CFD Modeling of Two Phase Flow in an Innovative Nebulizer Hood

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Introduction

Conventional aerosol delivery in nebulizer treatments involves the use of face mask which function as the interface between the aerosol generator (nebulizer) and the infant's mouth and nose. In order to achieve optimum aerosol therapy a perfect seal between the mask and the infant's face is required. It has been shown that even 1 cm gap between the mask and the infant's face reduces the drug delivery by 50%. A good seal is difficult to achieve in infant's because of squirming and crying, especially since nebulizer treatments take about 15 minutes, much longer than most infants tolerate. The drug delivery to the lungs is greatly reduced as the infant becomes impatient and obstreperous. This led to the development of more patient friendly interface for aerosol delivery, by means of a nebulizer hood. The aerosol is generated with a nebulizer that is attached to the top of the funnel, that is the pipe that delivers the drug to the patient, the hood consist of dome shape enclosure placed on the infants head. Aerosol therapy for wheezy infants by a nebulizer hood interface was proven to be as efficient as administration using a mask, in addition it was found to be preferred by parents, much better tolerated by infants, simple to operate and because treatment with nebulizer hood does not involve the use of a mask, the medication can readily be administered during sleep. A useful insight for further improvements of the nebulizer hood can be achieved with careful examination of the airflow and medical aerosol distribution inside the hood. Unstable breathing pattern is an inherent characteristic of normal healthy infants during sleep. The occurrence of short duration apneas is a physiological phenomenon that declines with advancing postnatal age. In this study we examine numerically the two phase flow, that is the air and the medical aerosol, inside the hood during three breathings phases: 1.inspiration 2. expiration 3. apnea. The conservation equations for the continuous phase, that is the air, and the dispersed phase, that is the medical aerosol was solved using the FLUENT 6.1 computational fluid dynamics (CFD) software. The geometry was generated with the GAMBIT software package.

Methods

The nebulizer hood consists of a hemispherical shaped plastic cape, four folding legs, and a funnel (the pipe that delivers the drug to the patient), with an effective volume of 238 cm^3. The nebulizer is attached to the top of the funnel with an adapter (Fig.1) . The nebulizer is driven by a small-sized compressor with flow rate of 7 l/min and has mass output of 0.25 g/min, and produces particles around 5μm in diameter.

Figure 1. The nebulizer hood.

In the present simulations, we considered an axisymmetric geometry that was generated and meshed using the GAMBIT software package (Fig.2). The mesh was generated using a scheme that creates a regular structured grid of mesh elements. The mesh is composed primarily of quadrilateral elements but includes also triangular corner elements. In order to achieve accurate calculations at the more complex regions, we used finer mesh between the exit of the funnel and the infant's mouth. In the base case, the tip of the funnel was set 2 cm above the mouth. The number of nodes in the calculation domain is 3232. The grid was constructed in a manner that the solution is grid independent. The length of the funnel is 0.173 m and the diameter of the mouth and head is 2 cm and 20 cm respectively. The governing equations was solved with FLUENT 6.1 Computational Fluid Dynamics (CFD) software package. It was assumed that the infant's tidal volume is 80 cm^3. The simulation was conducted with respect to three breathing phases:
1. inspiration 2. expiration 3. apnea. The simulation was conducted applying steady air flow for the air and transient motion for the aerosol. At inspiration and expiration a constant flow rate without pause was applied at the mouth in addition, a single injection of aerosol was considered instead of continuous injection. The above assumptions were checked using transient condition for both, the air and the aerosol, applying continuous injection of aerosol and in particular with respect to the temporal condition at the mouth, a physiologically superior periodic flow boundary condition was applied, the assumptions were found to be acceptable.

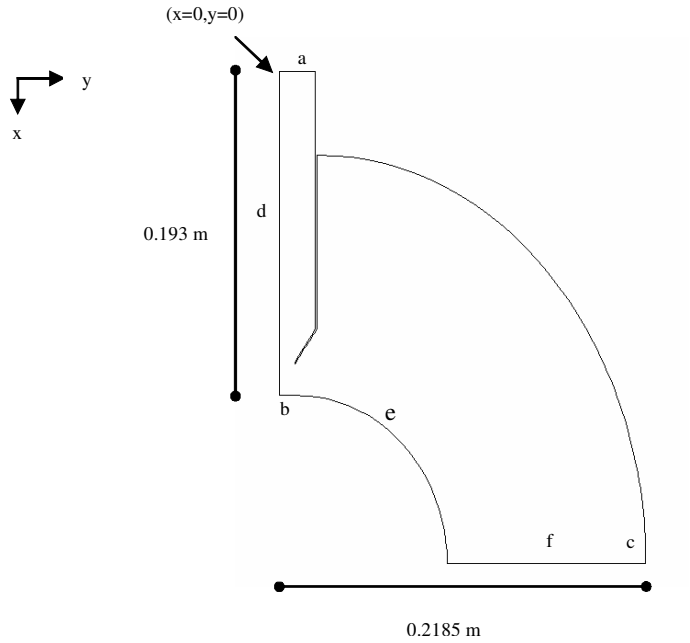

Figure 2. Hood geometry. The zone marked by a represents the exit of the nebulizer (the entrance to the computation domain), the zone marked by b represents the infant's mouth, and the zone marked by c represents the circumferential slit. The line d is the axis of symmetry; line e represents the head, and line f represents the surface that the infant is lying on.

The governing equations for the continuous phase are the continuity and Navier Stokes equations. The trajectories of the aerosol particles are calculated by accounting for the total force acting on the aerosol particles:

$$\frac{d\overline{u}_p}{dt} = F_D(\overline{u} - \overline{u}_p) + \overline{g}(\rho_p - \rho)/\rho_p + F_x \tag{1}$$

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

$$F_D = \frac{18\mu}{\rho_p d_p^{\,2}} \frac{C_D R_e}{24}, \tag{2}$$

$\overline{u}$ and $\overline{u}_p$ are the velocity vectors of the fluid phase and the dispersed phase respectively, ρ_p is the particle density, and d_p is the particle diameter. The particle Reynolds number Re is defined as

$$R_e = \frac{\rho d_p \left|\overline{u}_p - \overline{u}\right|}{\mu} \tag{3}$$

and the drag coefficient C_D is defined as

$$C_D = a_1 + \frac{a_2}{\mathrm{Re}} + \frac{a_3}{R_e^{\,2}}, \tag{4}$$

where the a's are empirical constants. The last term on the RHS of Eq. (1), F_x, represents additional forces that can be accounted for, such as inter-particle forces, but was not

addressed at this present study. Integration of Eq. (1) yields the components of the particle velocity $u_{p,i}$. The particle position x_i is calculated then by a second integration.
The boundary conditions for the two phase flow are as follow, for the air, air velocity was specified at the exit of the nebulizer, at the entrance to the infant's mouth, and on the walls of the funnel and the hood (no slip). At the circumferential slit where air exits the hood, i.e. the gap between the hood and the surface on which the infant is laying, atmospheric pressure was specified. The different breathing phases, inspiration, expiration and apnea are simulated by applying positive, negative, and zero air velocity at the infant's mouth, respectively. For the dispersed phase, particle size and cross-sectional distribution at the entrance to the funnel was given. At the solid boundaries of the calculation domain, except the funnel walls, a "trapped" condition is applied, that is when a particle touches a wall deposition occurs. At the funnel walls a "reflect" condition was applied, thus particles rebound when they touch the funnel's wall and eventually reach its exit in a manner that simulate realistic situation where particle that impacts the wall will stick on it and flow along it. This was achieved in the following way, particle that rebounds from the wall immediately will impact it again and then will rebound and so on until it will reach the funnel exit. At the circumferential slit an "escape" condition is applied, implying that a particle passing this boundary leaves the computation domain and is lost for further calculations.

Results

The dynamics of both the carrier air and the aerosol are analyzed. The validity of using a constant airflow during inspiration and expiration is tested against results of a more physiologically realistic time-varying solution, i.e. where periodic mouth breathing is implemented. The effect of manufacturing modifications of the hood and the effect of natural variability in the tidal volume on drug delivery is also examined. During inspiration the air accelerates as it moves through the funnel toward its narrow exit cross section, the air decelerate as it approaches the infant's mouth and achieves an average velocity that is approximately half its velocity at the funnel's exit. Air contours of velocity magnitude in the zone between the funnel's exit and the mouth are presented in Fig. 3. 5000 particles were introduced at the nebulizer exit. The results reveal that 84% of these particles penetrate the infant's mouth, 11% deposit on the head, and 5% deposit on the surface on which the infant is lying. During expiration there is a counter flow, resulting from the two opposing streams coming from the funnel and from the infant's mouth. As the two streams approaching the impact zone they forced to decelerate and the static pressure increase. These features may be somewhat affected by the air being non-isothermal due to temperature differences between air supplied by the funnel and the exhaled air. For this reason, the temperature of the air exhaled from the infant's mouth was fixed at 37^{o} C, the temperature of the emerging air from the nebulizer is set to 20^{o} C and the temperature of all other boundaries, surfaces, and fluxes was set to 25^{o} C. Apart from a narrow layer with T~37^{o} C near the mouth, the flow field in the hood seems unaffected due to an efficient convective mixing. The simulation revealed that all the particles escape through the circumferential slit. During Apnea the velocity at the mouth was set to zero, thus the air that comes from the funnel is forced to decelerate. The results reveal that 22% of the particles are trapped at the mouth, 24.6% , deposit on the head, 47% deposit on the surface on which the infant is lying, and 6.4% escape through the circumferential slit.

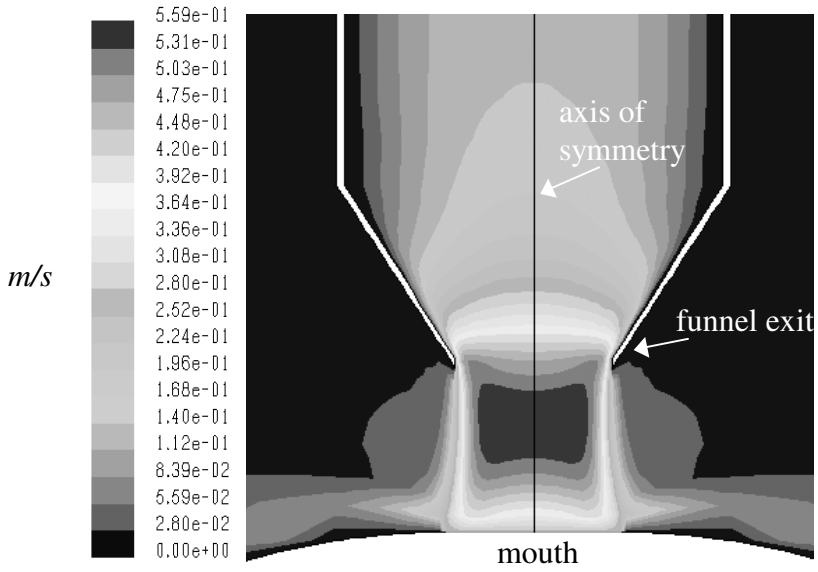

Figure 3. Air contours of velocity magnitude in the zone between the funnel's exit and the mouth during inspiration.

To simplify procedures, speed the simulations, and permit simple design analysis of the hood, the previous results were obtained by accounting for a steady air flow and a transient motion of the dispersed phase. This implies that the flow field of the dispersed phase changes much faster than that of the continuous phase (air). Indeed, the travel time of particles between the funnel's end and the mouth is approximately 2.5% of the breathing period. This suggested that a steady solution may be suitable for analyzing drug delivery in the hood. In addition, a constant flow at the mouth is forced during inspiration and expiration and the traced particles are introduced into the system simultaneously, thus not reflecting a continuous supply of aerosol particles by the nebulizer. In order to verify that the calculation and post processing procedures employed are reasonable, a more realistic configuration has been simulated. Specifically, the time variation of the air flow through the mouth was implemented using the POLYMATH software package. The periodicity is obtained by recalling this condition repeatedly during the multi-breath simulation, in addition continues injection of aerosol is implemented along with full transient simulation, that is, transient flow for both, the air and aerosol.

Two cases were examined. For a one breathing cycle (the second breath), 38.4% of the drug particles penetrate the mouth in the transient calculation as compared to 42% in the steady solution. When apnea of 4 sec was introduced after 6 consecutive breathing cycles, about 10% of the drug particles deposit on the head in both the steady and the transient simulations. These results indicate that the steady solution procedure is fairly reasonable and can be used for a further investigation of the hood. A study on the role of various design parameters on the flow field and drug distribution within the nebulizer hood was conducted. It was found that wider funnel exit decelerates the air compared to the base case. During inspiration, the average velocity of the air upon leaving the funnel continues to decrease and adjusts to the inhaled air velocity at the mouth. it was found that 81% of the particles are inhaled by the infant through the mouth , 11% deposit on the head and 8% deposit on the surface. During expiration. 2% of the particles deposit on the head, 14% deposit on the surface and the remaining 84% escape through the circumferential slit. For the apnea phase, the average velocity of the air that exits the funnel decreases to zero at the mouth. It was found that 7.6% of the particles are trapped at the mouth, 16% deposit on the head, 73% deposit on the surface and 3.4% escape via

the circumferential slit. Halving the slit width, increasing the hood diameter by 30%, and changing the geometry of the hood into a cube-shaped tent (initial design) showed minor effects on the flow field in the vicinity of the infant's face, and no effects whatsoever on particle penetration to the infant's mouth. Introducing inhomogeneous spatial aerosol distribution at the entrance to the domain in a manner that there is homogenous distribution only at three quarters of the entrance lead to 95% deposition at the mouth during inspiration. We also examined the effect of different tidal volumes. Two cases were studied: an increase and a decrease of 10% in the tidal volume with respect to the base case. For the decrease case, during inspiration, 80.4% of the particles were inhaled by the infant via the mouth, 10.6% deposit on the head, and 9% deposit on the surface. For expiration, 58.6% of the particles deposit on the surface and 41.4% escape via the circumferential slit. For the increase case, during inspiration, 87.4% of the particles were inhaled, 9.6% deposit on the head and 3% deposite on the surface. For expiration, there were no significant effects on the calculated flow field with respect to the base case.

Summary

The work presented here, which studies in detail a new nebulizer hood device devised to answer practical problems that arise when administering aerosolized medications to wheezy infants. In the basic configuration, the airflow within the funnel and at its exit is not affected by the breathing phase of the infant. Hence, the drug supply to the exit of the funnel is unaffected by the breathing phase, in all three breathing phases the air is forced to decelerates as it moves toward the infant’s mouth. This deceleration forced the aerosol to flow away from the mouth toward the periphery of the hood and out through the circumferential slit. Inhomogeneous air temperature has no effect on the delivery of the drug to the infant's mouth. As predicted, changing the geometry of the hood, but keeping the region between the funnel exit and the infant's mouth unaffected (i.e., same separation distance), has no effect on the drug-to-mouth delivery efficiency. If the distribution of the aerosol at the entrance to the funnel could be manipulated, a "core" enhanced distribution can increase the amount of drug arriving to the mouth. The analysis of the hood under steady breathing conditions was found suitable and accurate enough for further evaluation of the hood and its design. In order to further validate our results, we compared the amount of drug estimated to deposit on the head during 6 consecutive breathing cycles of inspiration, expiration, and apnea of 4 sec to experimental data. The simulations suggested that 37% of the drug that leaves the nebulizer reach the mouth (including particles that deposit at the mouth during apnea), 10.3% deposit on the head, 13.7% deposit on the surface, and the remaining drug (39%) exit the hood. These figures are in good agreement with the experimental data, although the geometry of the hood in the experiments was somewhat different from the one simulated . The work presented here can serve as an efficient tool for examining ways to further improve nebulizer hoods as an alternative drug administration tool to infants and young children who are unable to use efficiently masks, MDIs, and other standard apparatus used in aerosol therapy. Ample of cases in different fields proved that engineering-oriented CFD study is capable of improving product design and performance. It is our belief that such concepts can be utilized to improve the design of nebulizer hoods.