [5]. This model enables to investigate drug administration while the infant is breathing through the nose or the mouth, as well as when the funnel and the head are not tilted co-linearly. Moreover, a full transient solution has been calculated, which is necessary when dealing with realistic time-varying breathing functions like those implemented in this study at the openings of respiratory system. Normally, such a breathing pattern includes regular tidal breathing with inspiratory duty cycle (IDC) of 0.4(7) (the fraction of inspiration time to the breathing period). Using a hood device may adversely deliver unwanted medications to the eyes of the infant. The current study also addresses the extent of aerosol deposition at the infant's eye-zone.

The Hood

The hood system includes a funnel (effective volume of 238 cm³), a pneumatic nebulizer, a hemispherical and flexible plastic cape that encloses the infant's head, and four folding legs. The funnel delivers the aerosolized drug to the infant. It can be manually adjusted for better performance by moving it up and down and by tilting it in any direction at a wide range of angles (Fig. 1). The end of the funnel is narrower in order to direct the aerosol towards the openings of the infant's respiratory system. The nebulizer is attached at the top of the funnel with an adapter and is driven by a small-sized compressor that operates at a flow rate of 7 l/min and provides a mass flux of 0.25 g/min. Drug droplets of about 5 µm in diameter are produced by the nebulizer.

Method

A commercial computational fluid dynamics (CFD) software (FLUENT 6.1, Fluent Inc., USA), which is based on the finite volume method, was used to solve the governing equations subject to time varying boundary conditions. Specifically, the flow fields of the air and the discrete phase were taken to be non-steady, the injection of aerosol was assumed continuous throughout the cycle, and realistic breathing patterns were implemented at the openings of the respiratory system (the mouth and the nostrils). The flow field was obtained by solving the mass and momentum conservation equations. The continuity equation for the continuous phase (air) in Cartesian coordinate system reads:

\[
\frac{d\rho}{dt} = -\frac{\partial p u_i}{\partial x_i}
\]

where \( u_i \) is the i-th component of the velocity vector \( \vec{u} \) and \( \rho \) is the air density. The momentum equation for the air is:

\[
\rho(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u}) = -\nabla p + \rho \vec{g}
\]

and \( \mu \) is the dynamic viscosity of air. Since \( Gr/Re^2 \ll 1 \), where \( Gr \) is the Grashof number and \( Re \) is the flow Reynolds number, natural convection due to non isothermal conditions of the air can be neglected (i.e., apart from a narrow layer near the mouth and the nostrils, the flow field in the hood is unaffected by temperature disparity due to an efficient convective mixing). The dispersed phase is simulated using a Lagrangian frame of reference. This phase consists of spherical aerosol particles (droplets) dispersed in the continuous phase. Particle trajectories are calculated by accounting for the total force acting on the particles. Conservation of momentum for the particles reads,

\[
\frac{d\vec{u}_p}{dt} = F_D(\vec{u} - \vec{u}_p) + \vec{g}(\rho_p - \rho)/\rho_p
\]

where \( F_D(\vec{u} - \vec{u}_p) \) is the drag force per particle mass,

\[
F_D = \frac{18 \mu}{\rho_p d_p^2} \frac{C_D R_e}{24}
\]
\[ C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \]  \hspace{1cm} (6)

where the a's are empirical constants. Integration of Eq. 4 yields the particle velocity. The particle position is calculated then by a second integration,

\[ \frac{dx_i}{dt} = u_{p,i} \]  \hspace{1cm} (8)

Results

When the funnel is vertical and normal to the infant's face, the computational geometry is symmetrical (Fig. 2a). The air accelerates as it moves toward the funnel's narrow exit and the velocity field within the funnel and at short distances away from it is not affected by the infant's breathing pattern. For this base case configuration, model results revealed that after six complete breathing cycles with continuous injection of aerosol particles at the entrance to the computational domain (approximately 5000 particles per time step), 18% of the particles were inhaled through the nostrils by the infant. Since the lips perturb from the face to some degree, they may have a local effect on the flow field near the nostrils. In order to test whether this has any effect on aerosolized drug administration we implemented a computational geometry with lips. The amount of aerosol entering the respiratory system through the nostrils was identical to that calculated under the no-lips case, suggesting that the lips do not affect the aerosol inhalation through the nostrils. In fact, the funnel was positioned just above the infant's nose even when breathing through the mouth was considered. This breathing mode is not common among infants but may reflect special conditions, such as a rhinitis. Under mouth breathing, only 7% of the aerosol introduced at the entrance to the funnel penetrates the mouth. Under normal operation conditions we expected that the funnel, the head, or both will be inclined, therefore we chose to implement inclinations representing angles which frequently occur in realistic scenarios. When the funnel is tilted at 10° sideways (along the x-axis) while the head is at its base configuration (Fig. 2b), simulation of nasal breathing with IDC of 0.4 revealed a decrease in the amount of aerosol particles penetrating through the nostrils (3.5%). A considerable amount of drug is therefore lost, since most of the air that emanates from the funnel does not approach the nostrils but is rather drifted away. When the funnel is tilted at 10° along the z-axis (in the longitudinal direction) while the head is at its base configuration (Fig. 2c) the amount of drug delivered to the nostrils is 4.5%. The sharp decrease in drug delivery in these two last configurations relative to the base case one is due to the non-axisymmetric nature of the problem. In the more general case, when the funnel is positioned at an angle of 10° to the x-z plane (Fig. 2d) only about 5.5% of the particles reach the nostrils. This result shows the non-additive (i.e. non-linear) nature of the inhalability with respect to geometrical variations of elements that build the scenario. When the head is tilted sideways (in the x direction) and the funnel is kept vertical (Fig. 2e) only 6% of the particles introduced to the system penetrates the nostrils. Compared to the case when the funnel is tilted sideways and the head is at its base configuration, this result clearly shows that inhalability is non-commutative with respect to variations in the scene. In reality, oftentimes both the funnel and the head are non-collinear. This scenario was examined with both the head and the funnel tilted at 15° sideways towards the same direction (Fig. 2f). About 14.5% of the drug particles were inhaled through the nostrils. Another realistic configuration is when the head is tilted sideways while the funnel is inclined randomly with respect to the x-z plan. One possible configuration, simulated here, is when the head is tilted sideways at 15° and the funnel makes an angle of 15° with the normal to the x-z plan (Fig. 2g). Nasal breathing under such conditions results inhalability of about 1.5%. Regarding the deposition at the eyes, it was found that under optimal working conditions (i.e. when the infant's head is aligned to the funnel) the percentage of aerosol reaching the eyes zone is 0.48%. However, when the funnel is tilted toward the eyes the amount of aerosol reaching the eyes' zone is predicted to be 4.7%. An IDC of 0.4 is a general characteristic of infants' breathing. However, due to normal variability different infants will have slightly different IDCs. To study the effect of that variability on drug delivery, different IDC's were simulated (IDC=0.35, 0.45 and 0.5). A linear relationship between the IDC and the percentage of aerosol delivered to the infant's nostrils was found. This behavior is expected since as the inspiration period increase the amount of inhaled aerosols increase comparably.

Discussion

A three dimensional model for studying aerosolized drug delivery to infants using the nebulizer hood has been developed. The advantage of studying this system using a CFD model is the possibility to examine different realistic scenarios while avoiding confounding factor that are unavoidable in clinical experiments. As expected, the most efficient way to deliver aerosol particles to the openings of the respiratory system using the nebulizer hood is with the funnel normal to an infant's face. Any other configuration reduces the hood efficiency. In particular, a considerable decrease in the efficiency occurs when the funnel, the head, or both are
tilted. In such cases, the infant's breathing is not intense enough to overcome the inertia of the aerosol that emanates from the funnel. A major part of it (and its active agents) is therefore directed away from the openings of the respiratory system and is lost. When both the head and the funnel are tilted, an inclination of the funnel toward the face is obviously advantageous and succeeds in compensating somewhat for the non collinear configuration. However, when the funnel is directed away from the infant's face the overall system efficiency is reduced significantly. These results suggest that correct operation of the hood, more than variation of its design, is the key parameter for success in administering aerosolized therapeutics using the nebulizer hood. Thus, the caregiver should be advised to verify that during nebulizer hood treatments the funnel should always be positioned such that it is directed towards the head. Ignoring this rule will hamper the efficacy of the treatment considerably and require extended treatment durations to achieve the same results (dose). Experimental data was used to validate the model, it was found that the experiment results is in excellent agreement with the model results, suggesting that the numerical model is reasonably accurate and can indeed be used to study the efficiency of the hood nebulizer under a wide range of operating conditions.

References
Figure 1. The nebulizer hood inhaler. The arrows show possible modifications of the funnel.

Figure 2. Different configurations of the funnel and the infant's head [5]. (a) Base case - the funnel is normal to the infant's face, (b) the funnel is tilted sideways (along the $x$ axis), (c) the funnel is tilted in the longitudinal direction (along the $z$ axis), (d) the funnel takes a general inclination with respect to the vertical, (e) the head is tilted sideways (in the $x$ direction) while the funnel is vertical, (f) the head and funnel are tilted sideways towards each other, and (g) the head is tilted sideways (along the $x$ axis) and funnel is arbitrarily inclined to the vertical.