Computational Fluid Dynamics Modeling of Rollins7 Oxygen Mask

Abstract

This study's objective was to model the Rollins7 Oxygen Mask using Computational Fluid Dynamics (CFD). A three-dimensional CFD model was used to compute the flow dynamics of a simulated breathing patient. The numerical model was based on the finite volume method using an structured grid with tetrahedral cells. A low Reynolds number realizable k–ε viscous model was used to predict turbulence and the SIMPLE method was used to compute the pressure. To account for the influence of the three-dimensional form of the human body, a model that replicated the actual forms of a real human head was used. First, steady-state conditions were examined with the assumption of steady inhalation (peak inhalation velocity). Subsequently, an unsteady breathing model was introduced and analyzed.

A custom user-defined function (UDF) was used to compute sinusoidal breathing parameters for the patient model. The UDF, in additional to controlling the sinusoidal velocity profile, further controlled: temperature, O2 depletion, CO2 enrichment, and H2O enrichment during exhalation cycle.

The quantitative analyses showed gas flow compositions, velocity profiles, temperatures, and the mixing profiles of the Rollins7 Oxygen Mask under typical mask oxygen flow rates and patient breathing parameters.

Introduction

Rollins 7 Adult Oxygen Mask is a combination device that allows the delivery of aerosolized medication via a nebulizer or metered dose inhaler while providing oxygen therapy. The mask features an over-the-nose enclosed design with elastic straps to hold the mask in position on the patient's face. The Rollins 7 Adult Oxygen Mask is equipped with a single opening near the mouth to allow patients to imbibe food or drink during oxygen or nebulization therapy. This opening also helps to reduce CO2 buildup within the mask during oxygen therapy while still delivering high patient oxygen concentration.

The objective of the study was to fully characterize the performance of the mask under typical conditions using a computational fluid dynamics (CFD) model. The CFD model was used to illustrate mixing patterns, patient oxygen and carbon dioxide delivery concentrations and aerosol drug delivery rates under a variety of respiratory conditions and mask oxygen flow rates.

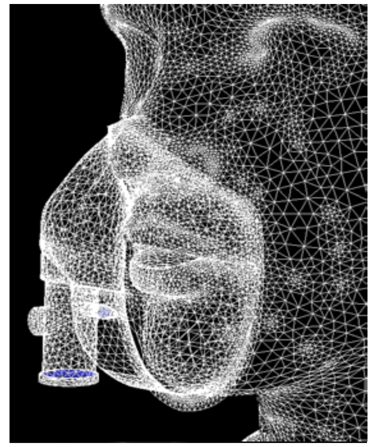
	Rollins7 Oxygen Mask	Mask and Head Model
Picture		
Model Features		
Manufacturer	Rollins Medical	
Model	Rollins7 Oxygen Mask	
Grid Construction	Gambit	
CFD Grid	600,000 Tretrahedral Cells	
Resolution	0.5 mm	

Figure 1: *General Features of the Aerosol Mask and CFD Model.*

General CFD Parameters

The CFD analysis was conducted using Ansys' Fluent package with custom source code generated by ARE Labs to control the breathing parameters of the simulated patient.

A CAD model of the Rollins7 Oxygen mask was obtained form Rollins Medical Solutions, Inc. A three-dimensional human head model was used to represent a patient in the CFD model. The human head model was modified to have an open mouth and throat tube for breathing. The mask was deformed to replicate the deformation that takes place when the mask is placed on a patient. Then the deformed mask was placed on the human head model and the head/mask model was placed in secondary room volume so that wall effects would not influence the results. The finite volume model consisted of approximately 600K tetrahedral cells; resolution at all wall surfaces was less than or equal to 0.1 mm.

The CFD analysis used a pressure based solver with a low Reynolds number realizable k–ε model for the viscous modeling with species transport. The solver used a 2nd order method to compute all values.

For unsteady state cases flow time was incremented in either 0.05 or 0.1 second intervals for a total for 30 seconds model time for each case.

Variation of the air-velocity distribution, species concentrations and influence of the exhalation re-breathing on the inhalation concentrations were examined for this study.

Breathing Model

A custom user-defined function (UDF) was coded for the CFD model to control various aspects of the human model breathing characteristics. The flow rate for the sinusoidal breathing model follows this equation:

$$FlowRate = a_x \sin(\beta t) \tag{1}$$

Where β and a_x are calculated from the below equations:

$$a_x = \frac{\beta V_t}{2} \tag{2}$$

Where V_t is the tidal volume and β is defined by:

$$\beta = \frac{\pi RF}{30} \qquad (3)$$

Where RF is the Respiratory Frequency in Breaths-Per-Minute (BPM). Figure 1 shows the flow rate in liter-per-second for one breathing cycle period using 11 BPM and a tidal volume of 700cc.

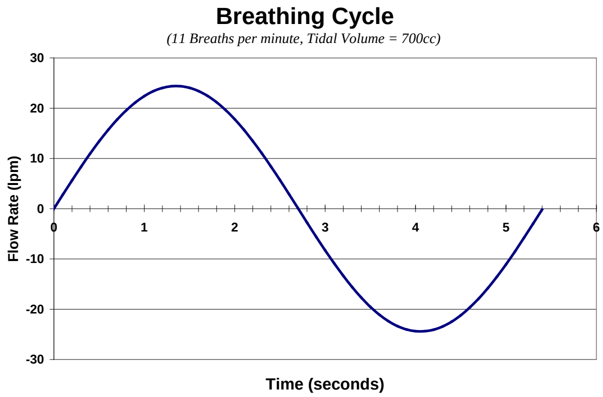


Figure 2: *Flow Rate vs. Time for CFD Model*

For a tidal volume of 700cc with a frequency of 11BPM the graph shows a peak inhalation flow rate of 0.4 lps (24 lpm) with a period of 5.4 seconds. This peak flow rate was used for the Steady State Models to obtain baseline performance.

Total minute volume for the above parameters can be calculated by equation 4 below:

$$MV = V_t \cdot RF \qquad (4)$$

Oxygen consumption was computed from the volume-weighted average of the inhalation oxygen concentration minus a constant use rate for metabolism. For the models a constant use rate of 4% oxygen depletion from the incoming stream was assumed which equates to an oxygen use rate of 0.310 lpm or 410mg/min.

Carbon dioxide enrichment in the exhalation cycle is computed in a similar manner. The exhalation is a function of the incoming carbon dioxide concentration plus a carbon dioxide generation rate. The generation rate was set equal to the oxygen molar consumption rate. The carbon dioxide generation rate for the model was 0.310 lpm or 565 mg/min. Water vapor in the exhaled gases were set to be fully saturated upon exit and temperature was assumed to equilibrate to a body temperature of 37°C (310K) and set for the exhalation cycle.

Steady-State Cases Overview

Initial steady-state models were run to investigate oxygen and aerosol delivery at peak inhalation velocities. The steady-state models were used to establish maximums/minimums and to compare against the unsteady state runs during peak inhalation/exhalation cycles. Although the steady-state runs were helpful in evaluating the CFD model all data in the report are from the unsteady state cases.

Un-Steady Cases Overview

The Unsteady State Model incorporates the full user-defined function (UDF) to control the simulated human patient breathing parameters. The unsteady state cases are divided into three main categories: (I) Oxygen delivery vs. Mask O2 flow rate, (II) Respiratory Parameter Effects on O2 delivery and (III) Validation of the CFD model using Nebulizer Test Data.

I. Mask O_2 Flow Rate Effects on O_2 and CO_2 Delivery

The first set of cases focused on oxygen and carbon dioxide concentrations delivered to the patient as the oxygen flow rate to the mask is increased. The mask oxygen flow was varied form 2 lpm up to 15 lpm.

II. Respiratory Parameters Effects on O_2 and CO_2 Delivery.

The second set of cases focuses on the effect of changing breath per minute (BPM) while leaving the tidal volume unchanged and the effect of changing tidal volume while leaving breaths-per-minute unchanged. Respiratory frequency was varied from 11 to 13 BPM and tidal volume was varied from 700cc to 880cc.

III. CFD Model Validation – Nebulizer Drug Delivery.

The last set of unsteady state cases were used to validate the model accuracy by comparing the model output to actual run data. The run directly compares the aerosol drug delivery rate (ug/min) to a patient when using a nebulizer at a flow rate of 8 lpm. The

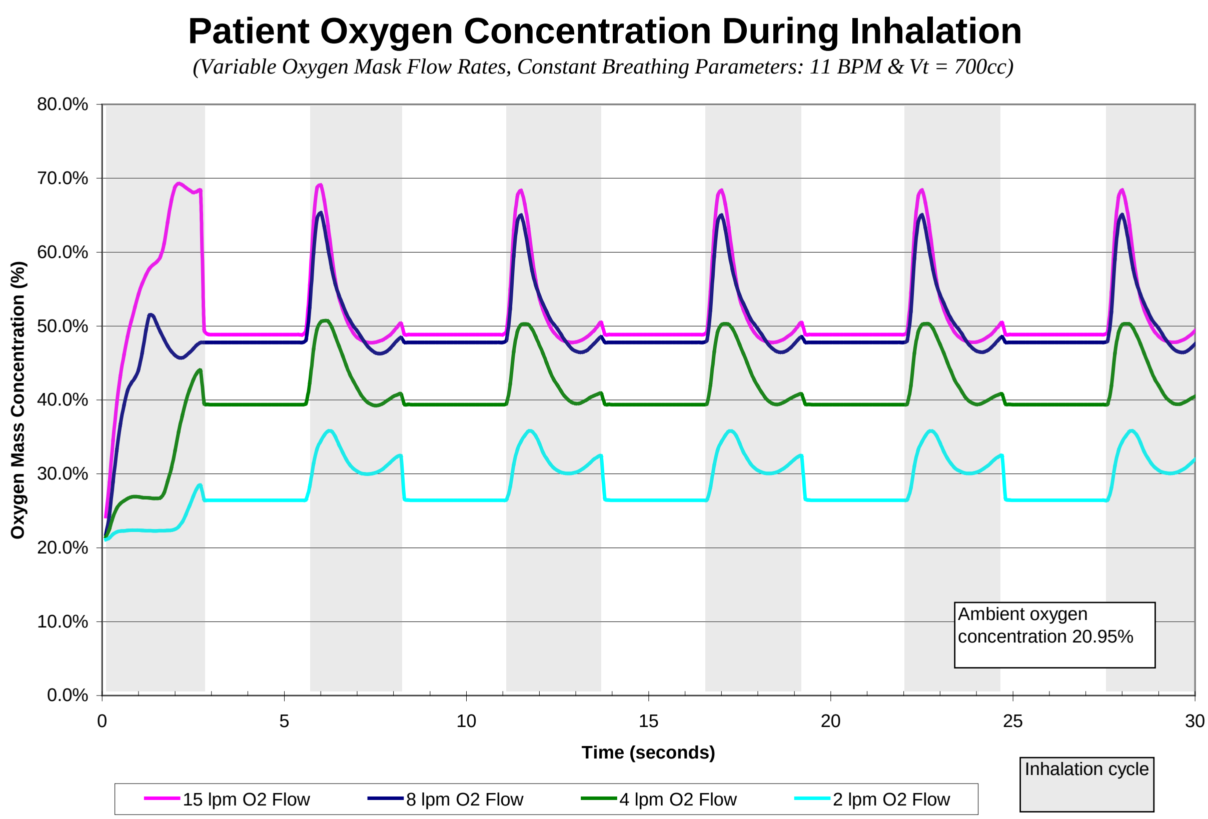


Figure 3: Oxygen Mass Concentration over Time for Various Mask Oxygen Feed Rates.

CFD predicted output was directly compared to test data performed in September 2012 using a ventilated mannequin with the Rollins7 Oxygen mask and albuterol sulfate as the nebulizing drug.

The breathing parameters used for both the model and the test data were 12 BPM and a tidal volume of 750cc for the male resting model and 14 BPM and a tidal volume of 480cc for the female resting model. The CFD model incorporates a discrete phase model with random walk and random eddy lifetime for particle tracking.

I. Mask O_2 Flow Rate Effects on O_2 and CO_2 Delivery

The initial unsteady modeling cases investigated the effects that varying the mask oxygen flow rate had on the oxygen delivery to the patient. The initial cases used identical breathing parameters of 11 BPM and 700cc tidal volume. Four separate cases were run with mask oxygen flow rates at 2, 4, 8 and 15 lpm. Figure 3 above shows the oxygen concentration measured from the back of the throat in the human model as a function of time.

The output of the CFD model shows that as the patient transitions from exhalation to inhalation a very high concentration of oxygen has built up in the mask. As the patient begins to inhale this high concentration of oxygen decreases due to the fact that peak inhalation flow rate is approximately 24.4 lpm. At peak inhalation the patient begins to draw in ambient air at a concentration of 20.95% thus causing the patient delivered oxygen concentration to decrease. The exhaled oxygen concentration is set to be homogenous with the output oxygen concentration determined by the total volume of oxygen inhaled minus the 310cc/min oxygen consumption rate. Additionally, a 310cc/min carbon dioxide generation rate for patient metabolism is also added to the exhaled gases.

Calculating the overall delivery of oxygen and carbon dioxide to the patient requires that the

CFD: Variations in O_2 Flow

	Model Input Parameters						Modeling Results	
Run	Mask O_2 flow (lpm)	Minute Volume (Lpm)	Frequency (bpm)	Tidal Volume (cc)	O_2 depletion (cc O_2 / min)	CO_2 generation (cc CO_2 / min)	Volume Weigted O_2 Concetration (mass%)	Vol-Weighted CO_2 Concetration (mass%)
1	2	7.77	11.1	700	310	310	***32.15%***	***1.091%***
2	4	7.77	11.1	700	310	310	***43.73%***	***0.942%***
3	8	7.77	11.1	700	310	310	***51.91%***	***0.712%***
4	15	7.77	11.1	700	310	310	***52.78%***	***0.397%***

Table 1: Oxygen Mass Concentration over Time for Various Mask Oxygen Feed Rates.

volume-weighted average over the entire inhalation cycle is calculated. The volume-weighted average concentration provides a true average delivered species concentration to the patient.

Due to the fact that the volumetric flow into the patient is sinusoidal, with flow starting at 0 and progressing to a peak, then declining back to zero, taking a simple average inhalation cycle would not yield true patient delivery values. Therefore values are volume-weighted to account for actual patient volumetric flow for each time step in the inhalation cycle.

The mathematical representation of this is a summation of the volumetric flow rate multiplied by the species mass concentration for each time step (for the entire intake period) divided by the total intake volume (tidal volume) for each breath.

$$MF_{Vol \cdot Weighted O_2} = \frac{1}{T_d} \sum_{i}^{i=30/RF} flowrate_i \cdot mf_i \qquad (5)$$

Where:

flowrate$_i$ is calculated by EQ(1) for each timestep, mf_i is the incremental mass fraction of the species at timestep i, and T_d is the tidal volume.

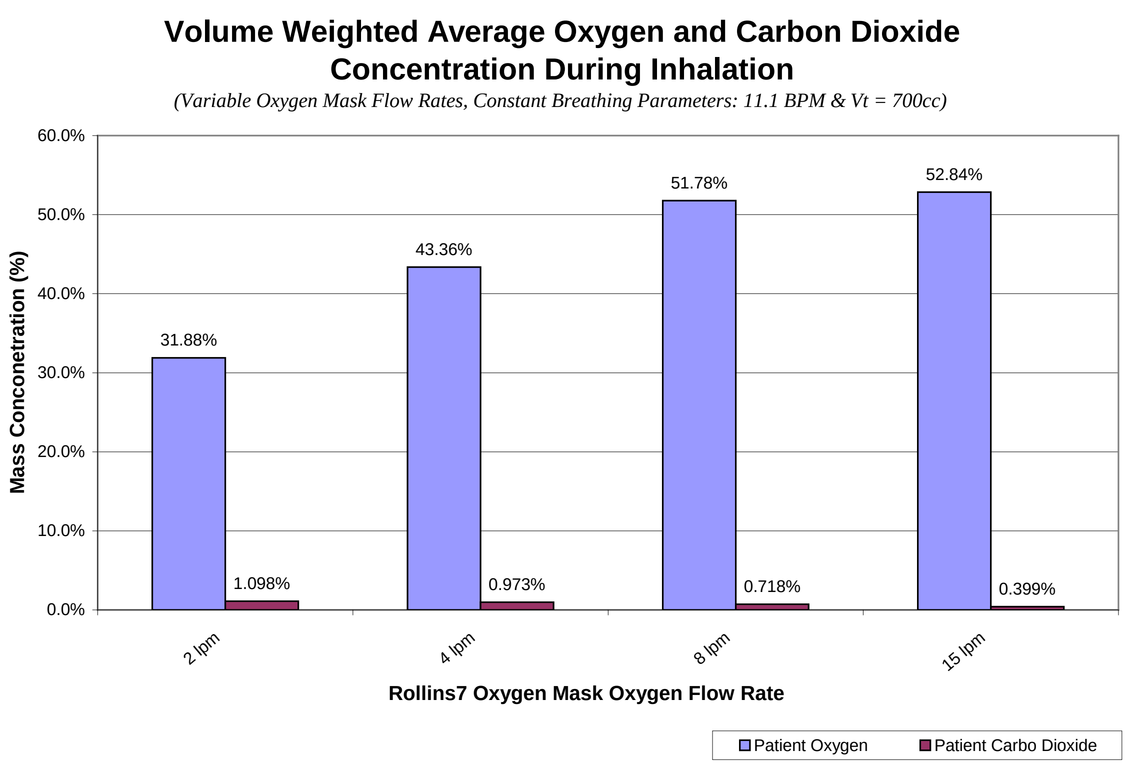


Figure 4: O_2 and CO_2 Volume-Weighted Concentrations vs. Oxygen Mask O_2 Feed Rates.

The summation of this term, from the start of the cycle to 30/RF, yields the volume-weighted average mass fraction of the species either inhaled or exhaled. Table 2 (page 7) shows the various runs that were modeled for a single set of breathing parameters

The CFD model shows that as mask oxygen feed rate is increased the patient volume-weighted average of oxygen increases and the volume-weighted carbon dioxide concentration decreases as expected. Figure 4 shows the result of the various oxygen feed rates under identical breathing parameters.

The CFD model shows that increasing the O_2 from 8 lpm to 15 lpm does not significantly increase the oxygen concentration delivered to the patient. This is probably due to losses to the atmosphere and inhalation of ambient air through the mask open mouth port. Carbon dioxide concentrations, however, do continue to decrease with high flow.

II. Respiratory Parameters Effects on O2 and CO2 Delivery.

The effects of changing breathing parameters on oxygen and carbon dioxide delivery to the patient were investigated in the following unsteady CFD cases. All cases use a constant mask oxygen flow rate of 8 lpm. For both sets of the data the minute-volume was increased at 1 lpm increments from the baseline of 7.77 lpm to 9.77 lpm.

The first set of comparison runs studies the effects of breathing frequency on oxygen delivery while maintaining a constant tidal volume of 700cc. Figure 5 shows the results of changing the breathing frequency on oxygen and carbon dioxide concentrations

The second set of comparison runs investigates the effects of changing tidal volume on oxygen and carbon dioxide delivery while maintaining a constant breathing frequency of 11 breaths-per-minute (BPM).

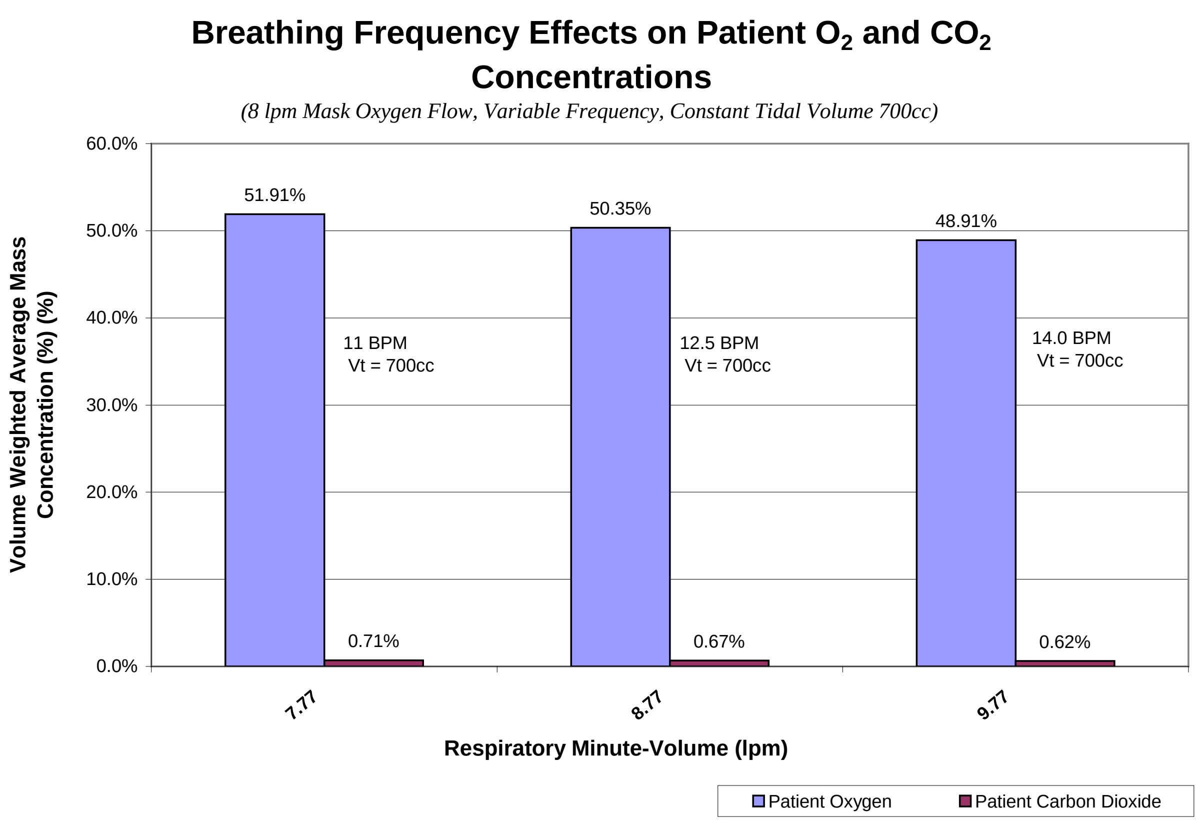


Figure 5: Breathing Frequency Effects on O_2 and CO_2 Delivery to the Patient.

CFD: Variations in Breathing Paramaters Model Summary

	Model Input Parameters						Modeling Results	
Run	Mask O_2 flow (lpm)	Minute Volume (Lpm)	Frequency (bpm)	Tidal Volume (cc)	O_2 depletion (cc O_2 / min)	CO_2 generation (cc CO_2 / min)	Volume Weigted O_2 Concetration (mass%)	Vol-Weighted CO_2 Concetration (mass%)
1	8	7.77	11.10	700	310	310	***51.91%***	***0.71%***
2	8	8.77	12.53	700	310	310	***50.42%***	***0.75%***
3	8	9.77	13.96	700	310	310	***49.50%***	***0.79%***
4	8	7.77	11.10	700	310	310	***51.91%***	***0.71%***
5	8	8.77	11.10	790	310	310	***50.35%***	***0.67%***
6	8	9.77	11.10	880	310	310	***48.91%***	***0.62%***

Table 2: Variations in Breathing Parameters Summary.

Figure 6 shows the results of increasing the tidal volume while maintaining a constant breathing frequency. The results show increasing the tidal volume decreases the patient volume-weighted oxygen concentration slightly. However, volume-weighted carbon dioxide concentrations actually increase as tidal volume increases with a constant breathing frequency.

Table 2 shows the complete summary for all unsteady state case runs investigating the effects of breathing parameters on patient oxygen and carbon dioxide delivery concentrations.

The CFD model shows that the overall effect of changing breathing frequency and tidal volume is minor in regards to affecting the delivered oxygen and carbon dioxide concentration to the patient.

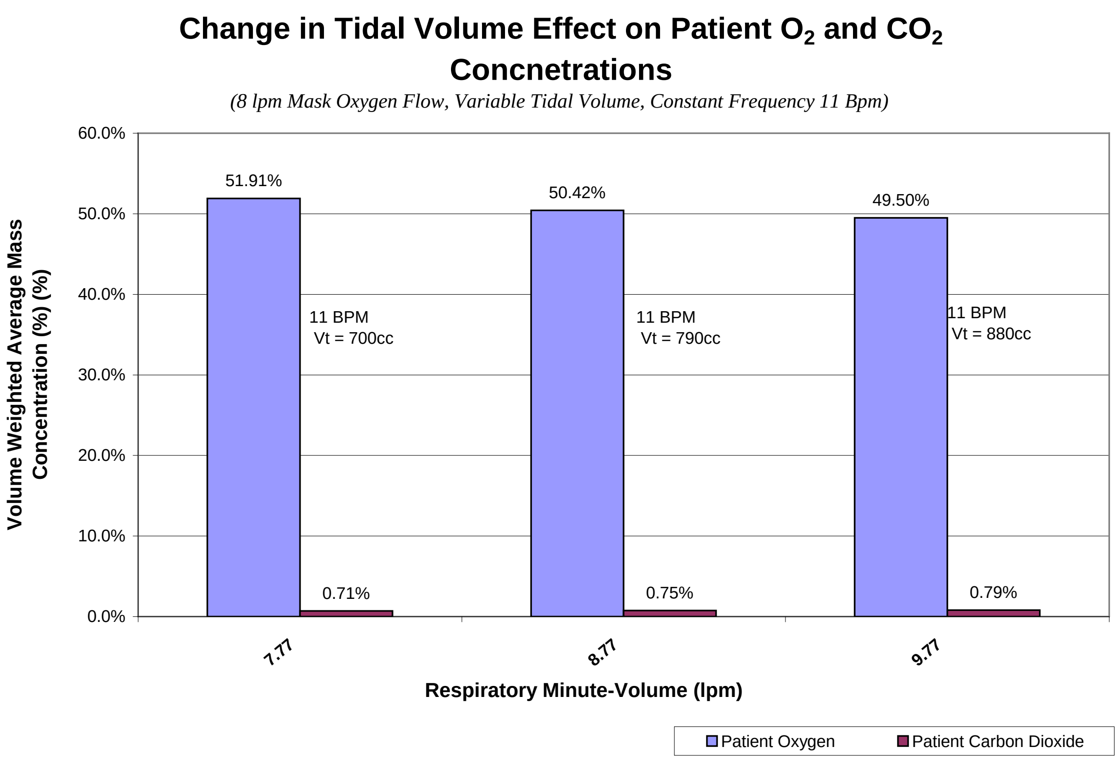


Figure 6: Breathing Tidal Volume Effects on O_2 and CO_2 Delivery to the Patient

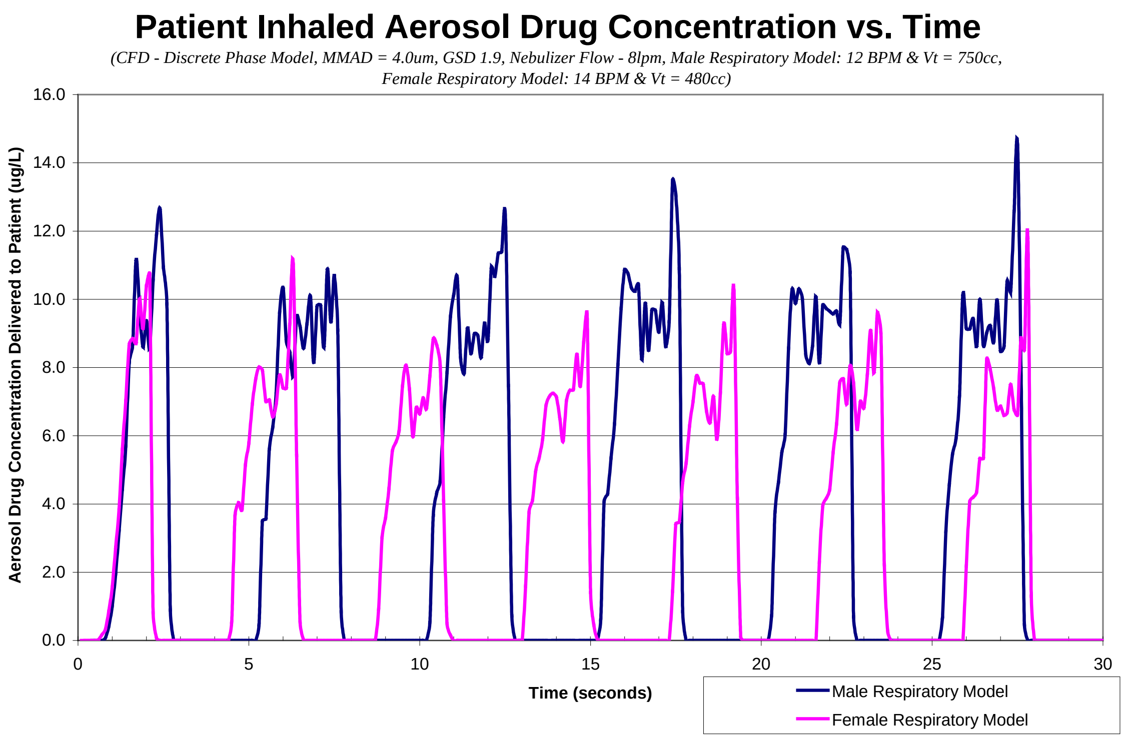


Figure 7: Patient Inhaled Aerosol Drug Concentration vs. Time.

III. CFD Model Validation – Nebulizer Drug Delivery.

The last set of unsteady state cases were used to validate the model accuracy by comparing the model output to actual run data. The CFD model was used to predict patient nebulized drug delivery rates for two different respiratory models. The CFD predicted output was directly compared to test data performed in September 2012 using a ventilated mannequin with the Rollins7 Oxygen Mask.

The testing was conducted on a modified CRP mannequin equipped with a throat tube to an absolute collection filter. The mannequin simulated breathing patterns were controlled via Philips Respironics Life-Care PLV-100 (Andover, MA) piston ventilator. The mask was placed onto the mannequin, ventilation parameters were set and a nebulizer was filled with 5ml of albuterol sulfate nebulizer solution. The ventilator and the nebulizer were initialed and allowed to run for 5 minutes. The nebulizer pre/post fluid and the capture filter were analyzed via HPLC to determine nebulization rate and aerosol drug delivered to the simulated patient. Table 4 below shows the results of the testing conducted at ARE Labs in 2012.

The CFD model incorporates a discrete phase model with random walk and random eddy lifetime for unsteady particle tracking. Additional modeling inputs such as: particle MMAD, GSD and Mass rates are shown below in Table 3.

CFD: Nebulizer Model Parameters

	Breathing Input Parameters				Nebulizer Input Parameters			
Run	Respiratory Model	Minute Volume (Lpm)	Frequency (bpm)	Tidal Volume (cc)	Nebulizer Flow (lpm)	Aerosol Output (ug/min)	MMAD (um)	GSD (um)
1	**Male, resting**	9.0	12	750	8	288.9	4.0	1.9
2	**Female, resting**	6.7	14	480	8	219.6	4.0	1.9

Table 3: *Modeling Input Parameters for Nebulizer Validation Runs.*

Adult Mask Nebulizer Testing Summary

Features	Respiratory Model	Rollins7 Adult	CFD Model
Nebulizer Fill (ug) *(Albuterol Sulfate)*	Adult Male, resting Adult Female, resting	4893.6 +/- 46.8 4896.7 +/- 72.6	
Nebulizer Residual (ug) *(Albuterol Sulfate)*	Adult Male, resting Adult Female, resting	3449.6 +/- 164.9 3798.3 +/- 58.8	
Treatment Time *(minutes)*	Adult Male, resting Adult Female, resting	5.019 +/- 0.02 5.017 +/- 0.00	
Nebulization Rate *(ug/min)*	Adult Male, resting Adult Female, resting	**288.8 +/- 27.8** **219.6 +/- 12.5**	**288.9** *(input)* **219.6** *(input)*
Patient Delivery Rate *(ug/min)*	Adult Male, resting Adult Female, resting	**69.1 +/- 5.5** **39.3 +/- 3.7**	
Confidence level of testing		The test and number of samples (3) tested provide 95% confidence level	

All values Mean +/- SD

Table 4: Previous Testing Data Summary (Albuterol Sulfate).

Two different respiratory models were used for the testing. The first set of parameters represented a male resting model at 12 breath-per-minute (BPM) and a tidal volume of 750cc. The second set represented a female resting model with 14 BPM and a tidal volume of 480cc.

Figure 7 (page 8) shows the results obtained form the CFD model for aerosol concentrations delivered to the patient vs. time for both the male and female respiratory model. The average drug concentration during inhalation for the male respiratory model is around 9.0 ug/l while the female model shows an average of around 7.0 ug/l.

The overall inhaled drug per breath was calculated on a volume-average basis and shows that for the male respiratory model the patient received an average dose of 5.99 ug/breath for the entire 30 second model time. The female model showed an average dose of 3.05 ug/breath.

The testing results showed that, for the male respiratory model, the delivered dose rate to the patient was 69.1 ± 5.5 ug/min. This value is extremely close to the predicted CFD value of 71.9 ug/min. The female respiratory model testing showed delivered dose rates of 39.3 ± 3.7 ug/min. This value is again extremely close to the CFD predicted results of 42.7 ug./min.

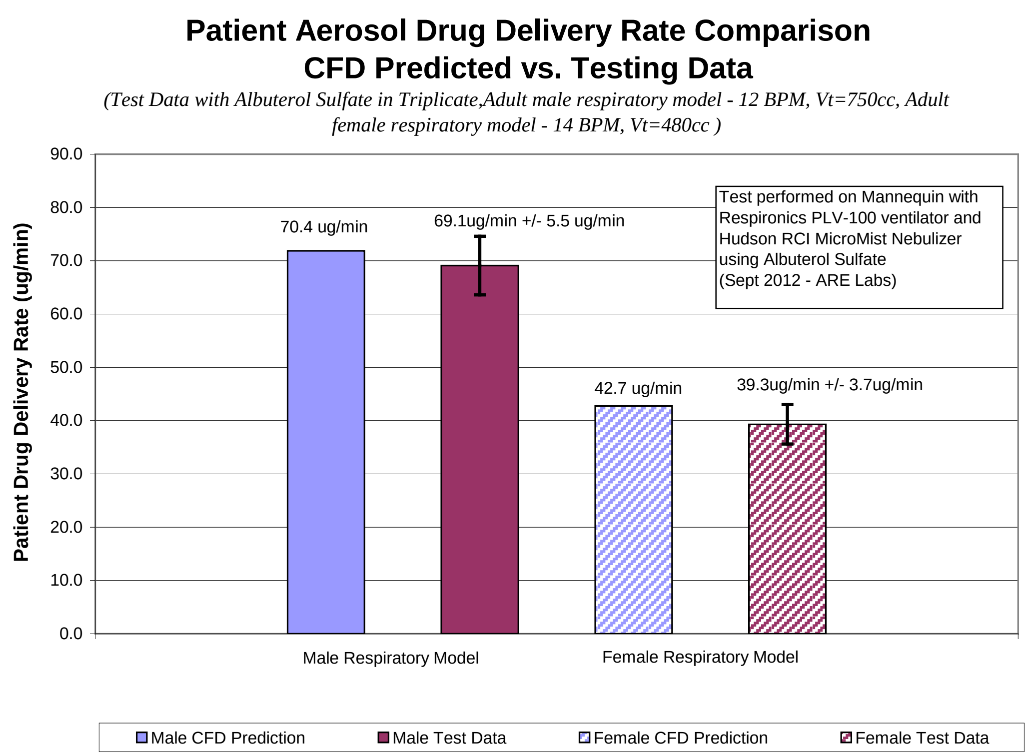


Figure 8: Patient Inhaled Aerosol Drug Concentration vs. Time.

The average delivered dose per minute is calculated by multiplying the average dose received per breath times the breathing frequency. For the male model this corresponds to 71.9 ug/min delivered dose to the patient. For the female model the delivered dose rate was 42.7 ug/min.

The CFD predicted results are within the testing data uncertainty and validates the CFD models accuracy.

Conclusions

The computation fluid dynamics model shows excellent agreement with test data used to predict total patient drug delivery rates (ug/min). This validation of the model gives confidence for the other predicted variables such as oxygen and carbon dioxide delivery rates under various breathing conditions.

The CFD model shows that the Rollins7 Oxygen Mask has a very high delivery of oxygen to the patient despite the large mouth port in the mask. The volume-averaged mass concentration of oxygen delivered to the patient was 31.9% at 2 lpm oxygen flow, 43.4% at 4 lpm oxygen flow, 51.8% at 8 lpm oxygen flow and 52.3% at 15lpm oxygen flow. This is under typical resting breathing parameters of 11 breath-per-minute with a tidal volume of 700cc. These results also show the diminishing return of patient delivered oxygen when the flow rate is increased above 8 lpm.

The results also show that variations in breathing frequency and tidal volume have only a slight effect on the average oxygen delivery to the patient. Patient minute-volumes ranged from 7.8 lpm to 9.8 lpm while the volume-averaged patient oxygen concentration only varied from 48.9% to 51.9% with an oxygen mask feed rate of 8lpm. From the data we can see that even with a fairly high resting minute-volume of 9.8 lpm the Rollins7 Oxygen Mask was still able to deliver a 48.9% average oxygen concentration to the patient.

The Rollins7 Oxygen Mask also showed excellent results at reducing the patient carbon dioxide re-uptake. This is due to the open mouth design which allows patient expired gases to more easily escape the mask. The volume averaged patient carbon dioxide concentrations ranged was 1.1% at 2 lpm oxygen flow, 0.97% at 4 lpm oxygen flow, 0.72% at 8 lpm oxygen flow and 0.4% at 15lpm oxygen flow. This is under typical resting breathing parameters of 11 breath-per-minute with a tidal volume of 700cc.

The results are similar to that of the oxygen delivery rates except that high oxygen flows to the mask continue to lower the carbon dioxide re-uptake due to the persistent flushing of the exhaled gases.

The computation fluid dynamics model shows that the Rollins7 Oxygen Mask not only provides the patients with high oxygen delivery rates but also significantly reduces carbon dioxide re-uptake by the patient.

References

Aerosol Research and Engineering Laboratory Inc. "Drug Delivery Comparison using the Adult Rollins 7 Oxygen Mask on a Ventilated Human Model." Project 10766.1 for Rollins Medical. Sept 2012

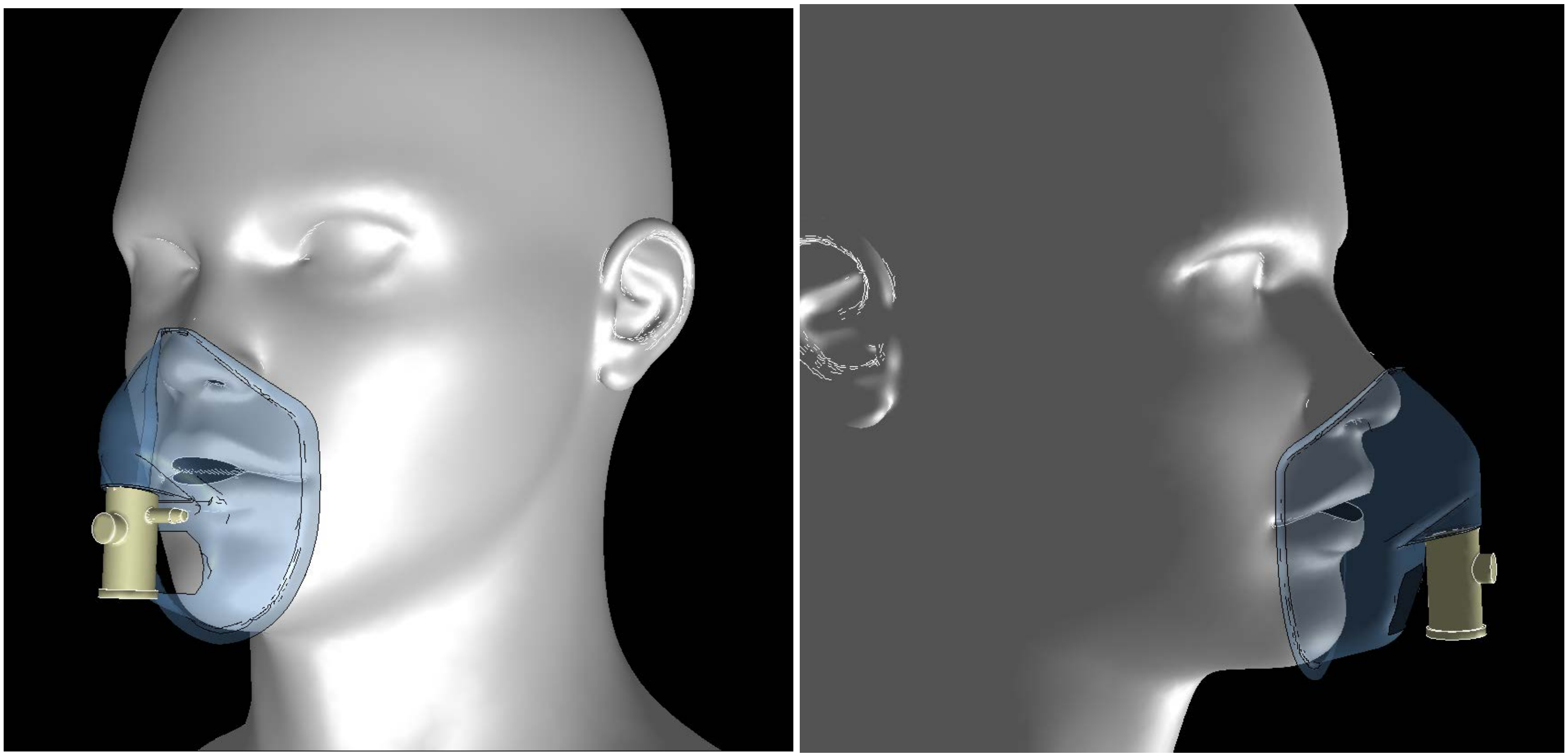
Gupta, J.K., Lin, C.-H., and Chen, Q. 2010. "Characterizing exhaled airflow from breathing and talking,"Indoor Air, 20, 31-39.

Gao, N. and Niu, J. (2006) Transient CFD simulation of the respiration process and interpersonal exposure assessment. Building and Environment, 41 (9), 1214-1222.

Appendix A

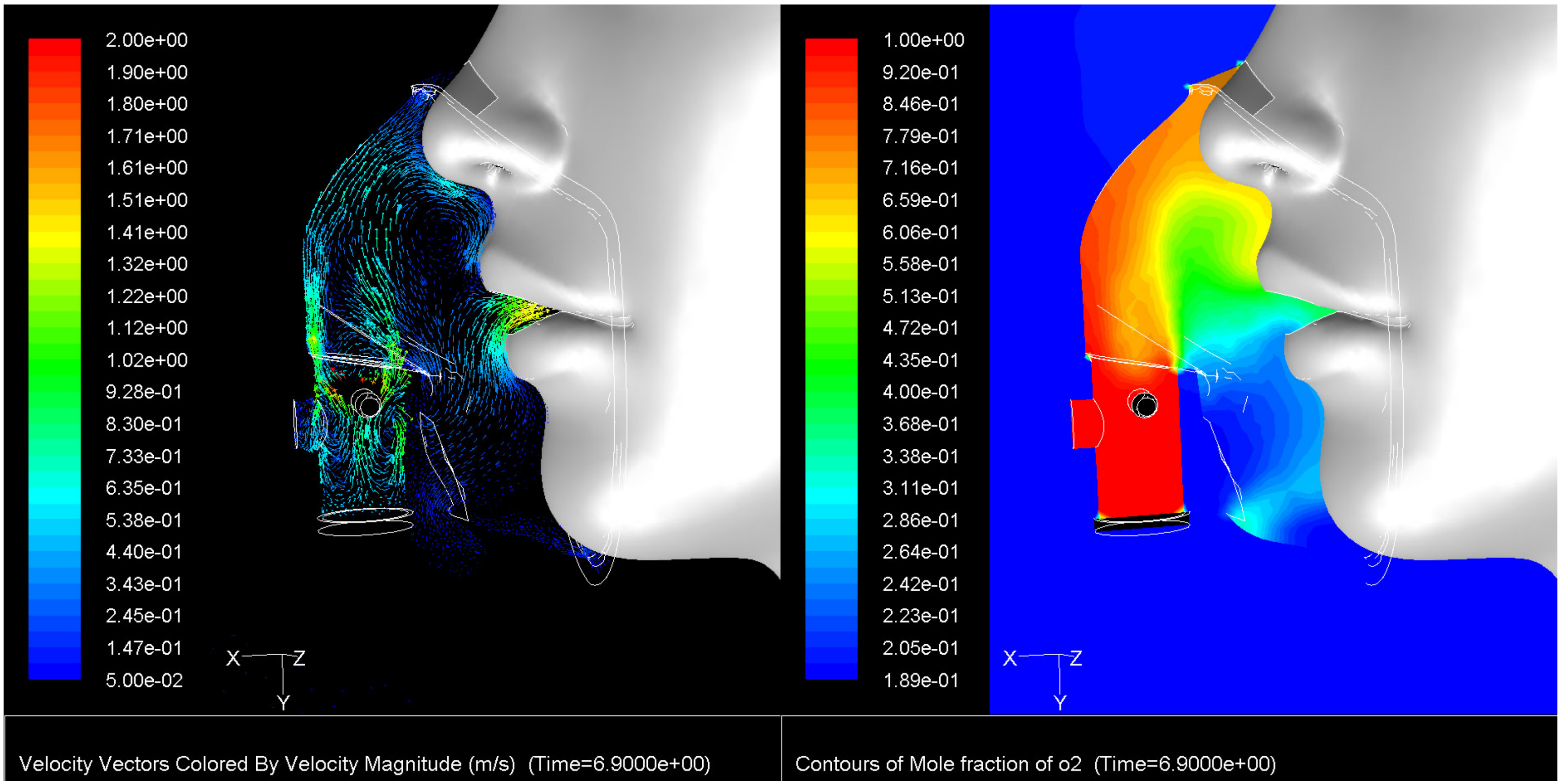
Select Images from CFD runs

Rollins7 Oxygen Mask: Mask and Human Model



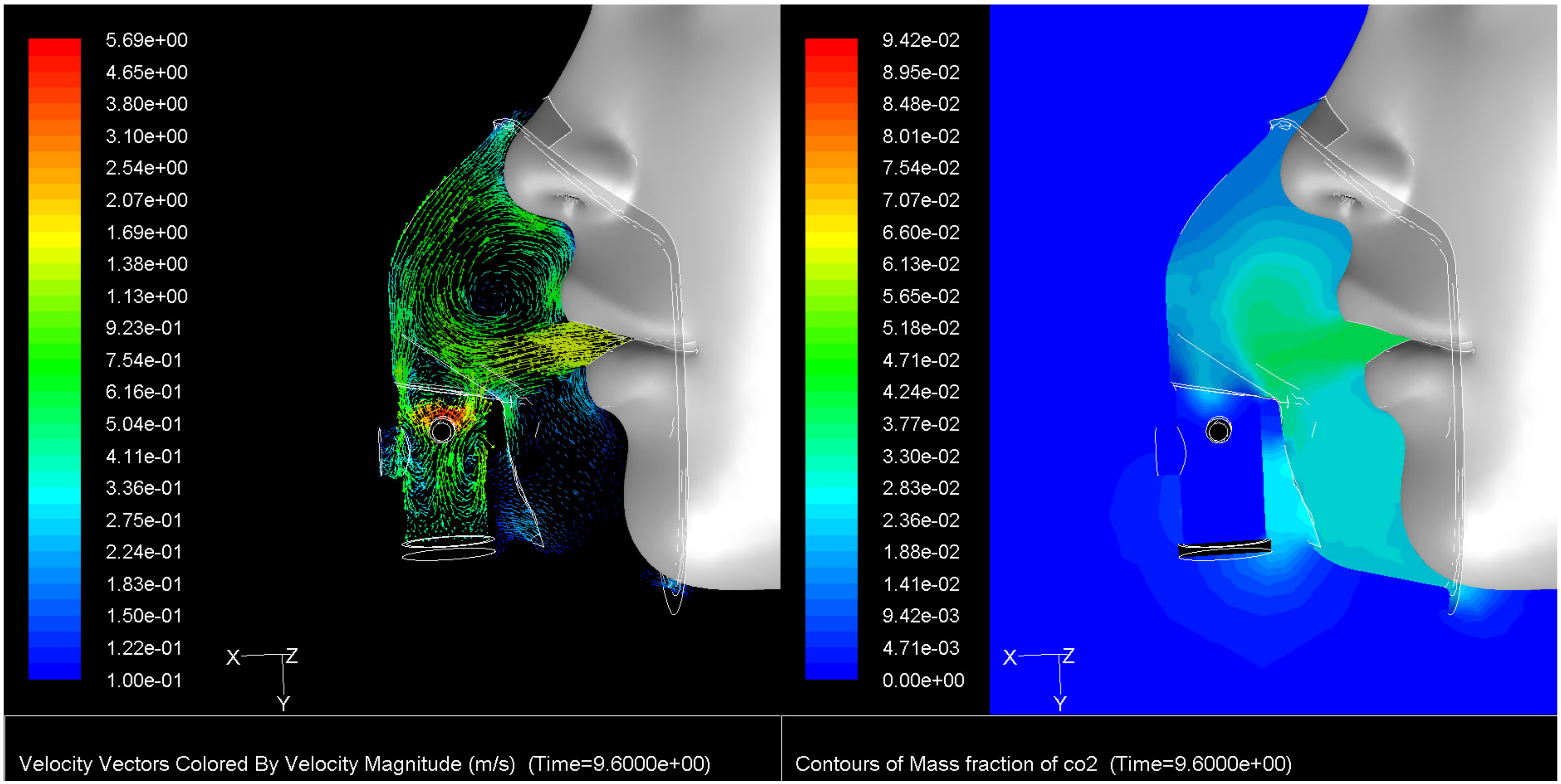
Rollins7 Oxygen Mask: Velocity Vectors and O2 fraction

(Sagittal plane, Peak inhalation, RF = 11 BPM, T_v = 750cc, Mask O_2 flow rate 8 lpm)



Rollins7 Oxygen Mask: Velocity Vectors and CO2 fraction

(Sagittal plane, Peak Exhalation, RF = 11 BPM, T_v = 750cc, Mask O_2 flow rate 8 lpm)



Rollins7 Oxygen Mask: Velocity Vectors and CO2 fraction Close-up of Mouth Opening

(Sagittal plane, Peak Exhalation, RF = 11 BPM, T_v = 750cc, Mask O_2 flow rate 8 lpm)