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Particle and Fiber Transport and Deposition in Human Respiratory Track

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Outline

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- Human Airway passages
- Particle and Fiber Transport and Deposition
- Computational Models for Spherical and Fiber Transport and Deposition in Human Airways
- Concluding Remarks

Motivation

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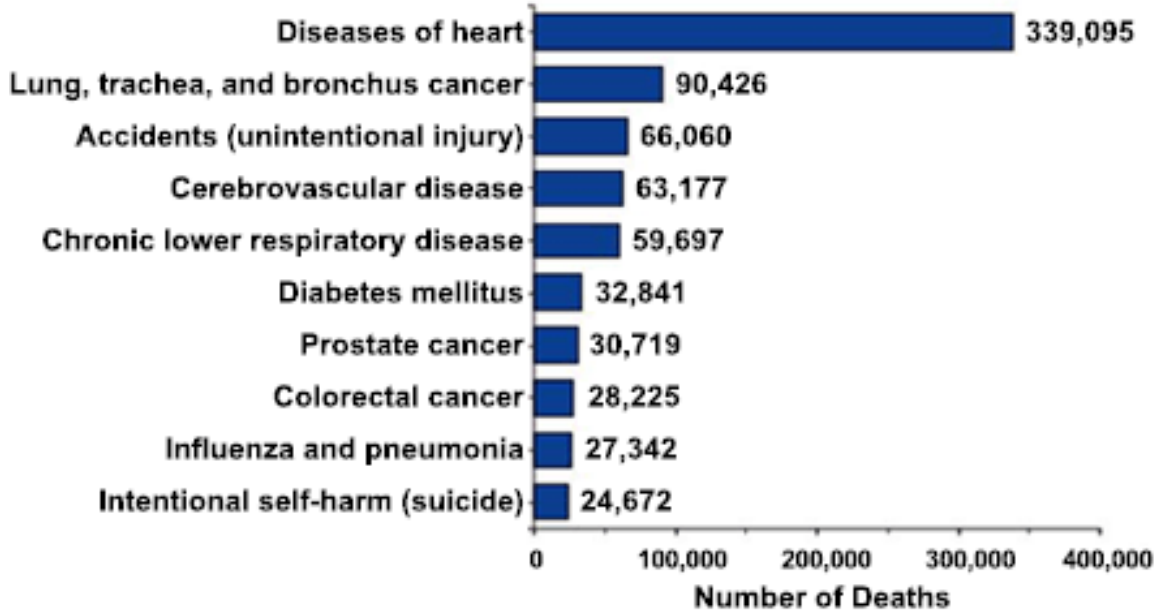
Ten Leading Causes of Death Among Men in the U.S. 2001



- Lung cancer facts (2005): estimated 163,510 deaths, 172,570 new diagnoses, 3rd most common type of cancer in the U.S., more people die from lung cancer than any other type of cancer

- Research has found inhaled toxic aerosol substances are the major cause of lung diseases.

* Source: National Vital Statistics Report, Vol. 52, No. 3, 2003.
* Department of Health and Human Service, Centers for Disease Control and Prevention

Lung Function and Anatomy

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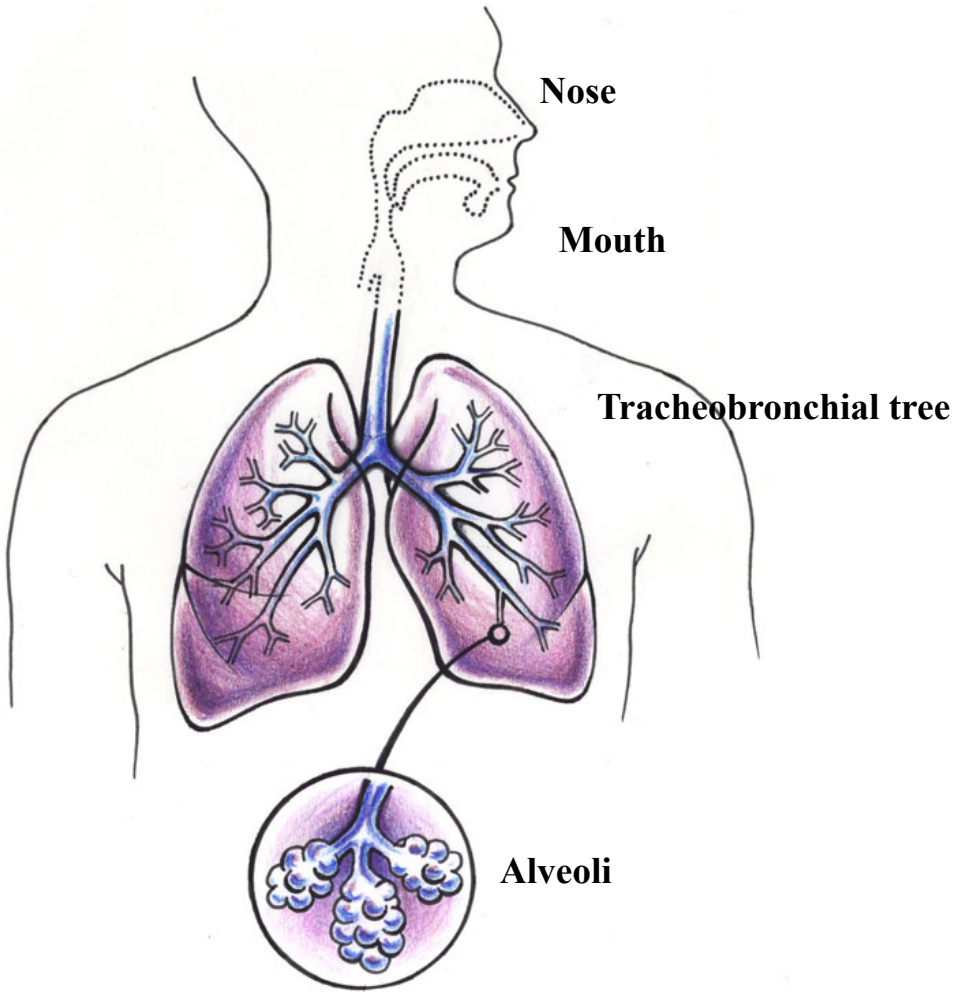

Respiratory systems

Respiratory Cycle:

- **7–60 L /min volume rate**
- **Throughout the life**

- **Humidification**
- **Temperature Regulation**
- **Trap Particles**
- **Remove Particles**

- **Gas exchange (O_2, CO_2)**
- **Immunology defense**

Objectives

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- Develop a computational model for predicting the transport and deposition of inhaled aerosols in human airways
- Develop an efficient computational model on particles and fibers Deposition.
- Identify the deposition mechanism and deposition pattern
- Quantify the effects of the breathing rate, aerosol size, aerosol shape (compact or elongated), and airway features on aerosols transport and deposition processes
- More effective prevention of human respiratory health problem in hazardous environment
- Better control of efficient drug delivery to the targeted disease sites

Particle Deposition in a Duct

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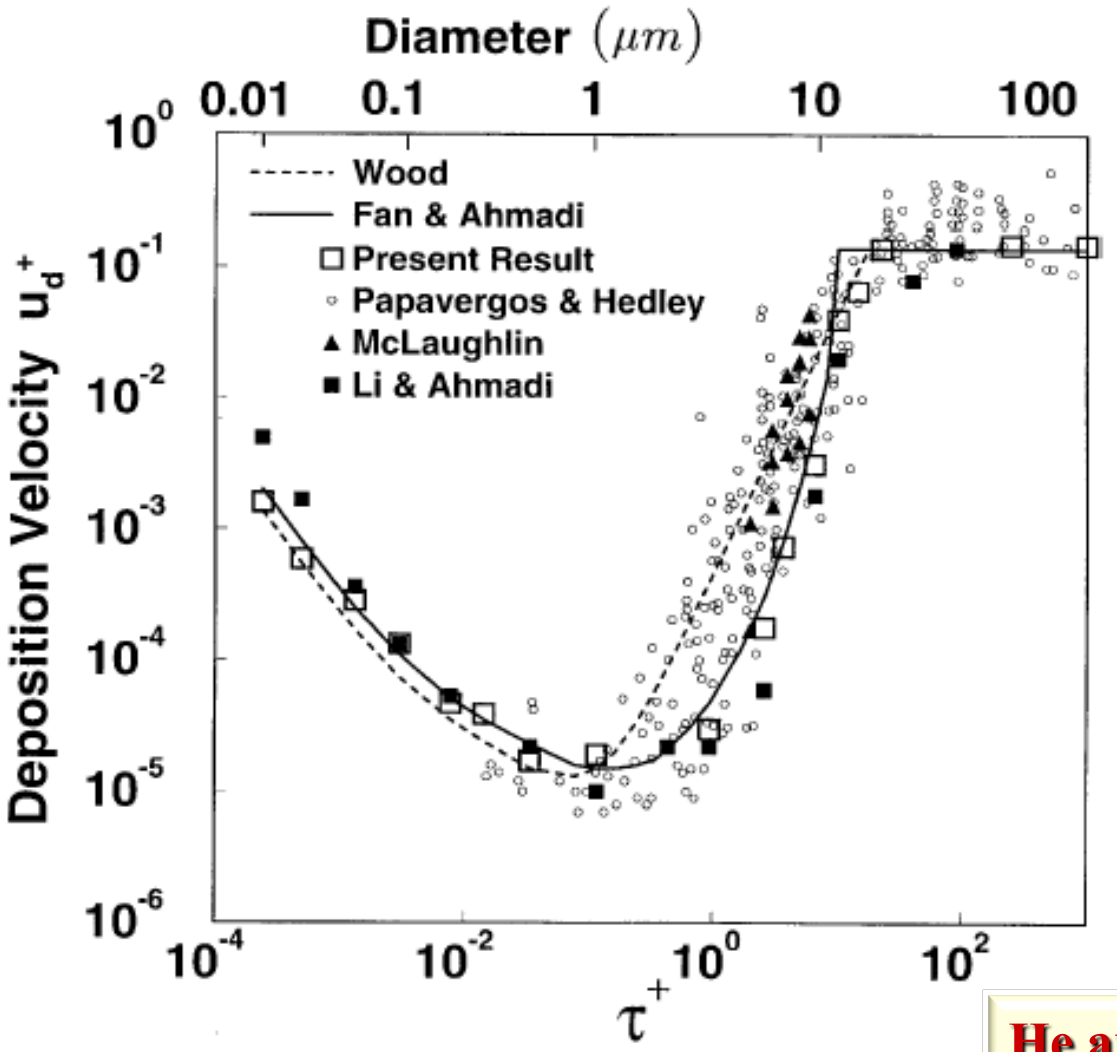

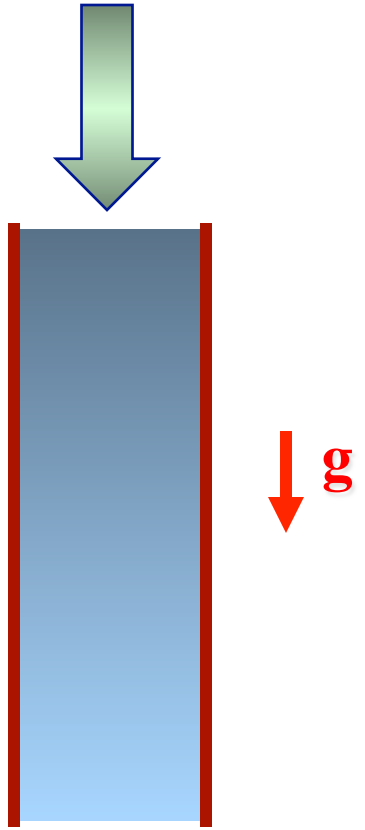

He and Ahmadi (1999)

Particle Deposition in a Duct

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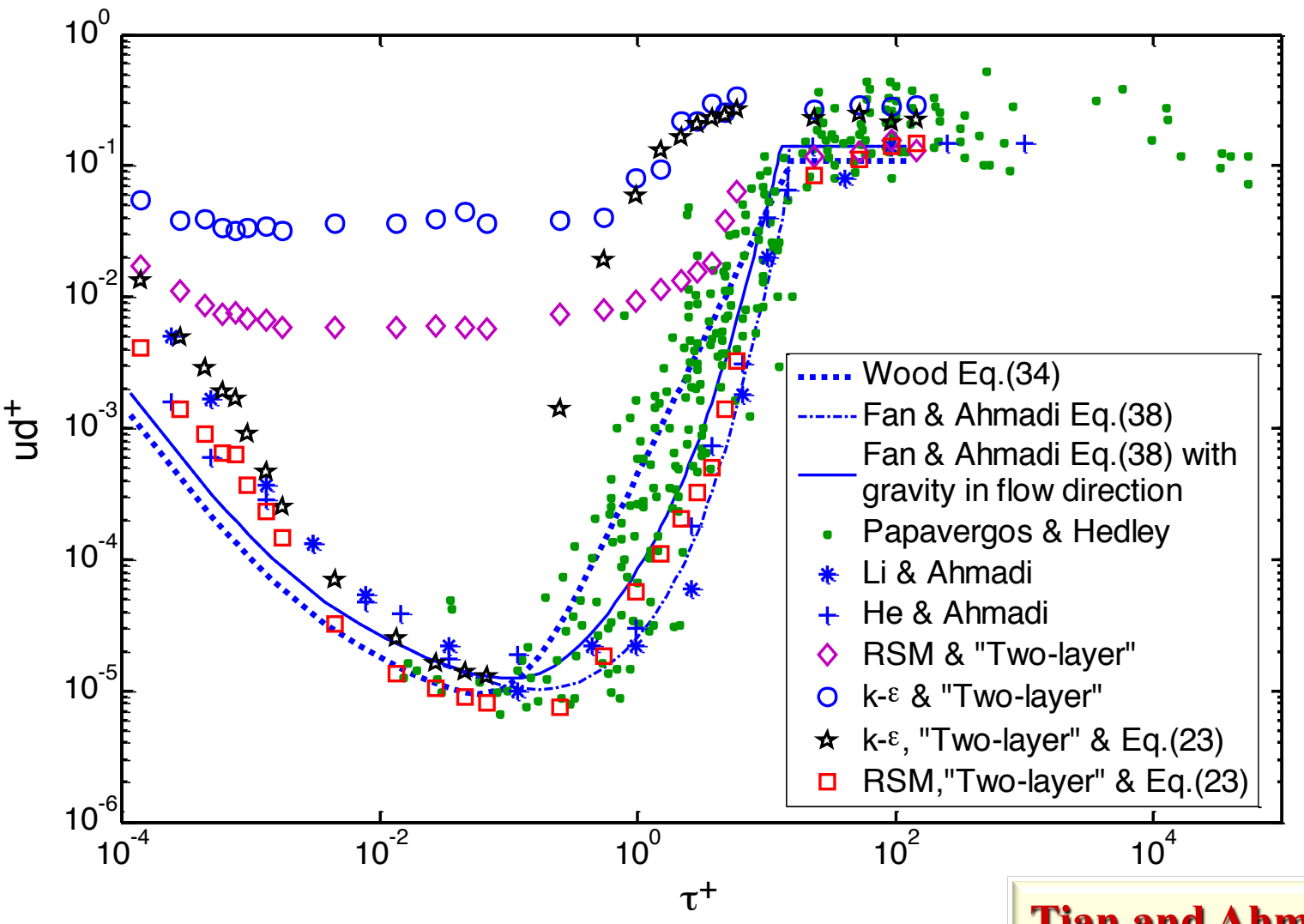

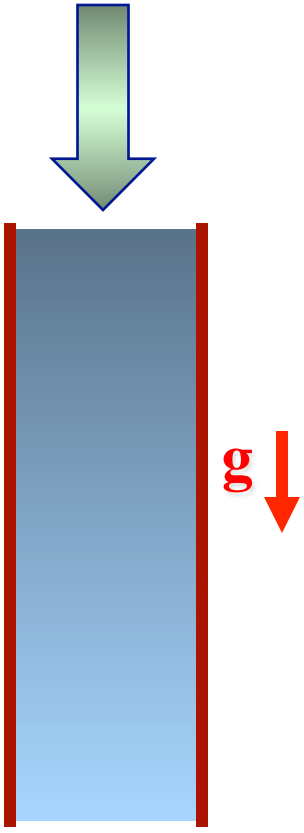

Tian and Ahmadi (2007)

Respiratory Deposition

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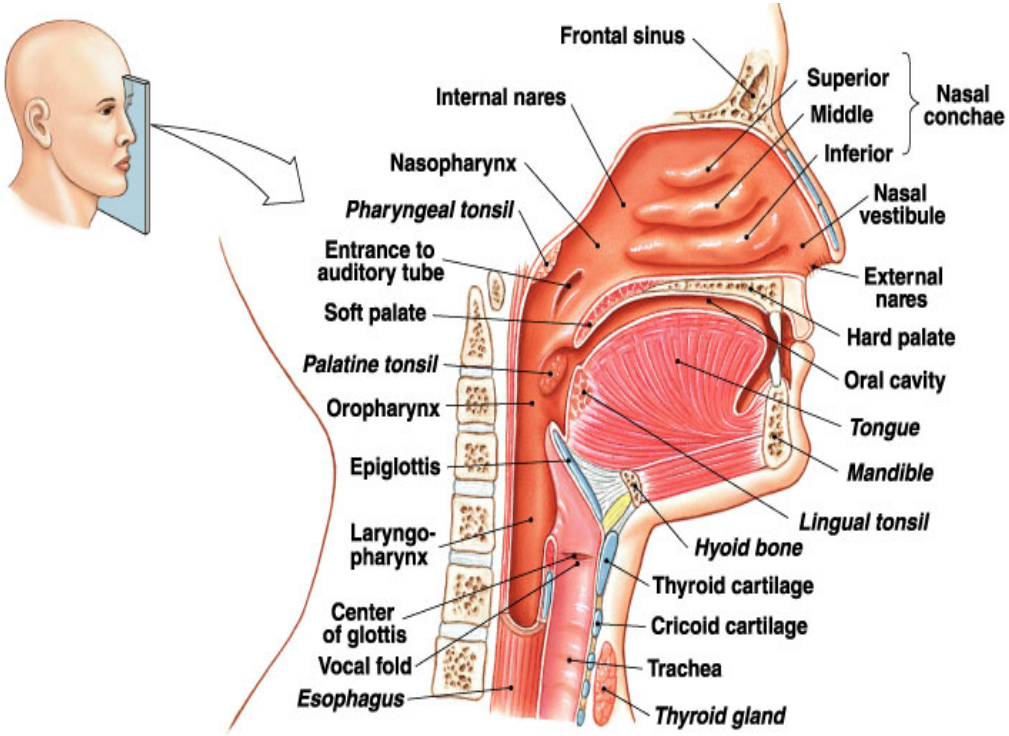
Particle and fiber deposition in human lung and nose

EPA

NIOSH



Asbestos Fibers

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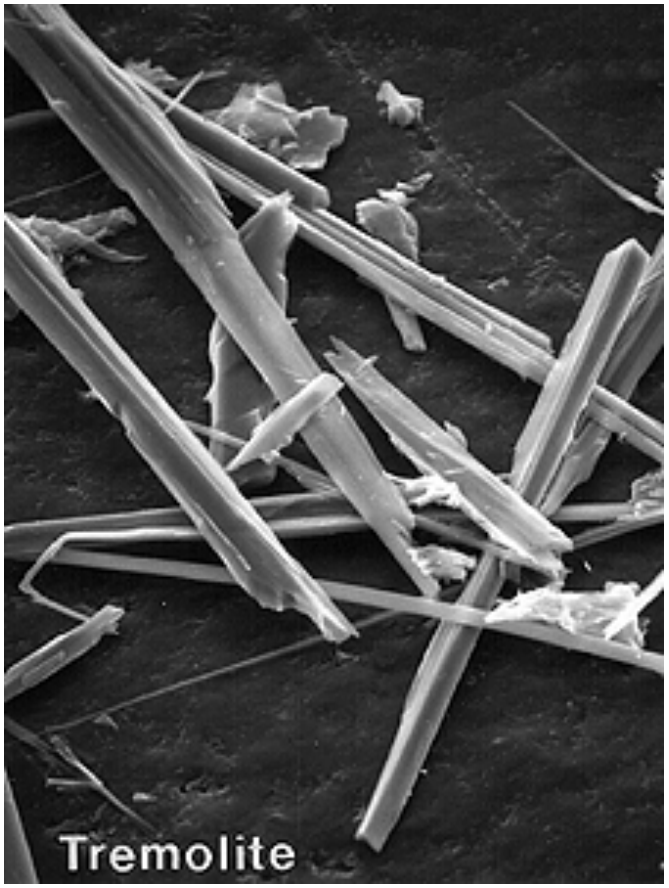
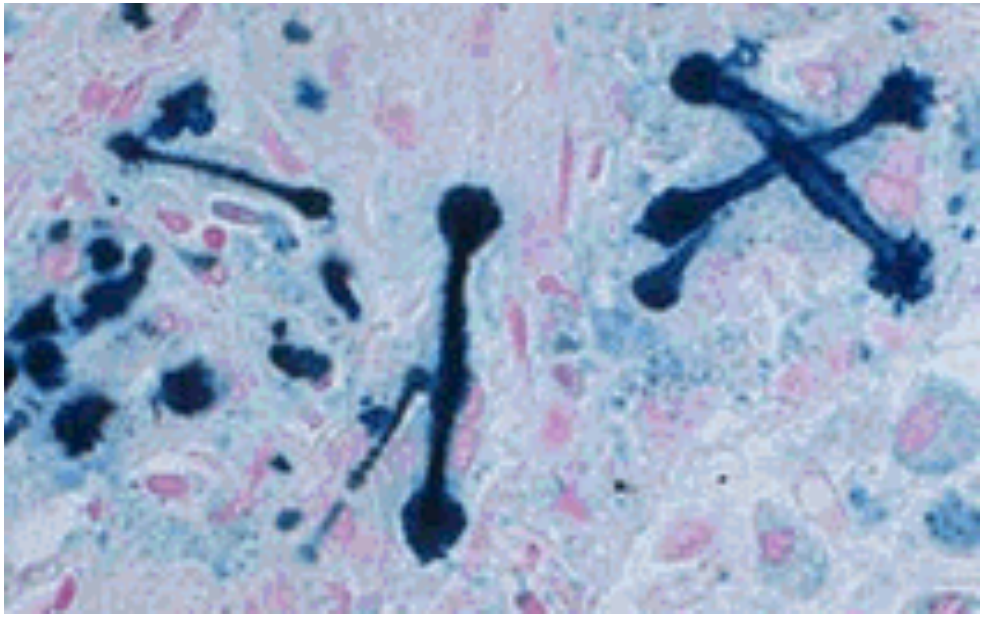


Asbestos



Asbestos in the Lung

Lung Deposition

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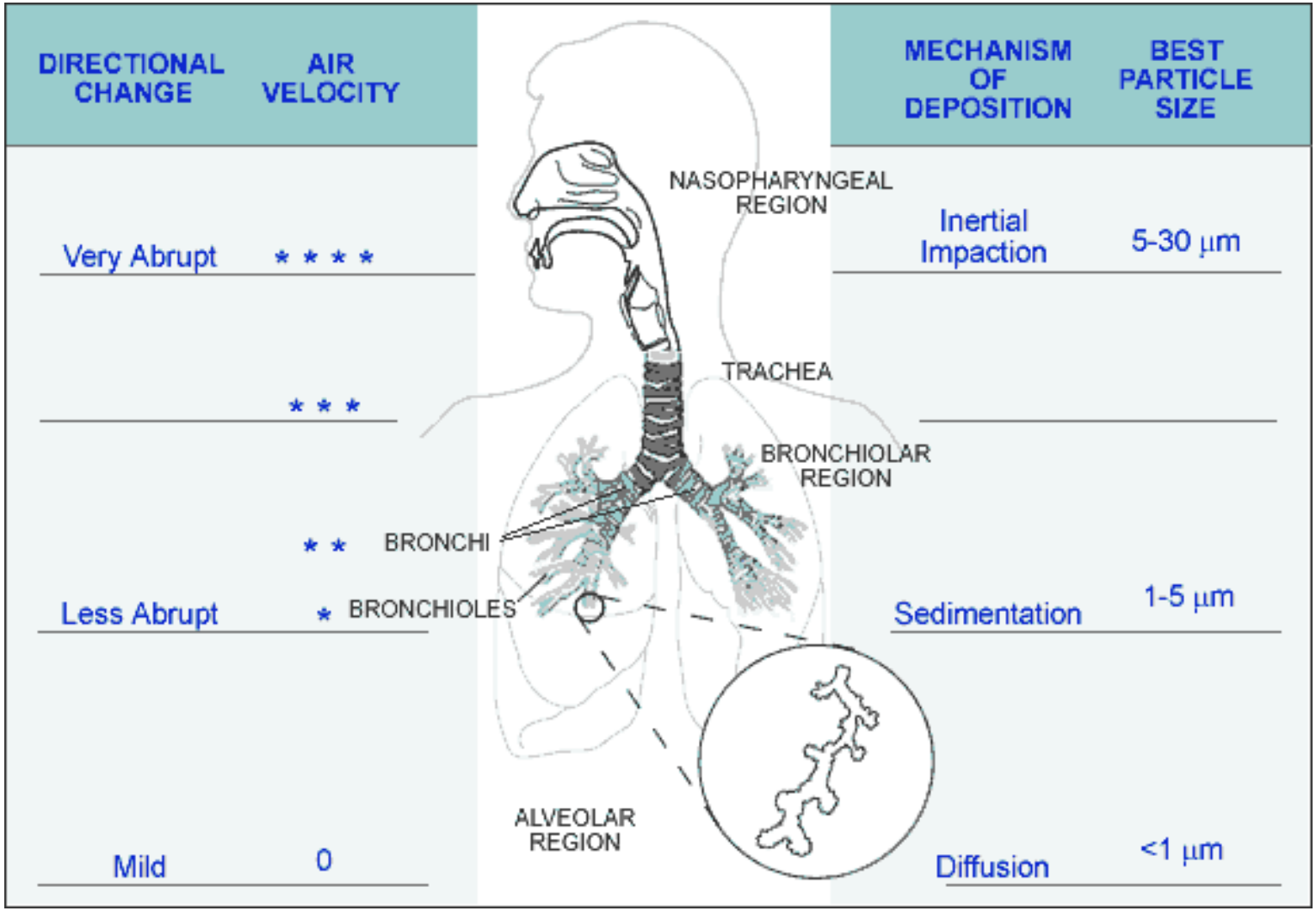
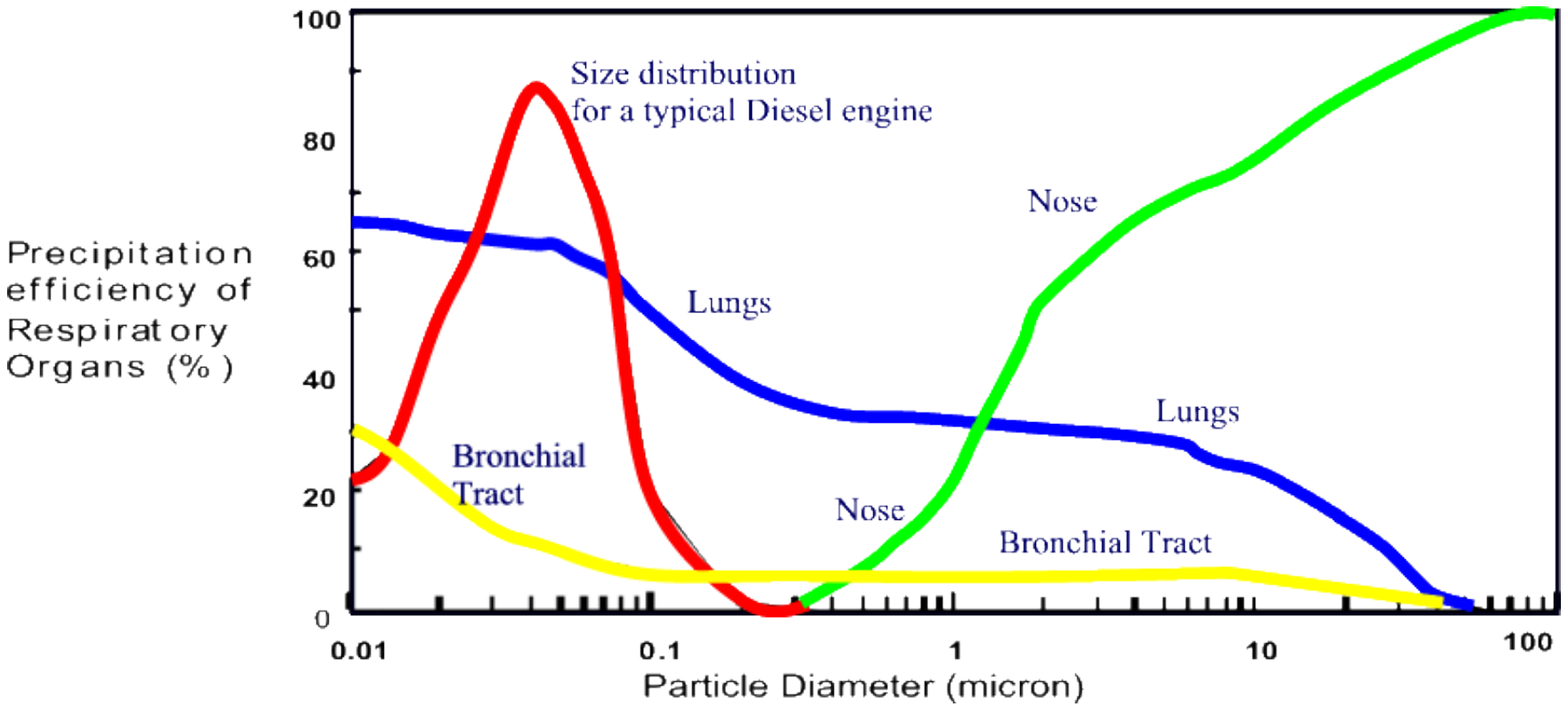


Lung Deposition

Clarkson University



Variations of Capture Efficiency with Stokes Number

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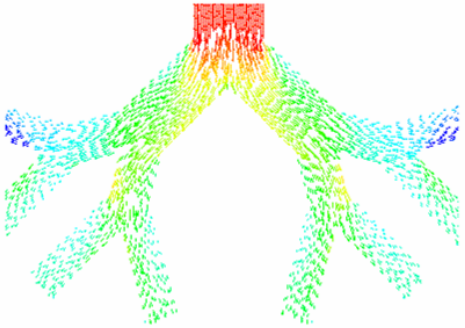
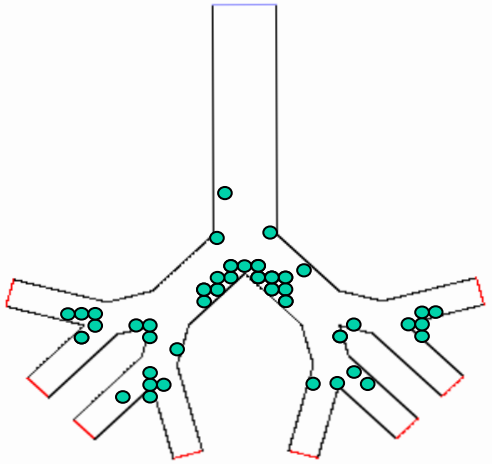
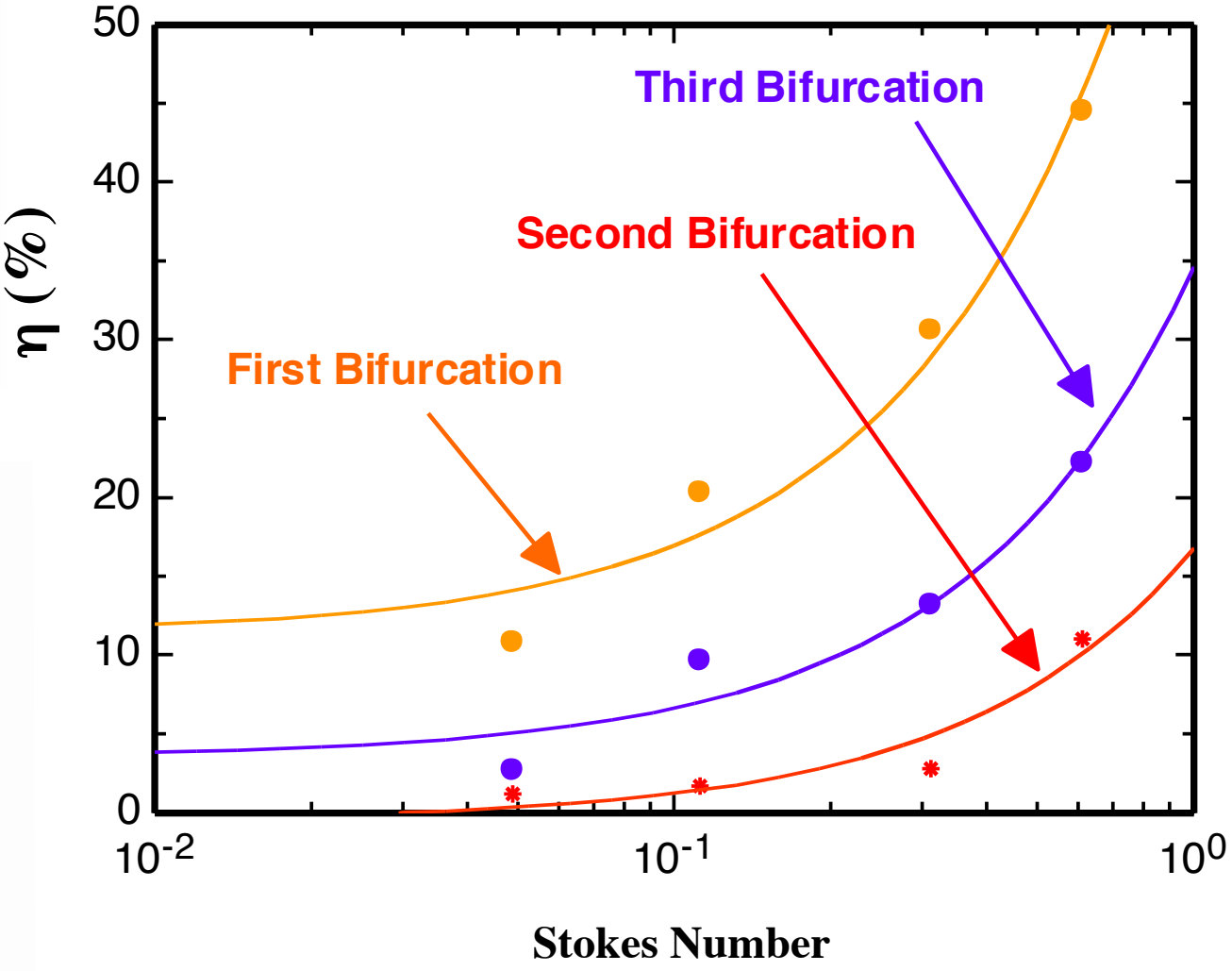


Turbulent





Mean Velocity Contours

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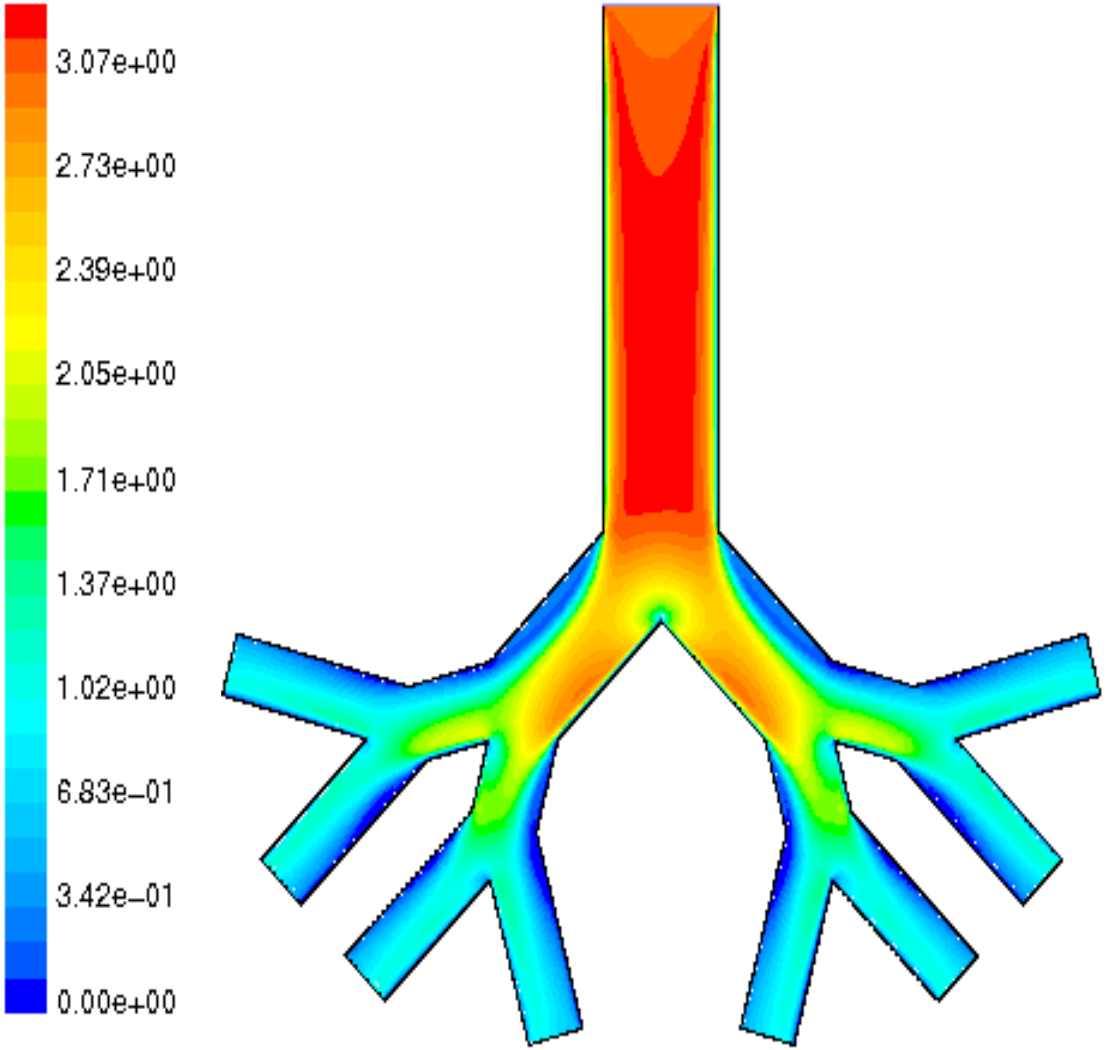
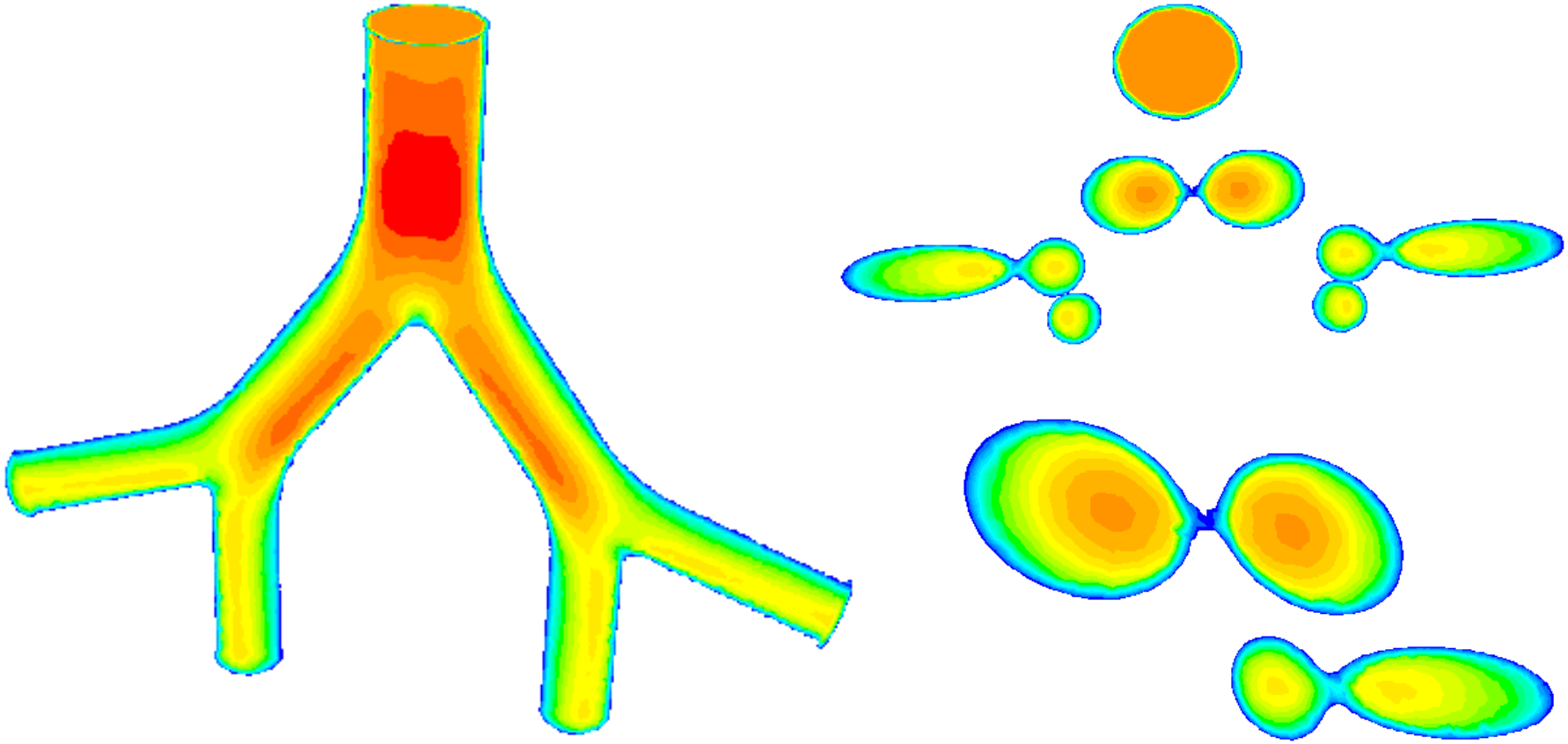


Lung Deposition

Clarkson University



Velocity Magnitude Contours

Lung Deposition

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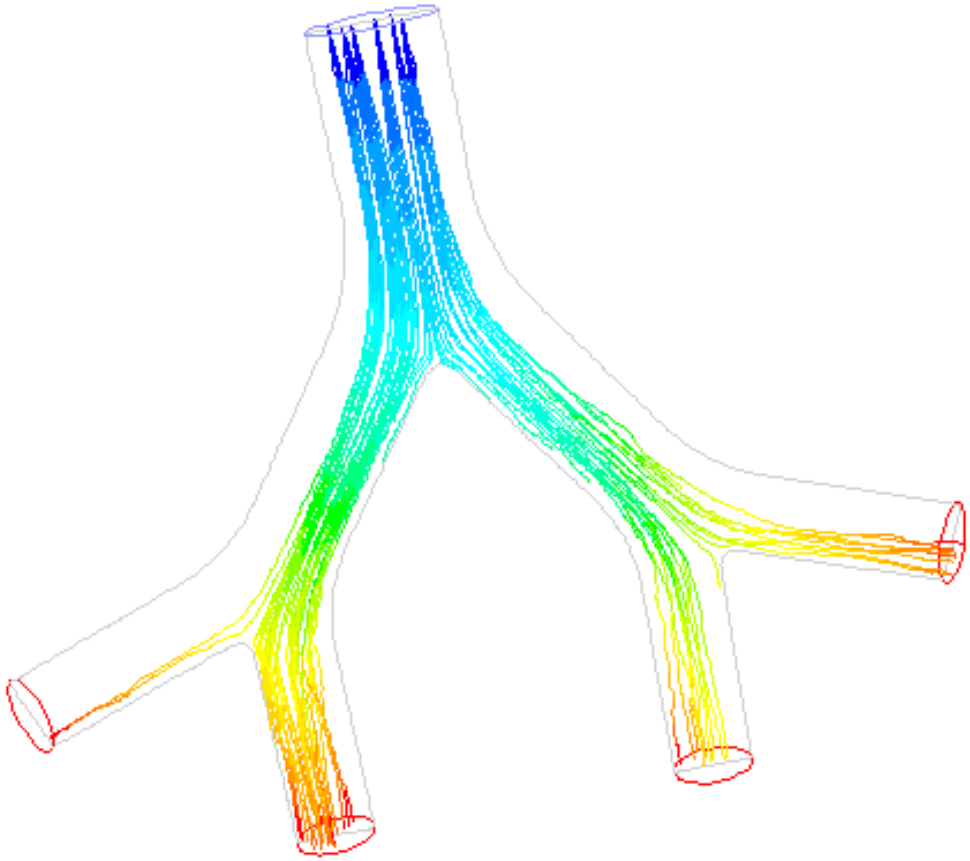

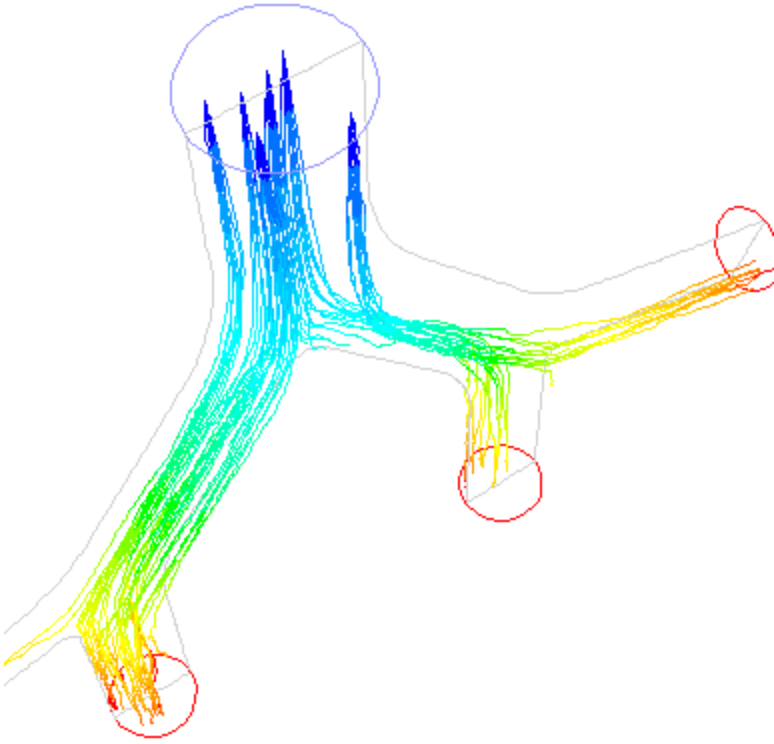

Sample 1 µm Particle Trajectories

Multi-Level Lung Model

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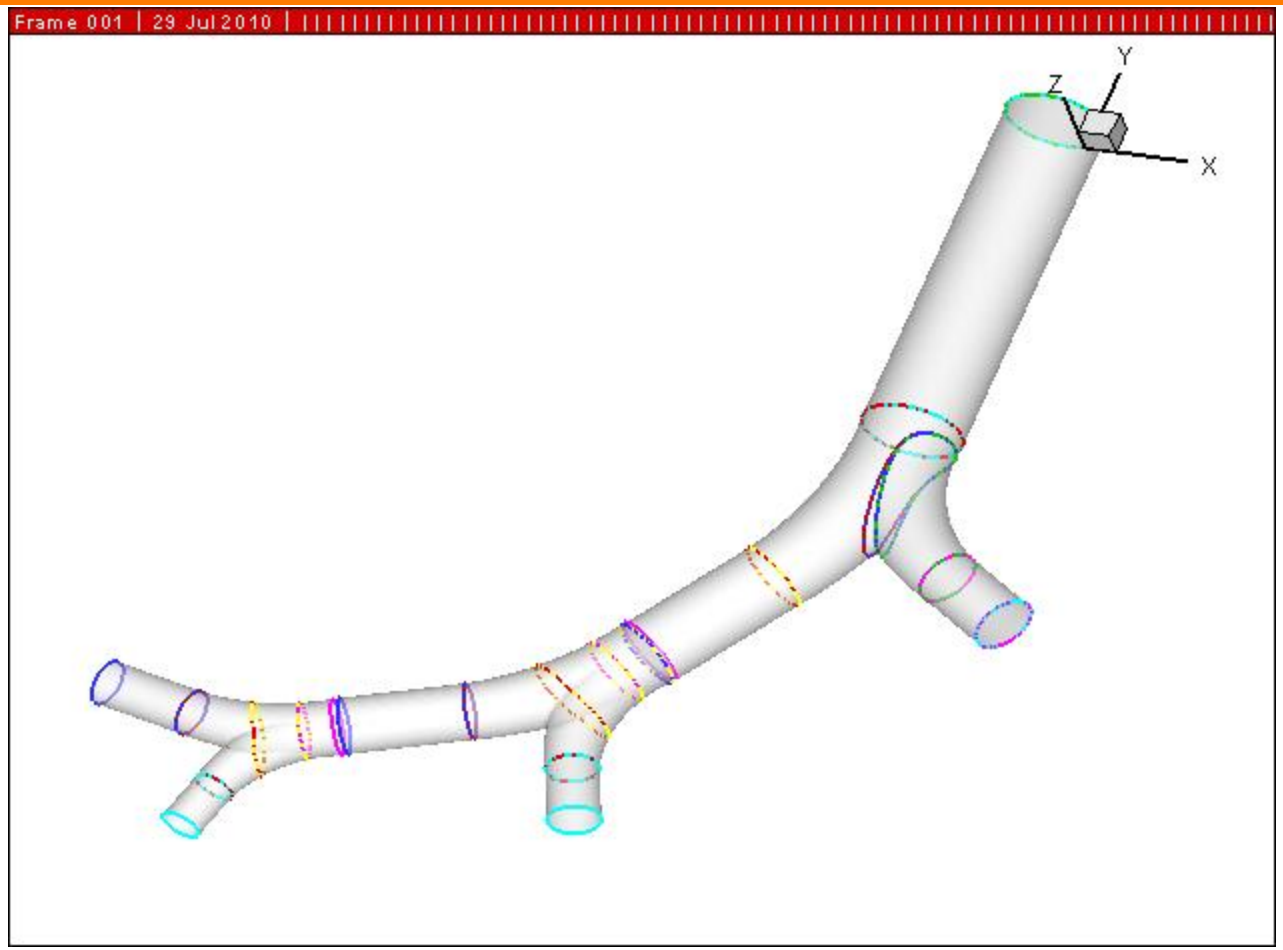

Multi-Level Bifurcation Model

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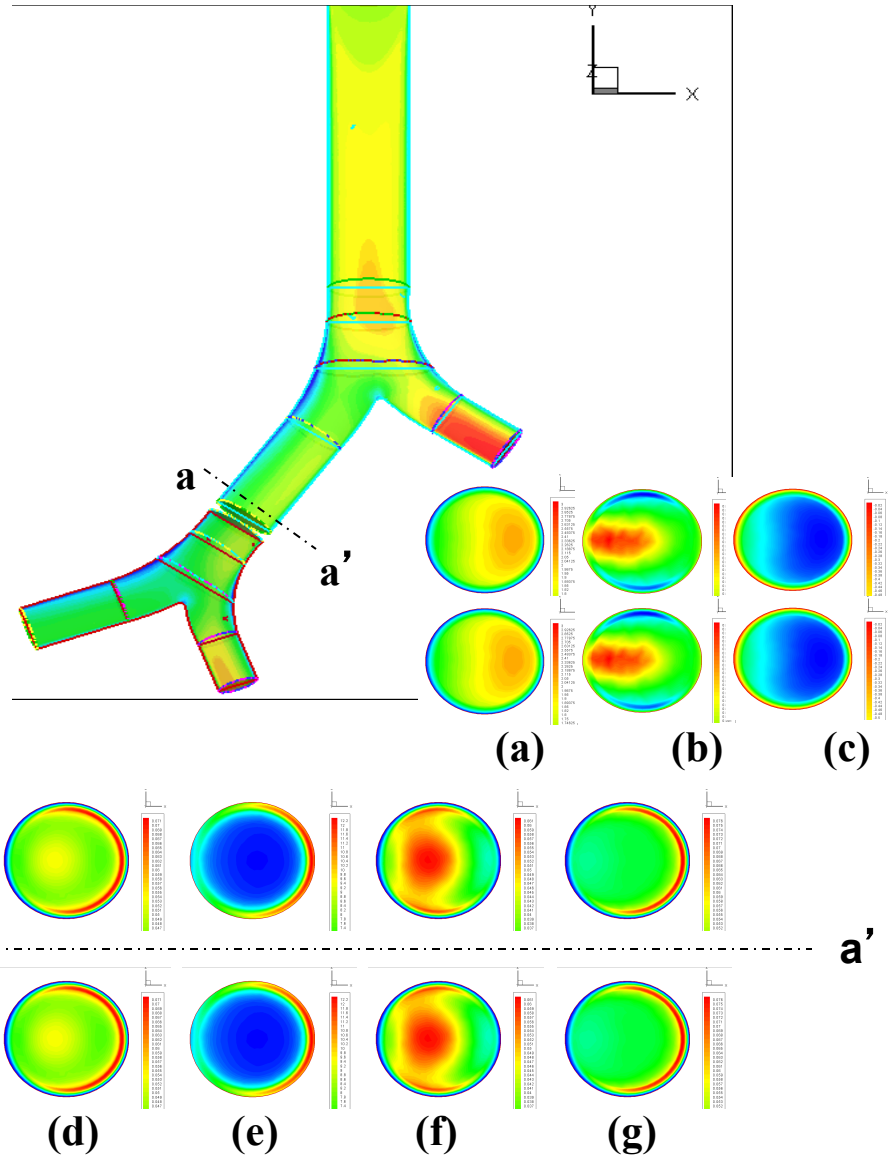
The schematics of multi-level bifurcation model

At interface aa’:

- (a) velocity magnitude
- (b) x- velocity
- (c) y- velocity
- (d) turbulence kinetic energy
- (e) turbulence dissipation rate
- (f) Reynolds stress uu
- (g) Reynolds stress vv



Lung Deposition

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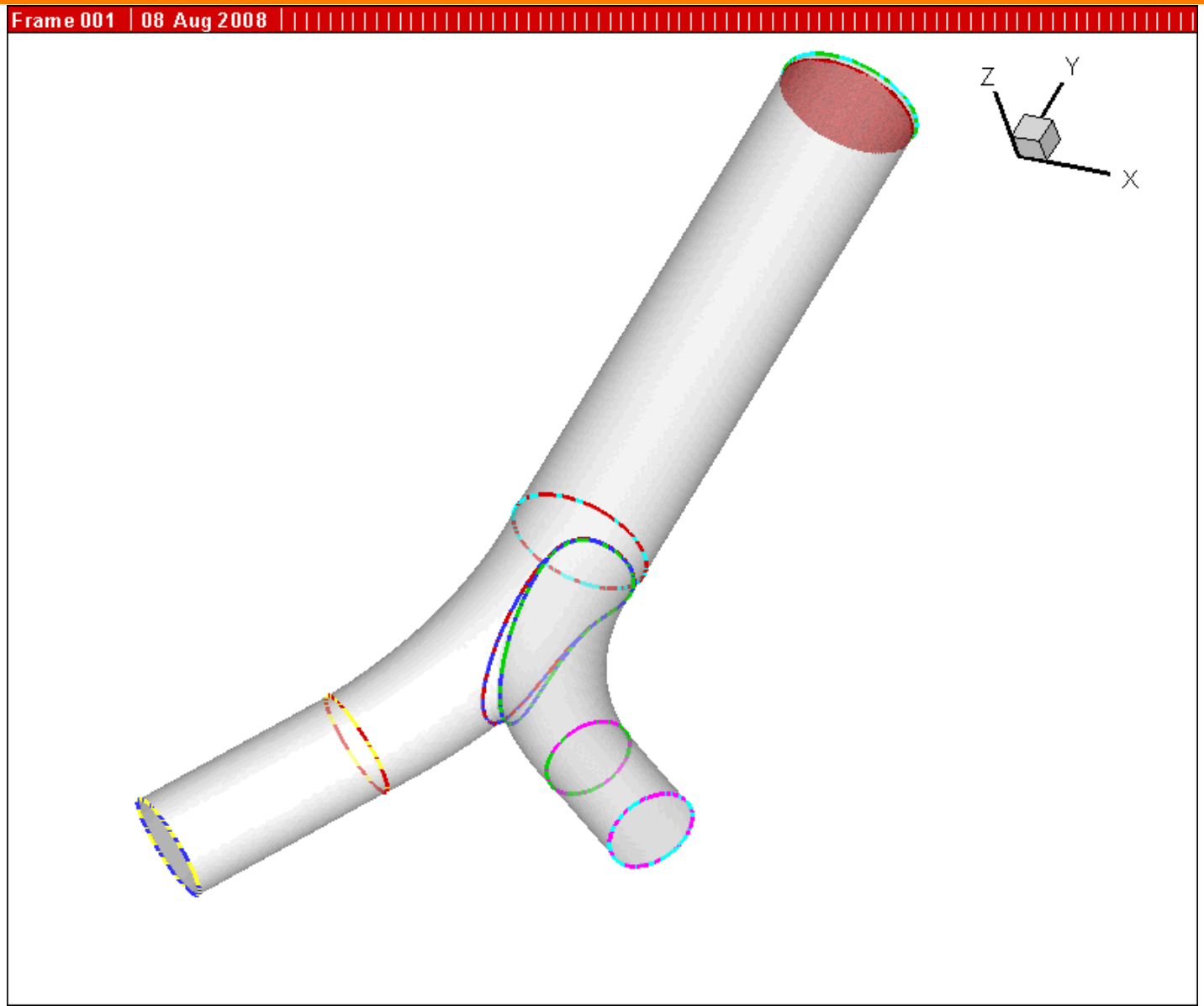

1 µm

Lung Deposition

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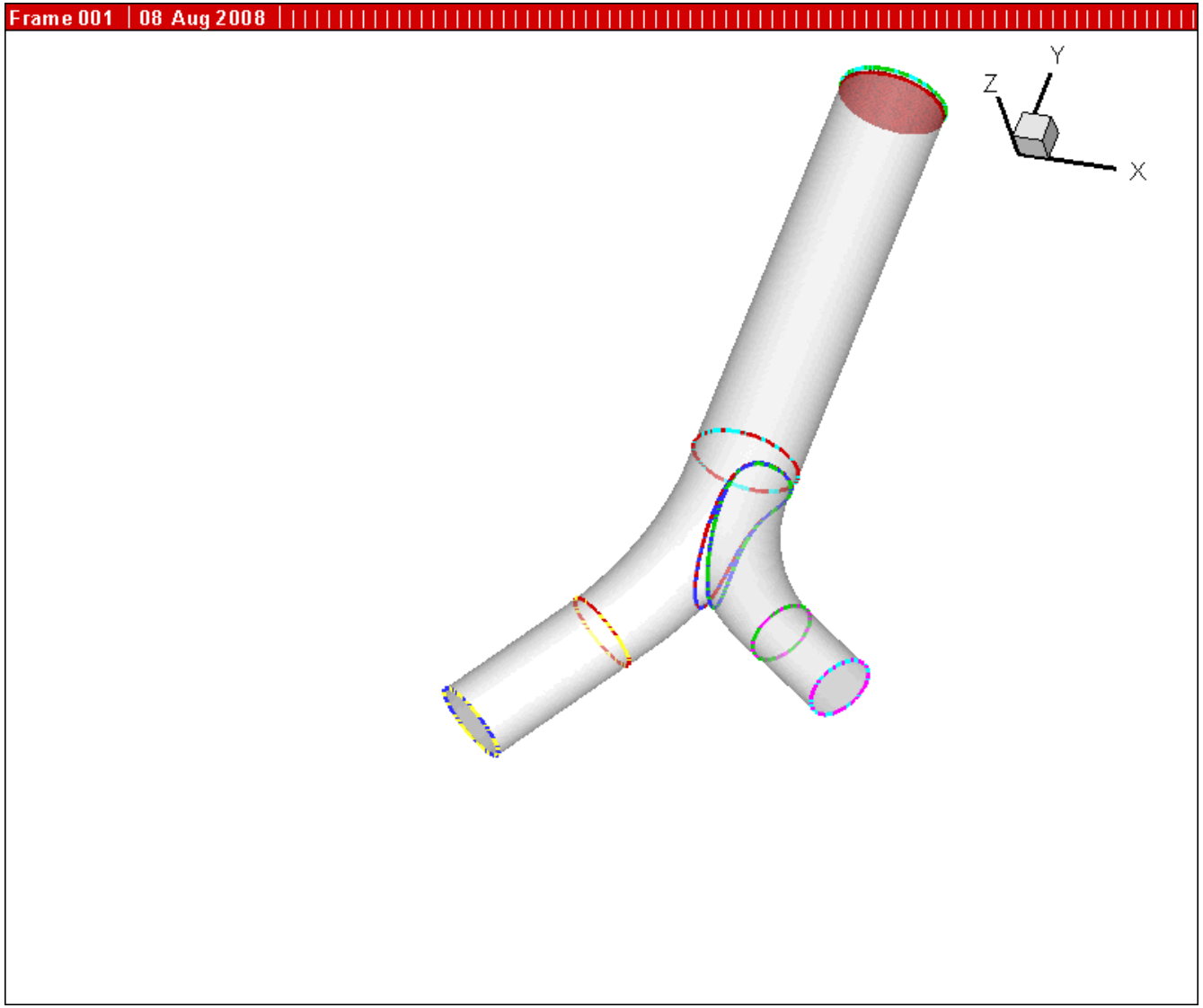

Lung Deposition Efficiency

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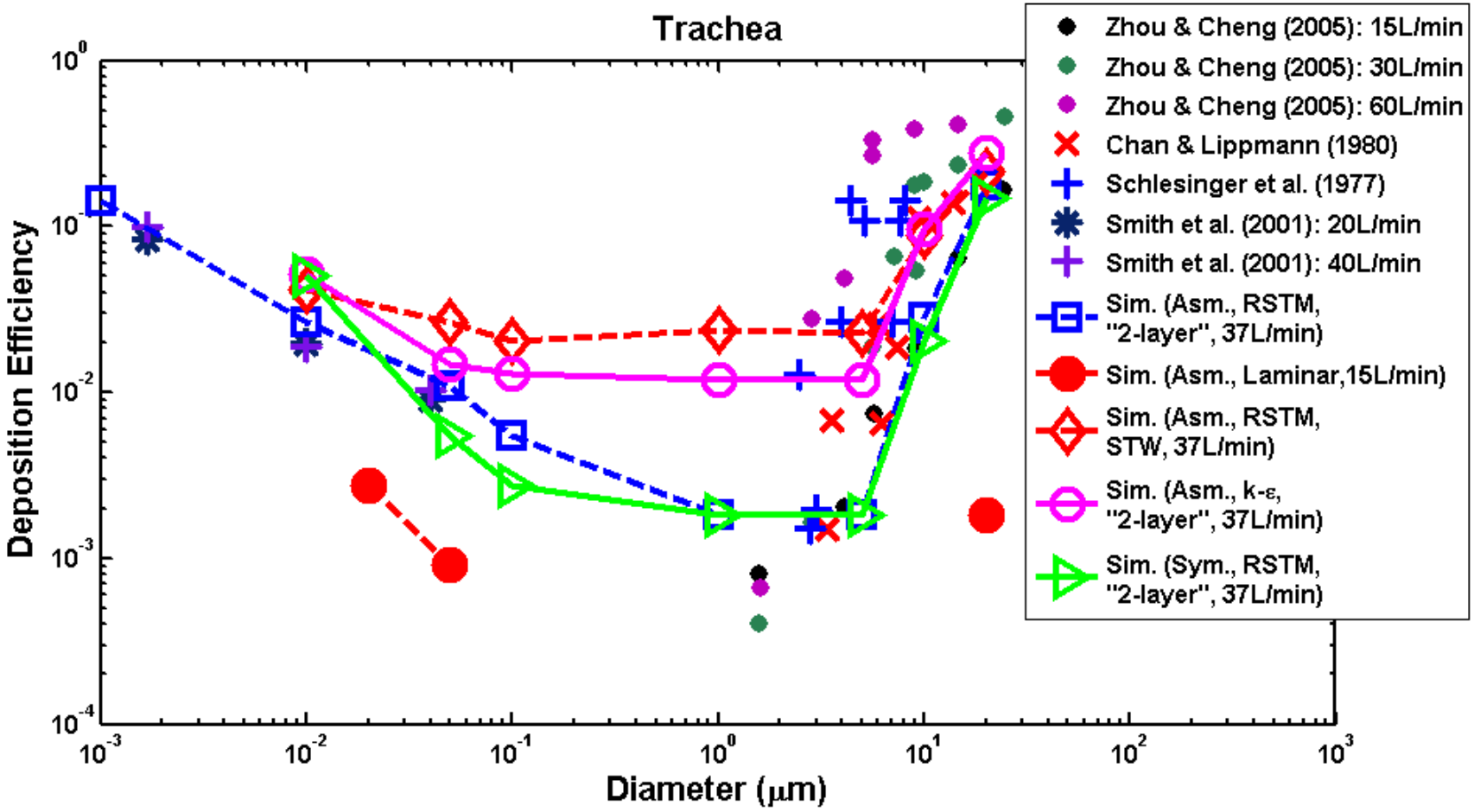
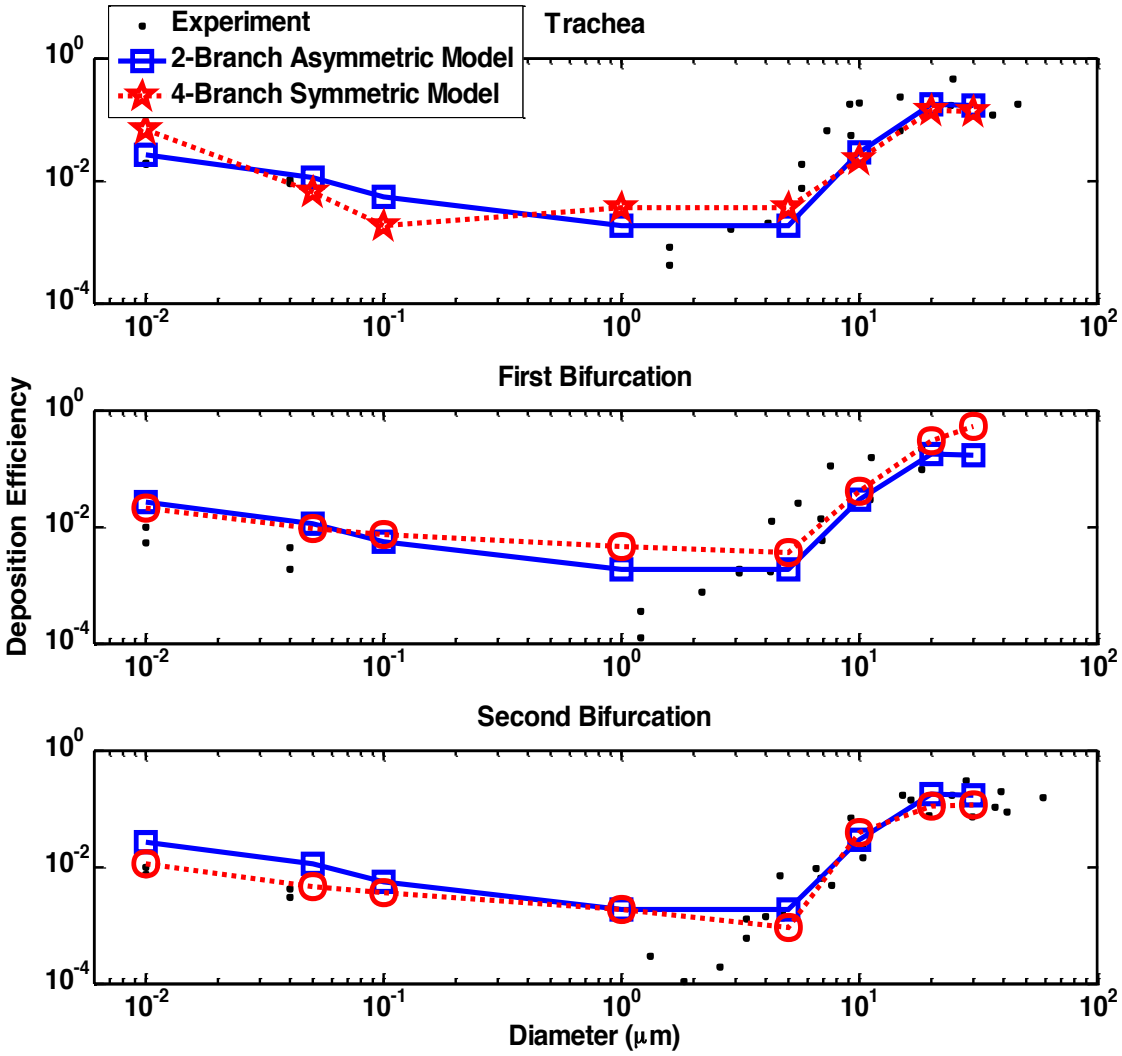


Lung Deposition Efficiency

Clarkson University



Fiber Transport Model

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Translational Motion

$$m^p \frac{d\mathbf{v}}{dt} = (m^p - m^f)\mathbf{g} + \mathbf{f}^h + \mathbf{f}^L + \mathbf{f}^B(t),$$

Rotational Motion

$$I_{\hat{x}} \frac{d\omega_{\hat{x}}}{dt} - \omega_{\hat{y}}\omega_{\hat{z}}(I_{\hat{y}} - I_{\hat{z}}) = T_{\hat{x}}^h + T_{\hat{x}}^B(t),$$

$$I_{\hat{y}} \frac{d\omega_{\hat{y}}}{dt} - \omega_{\hat{z}}\omega_{\hat{x}}(I_{\hat{z}} - I_{\hat{x}}) = T_{\hat{y}}^h + T_{\hat{y}}^B(t),$$

$$I_{\hat{z}} \frac{d\omega_{\hat{z}}}{dt} - \omega_{\hat{x}}\omega_{\hat{y}}(I_{\hat{x}} - I_{\hat{y}}) = T_{\hat{z}}^h + T_{\hat{z}}^B(t),$$

Fiber Transport Model

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Translational Brownian Force

$$< \hat{\mathbf{f}}^B(t) >= 0, \quad < \hat{\mathbf{f}}^B(t) \otimes \hat{\mathbf{f}}^B(t+t') >= \pi S^t \delta(t')$$

$$S^t_{\hat{i}\hat{i}} = 2KTR^t_{\hat{i}\hat{i}} / \pi$$

Rotational Brownian Torque

$$< \hat{\mathbf{T}}^B(t) >= 0, \quad < \hat{\mathbf{T}}^B(t) \otimes \hat{\mathbf{T}}^B(t+t') >= \pi S^r \delta(t')$$

$$S^r_{\hat{i}\hat{i}} = 2KTR^r_{\hat{i}\hat{i}} / \pi$$

Fiber Transport and Deposition

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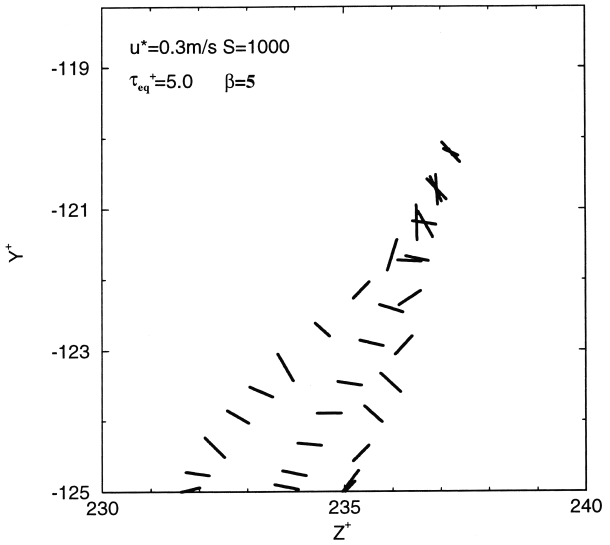

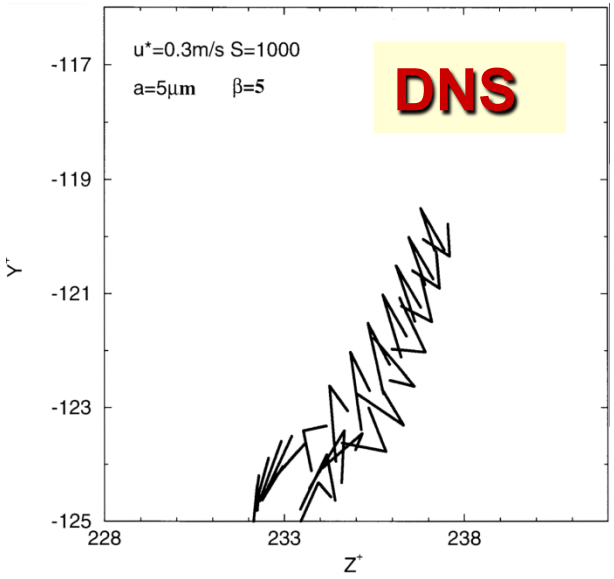

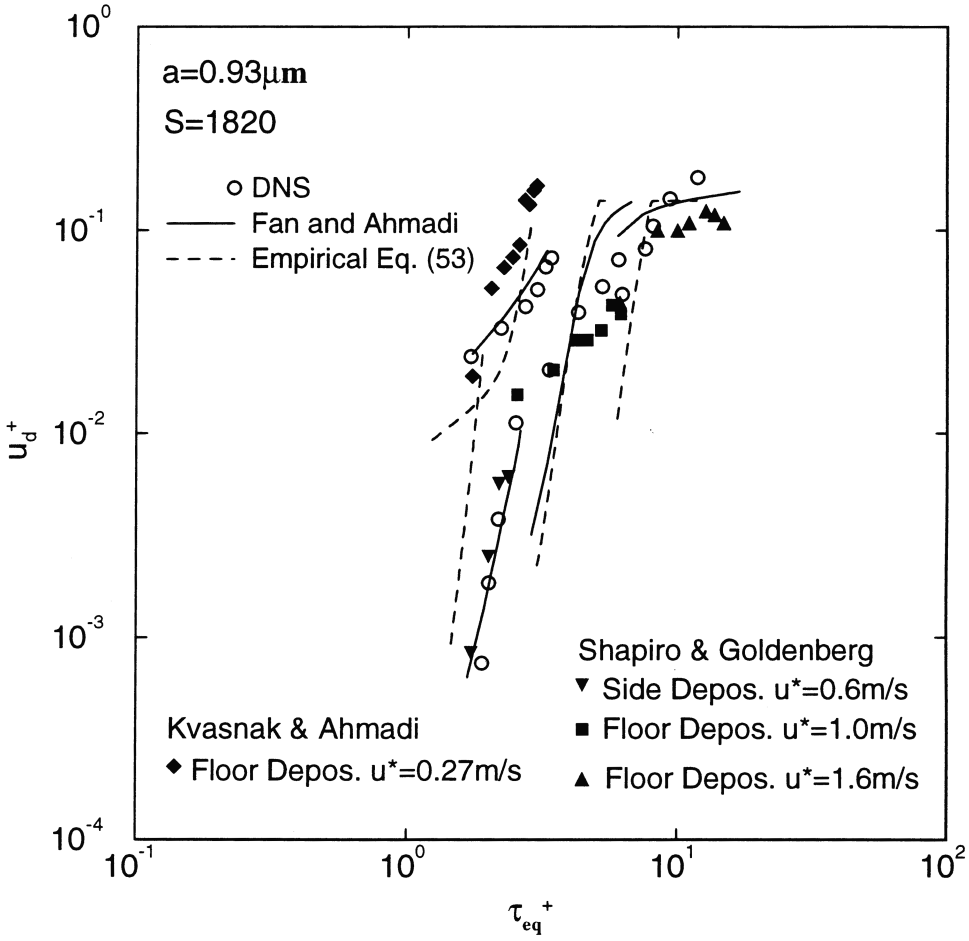

Ellipsoidal Fibers
Duct Flows

Flow Simulations

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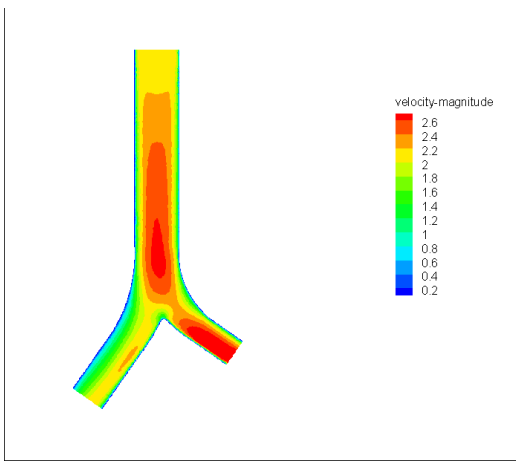
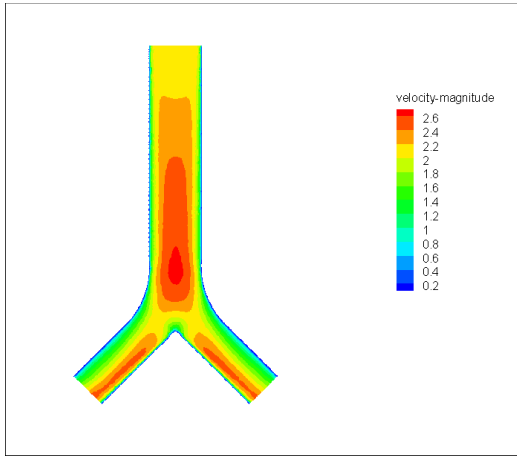
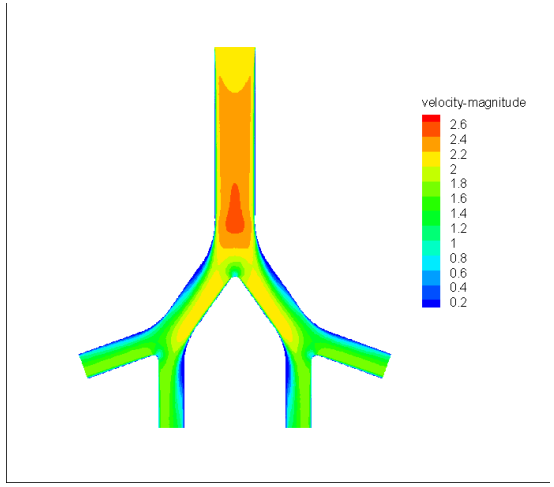
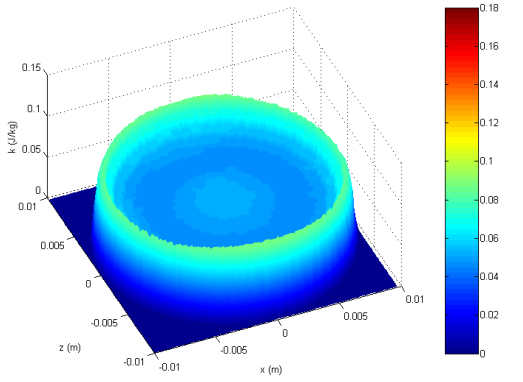
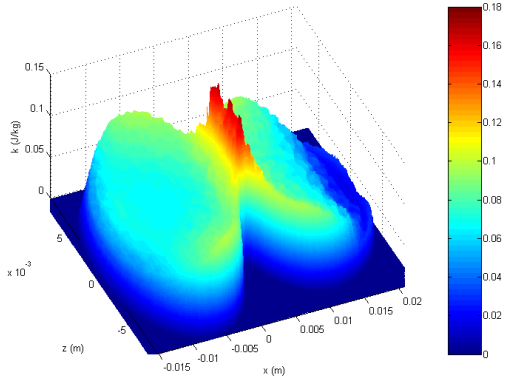


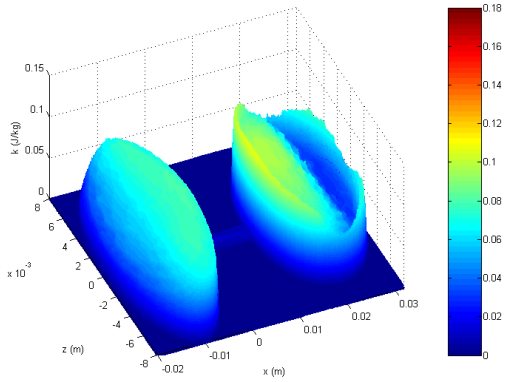




Velocity magnitude contour. Breathing rate = 37L/min







Turbulence kinetic energy. Breathing rate = 37L/min

Fiber Motion Simulations

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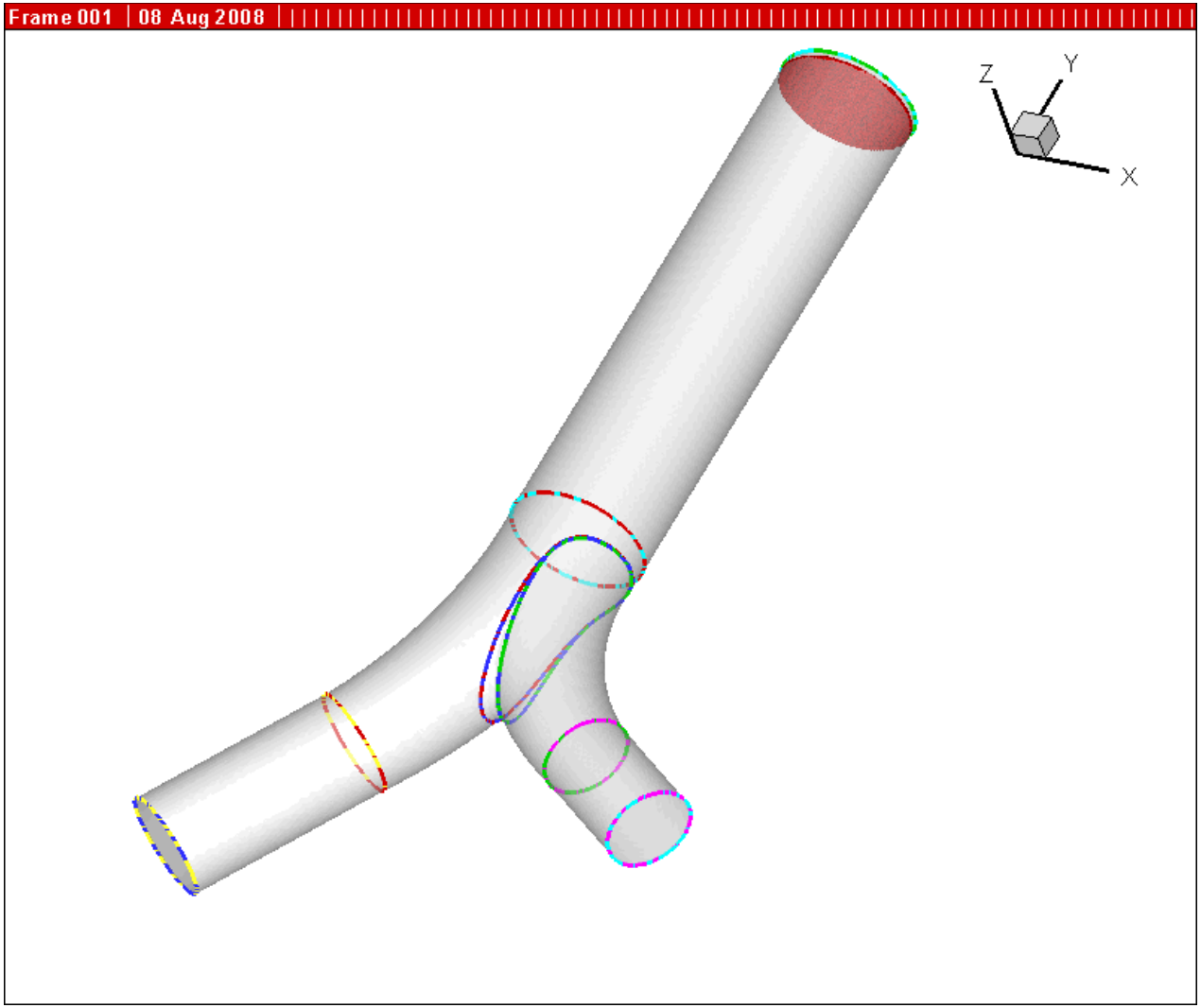

Trachea and the first bifurcation (37L/min) β = 15, d = 3.66 μm

Fiber Motion Simulations

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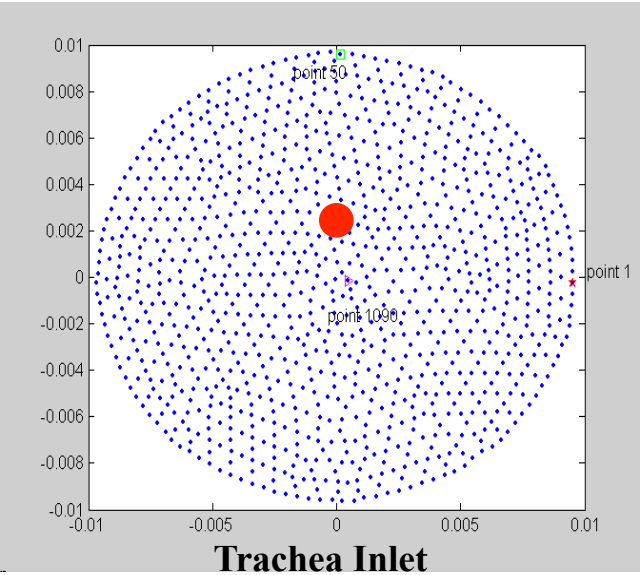
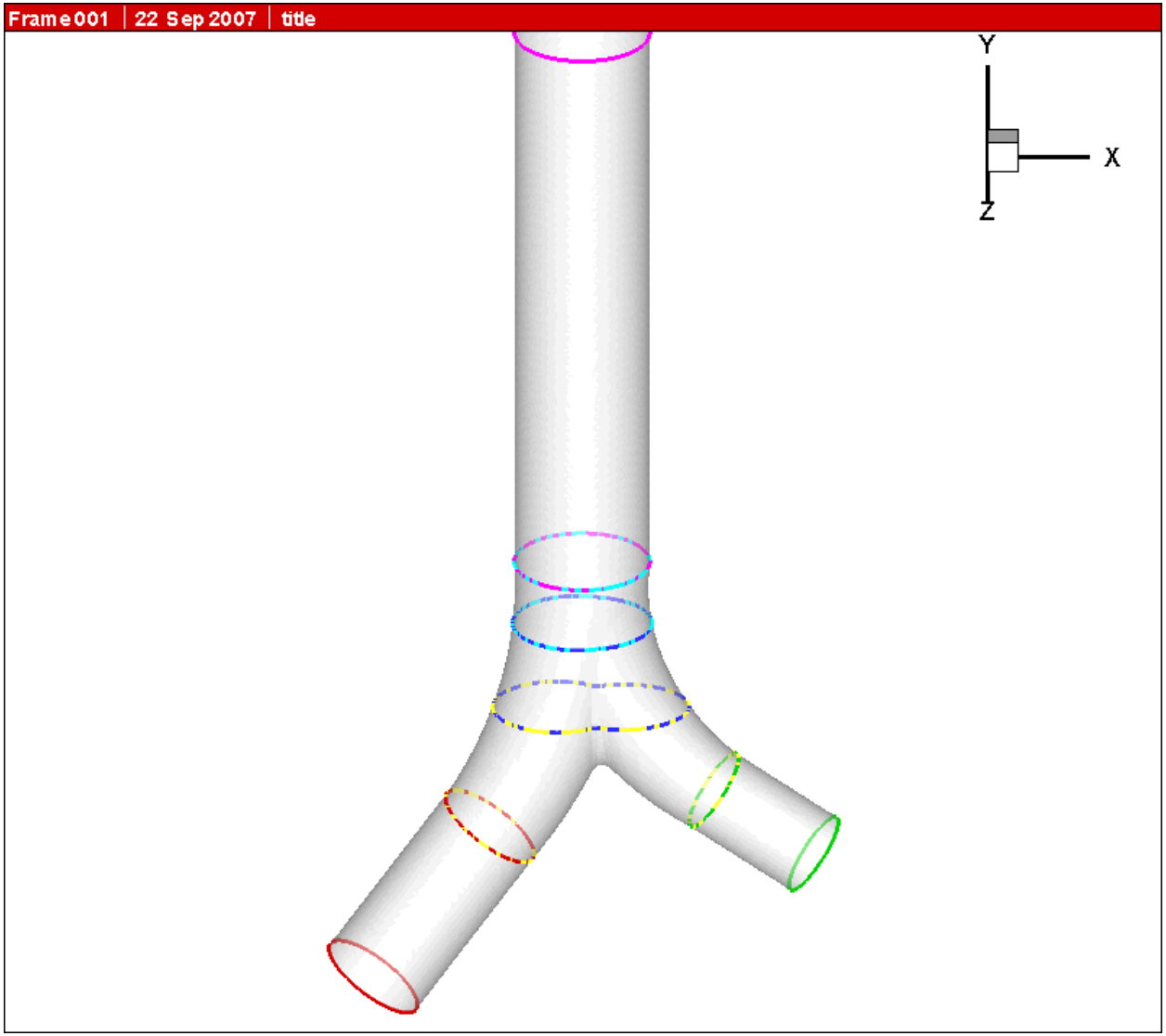


Trachea Inlet



Fiber Motion Simulations

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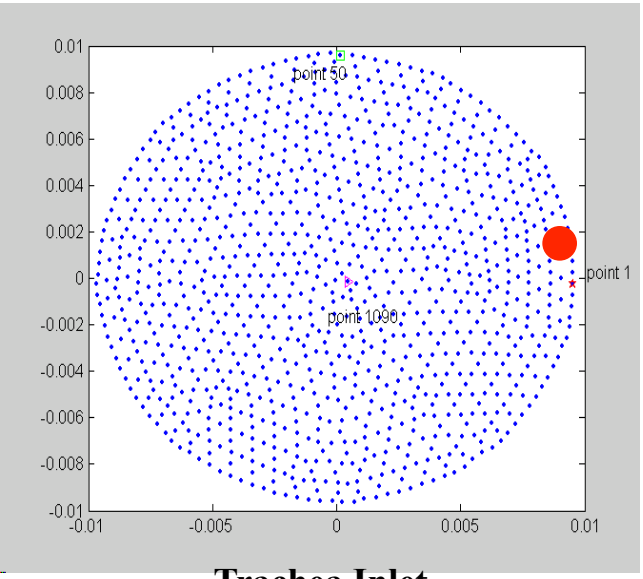
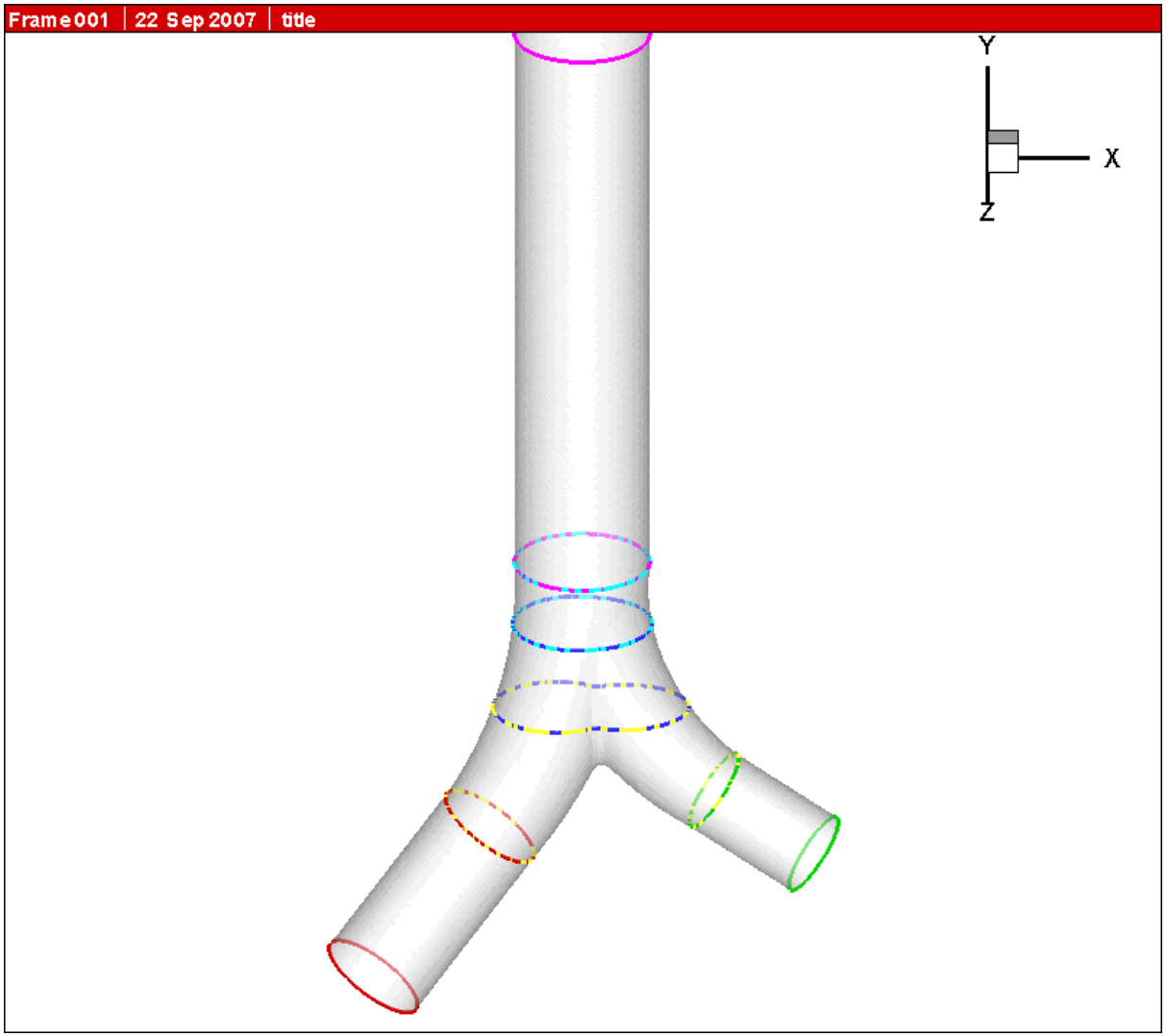
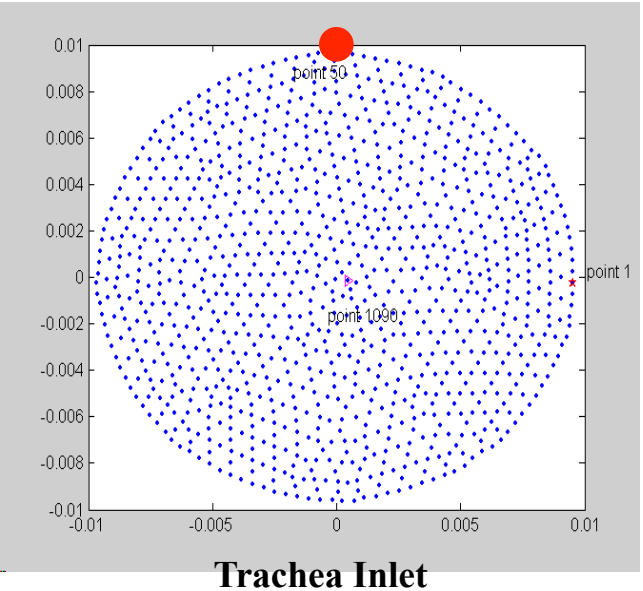


Trachea Inlet

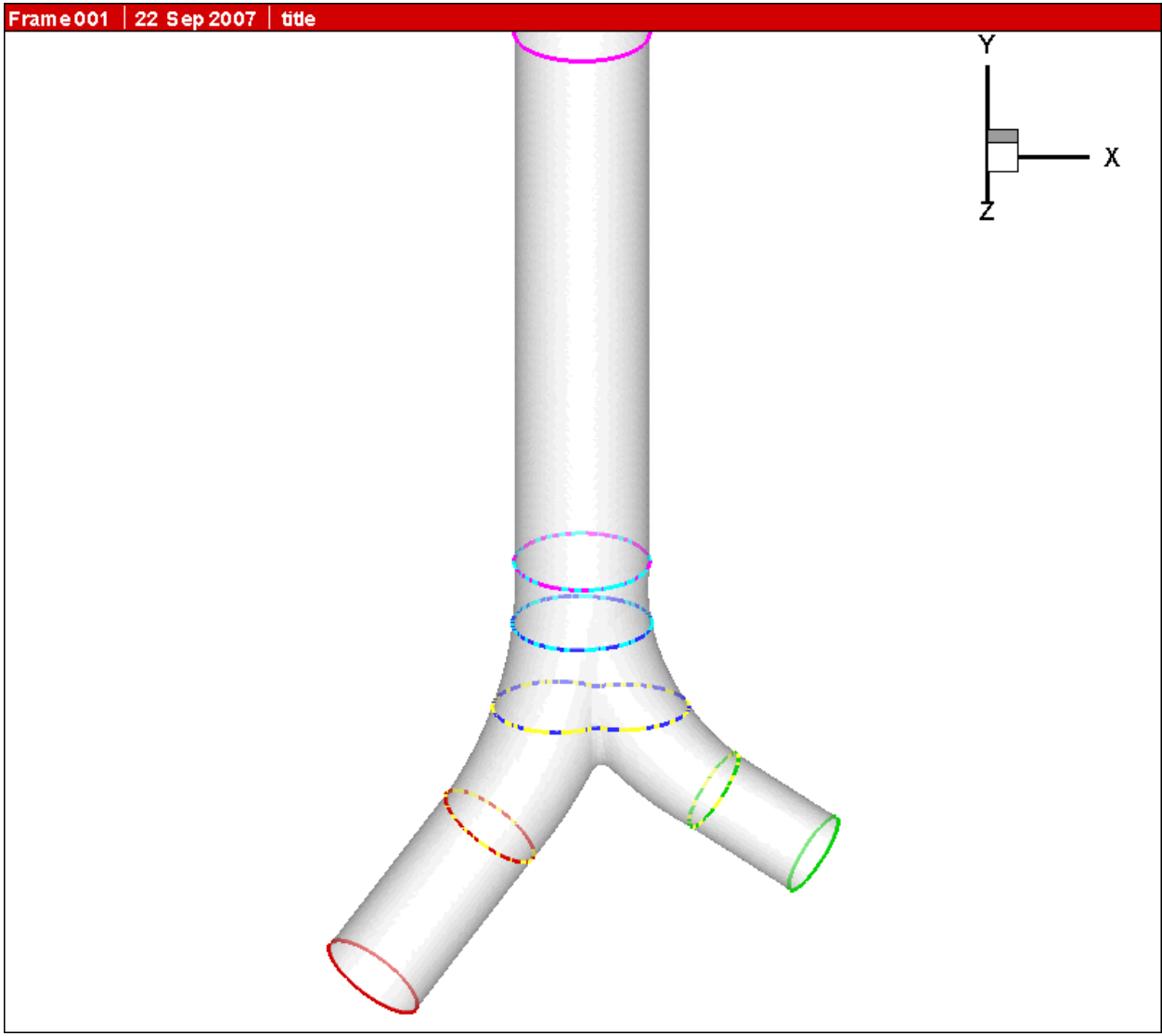


Fiber Motion Simulations

Clarkson University



Trachea Inlet



Fiber Deposition Pattern

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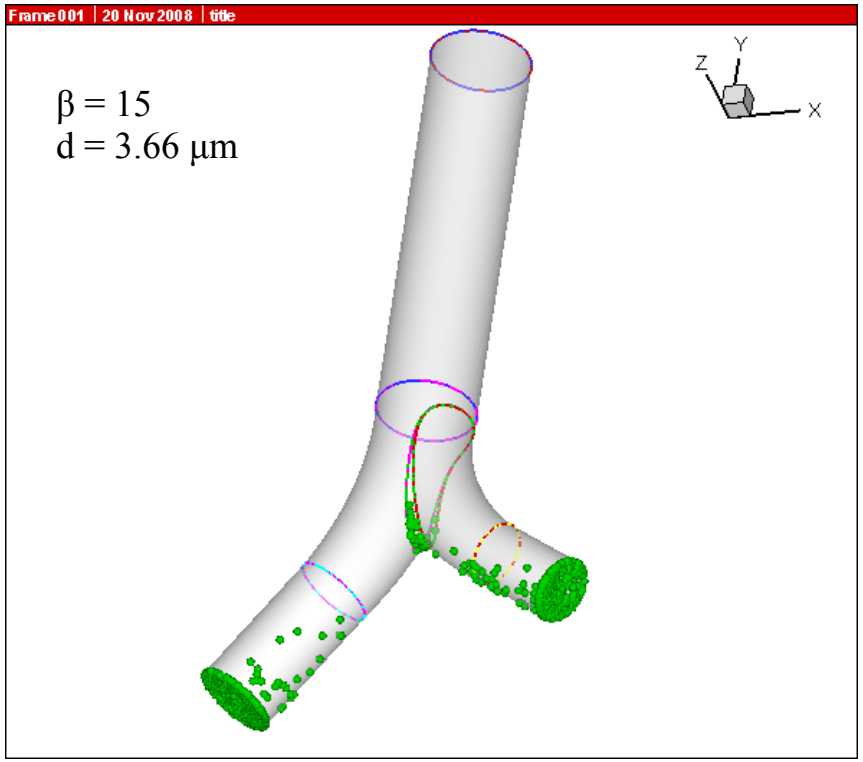
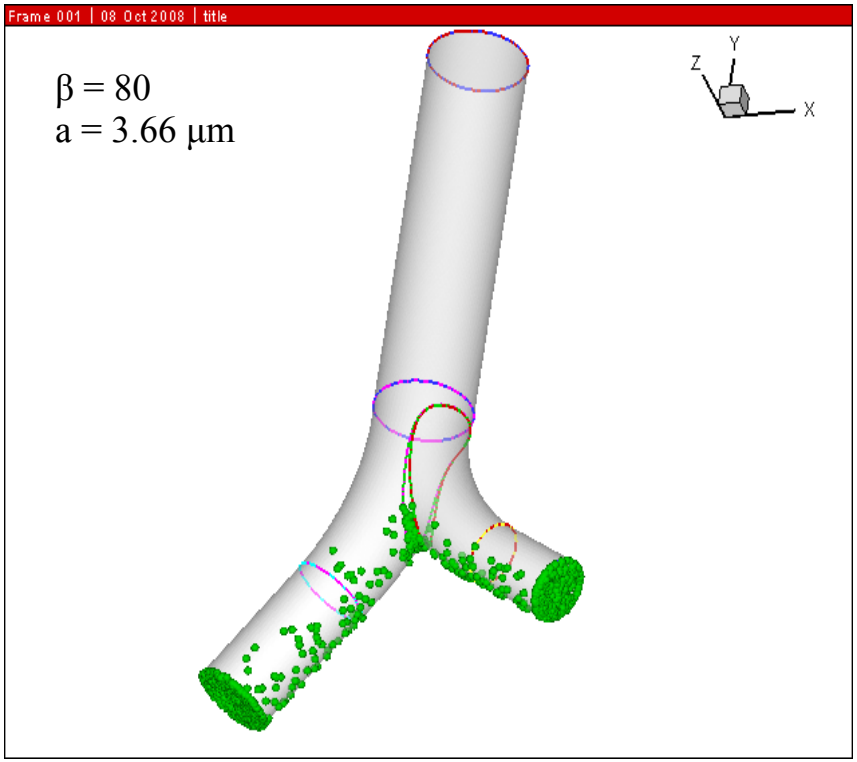


Trachea and the first bifurcation (37L/min)
β = 15, d = 3.66 μm



Trachea and the first bifurcation (37L/min)
β = 80, d = 3.66 μm

Comparison with Experimental Data

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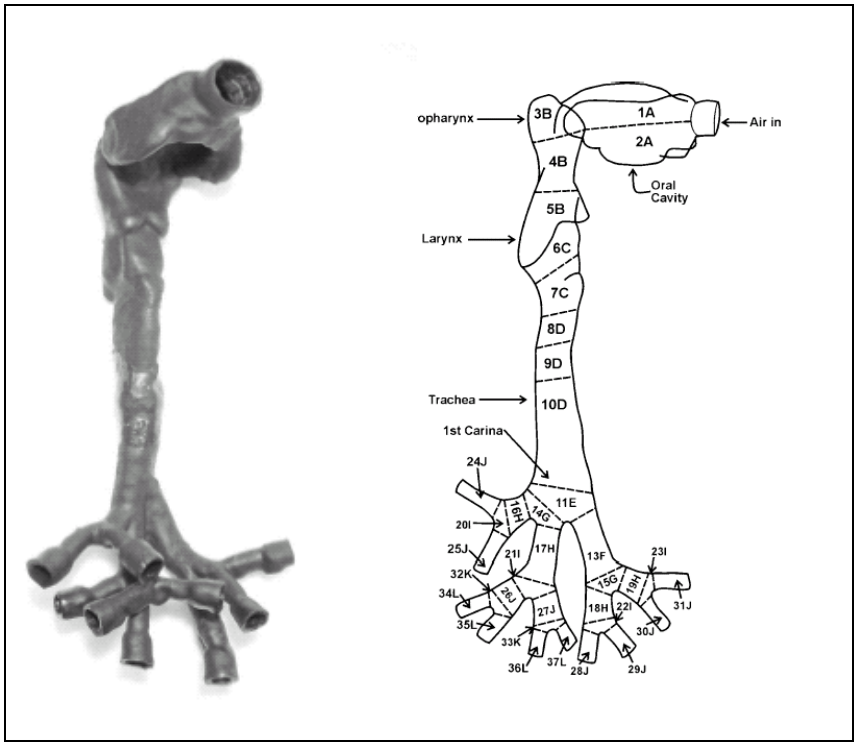
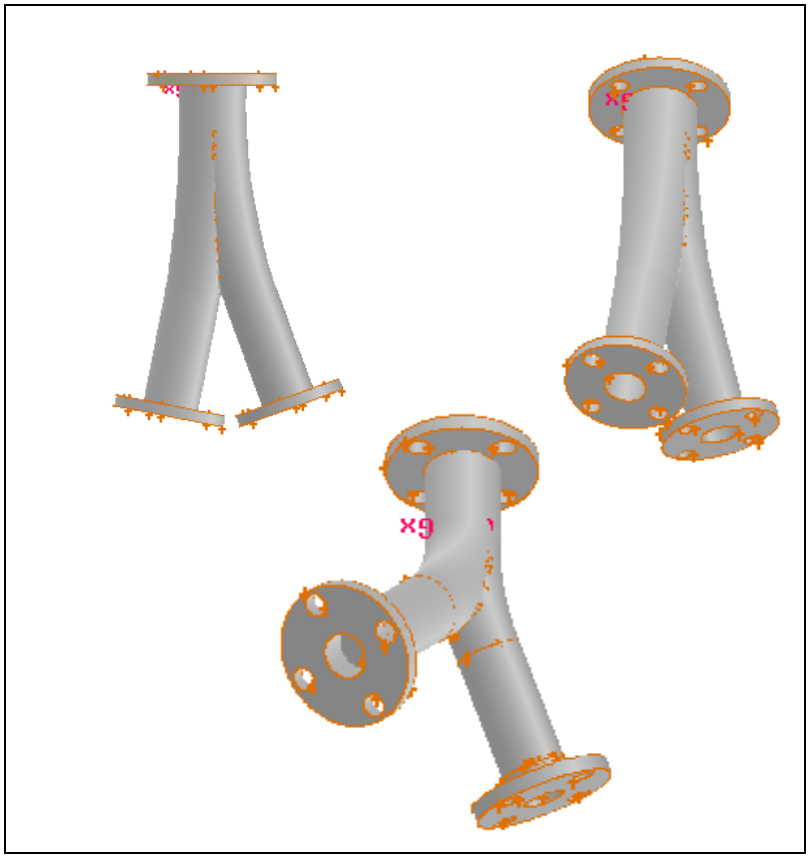


Human tracheobronchial cast of Zhou and Cheng, 2007



Human Tracheobronchial airway model of Wang and Hopke, 2008

Simulation Conditions

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- **Breathing rate**
  - **15, 40, 60 L/min**

- **Fiber property**
  - **Carbon fiber (1830kg/m^3),**
  - **Semi-minor diameter 3.66 µm, 1, 2, 8, 16 µm**
  - **Aspect ratios: 1 – 80**

- **Fiber non-dimensional relaxation time**

$$\tau_{eq}^{+} = \frac{4\beta Sa^{+2}}{k_{\hat{x}\hat{x}} + k_{\hat{y}\hat{y}} + k_{\hat{z}\hat{z}}}$$

Fiber Deposition

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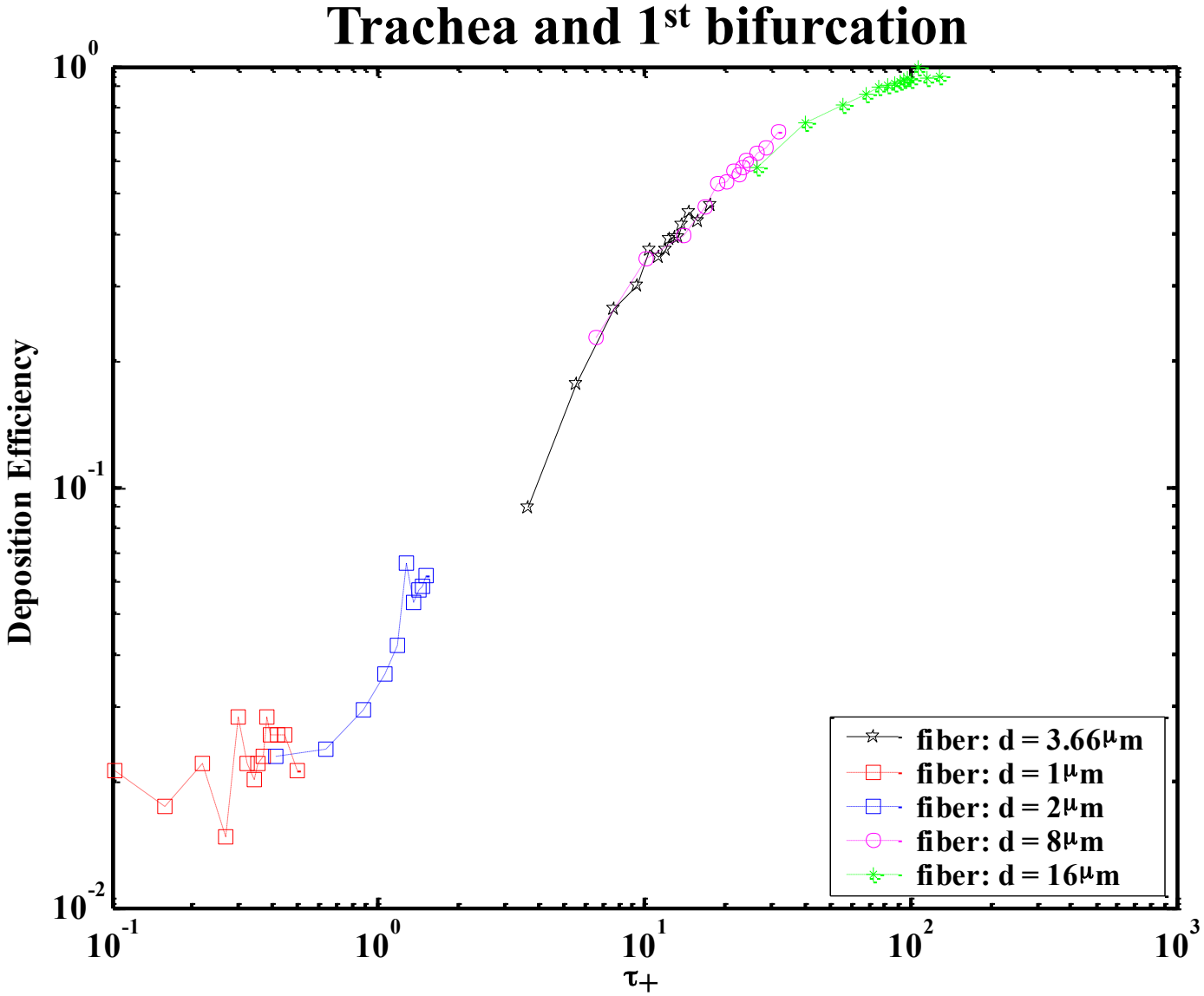
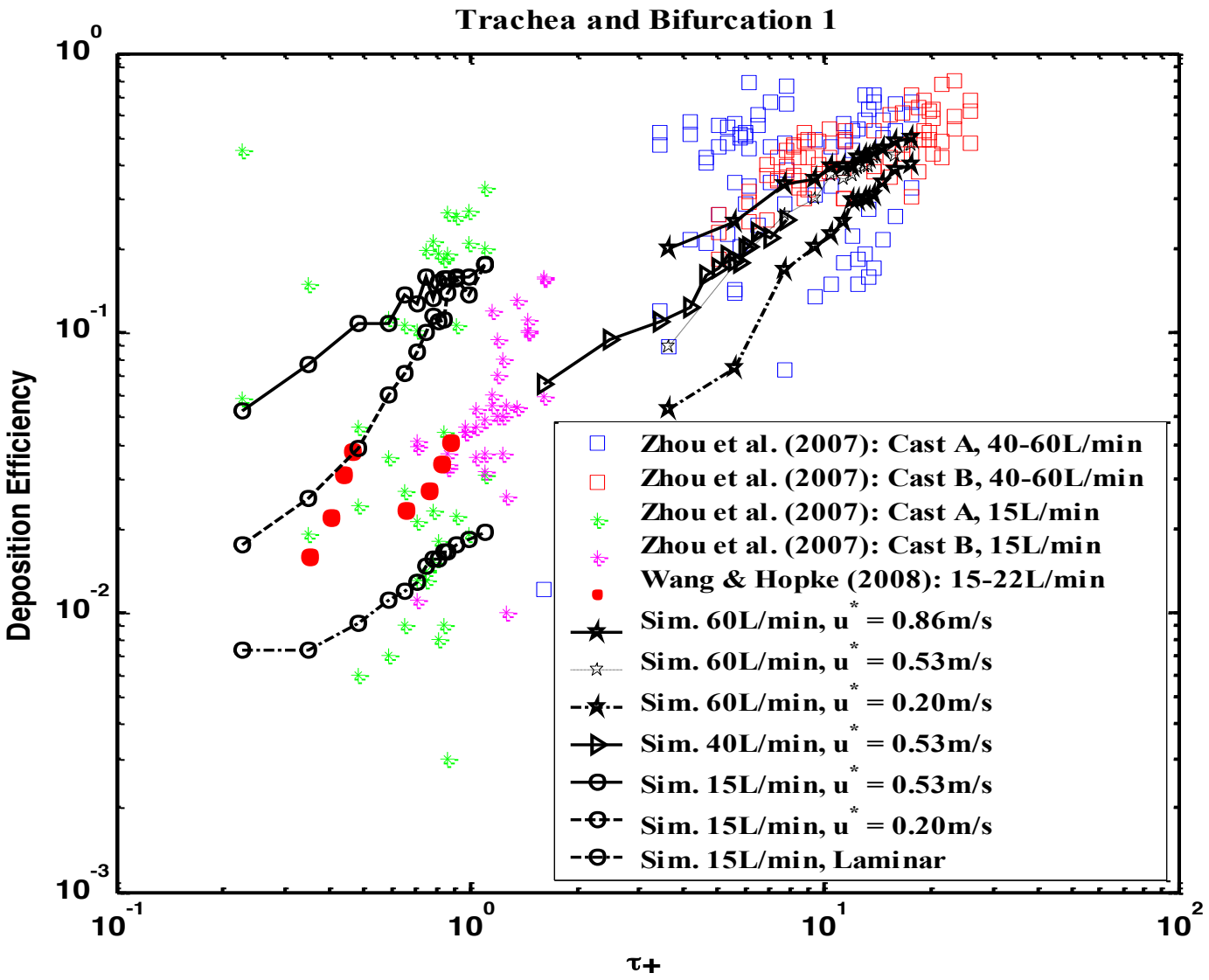


Fiber Deposition

Clarkson University



Comparison with Equivalent Spheres

Clarkson University

- Comparison are made between fiber and
  - Equivalent volume (D_eqv)
  - Equivalent Stokes by Fan and Ahmadi, 1995 (D_stk)

- Comparison data

Semi-minor diameter (μm)	Aspect ratio	D_eqv (μm)	D_Stk (μm)
1	1 – 80	---	---
2	1 – 80	2 – 8	2 – 4
3.66	1 – 80	3.66 – 15	3.66 – 8
8	1 – 80	8 – 34	8 – 17
16	1 – 80	16 – 70	16 – 35

Equivalent Spheres Diameter

Clarkson University

Equivalent Volume

$$d_{ev} = 2a\beta^{\frac{1}{3}}$$

Equivalent Stokes diameter Shapiro and Goldenburg (1993)

$$d_{Stokes_Shapiro} = 2a\sqrt{\frac{\beta \ln(\beta + \sqrt{\beta^2 - 1})}{\sqrt{\beta^2 - 1}}}$$

Equivalent Stokes diameter Fan and Ahmadi (1995)

$$d_{Stokes_Fan} = 6a\sqrt{\frac{2\beta}{k_{xx} + k_{yy} + k_{zz}}}$$

Equivalent Aerodynamic diameter, Stober (1972)

$$d_{Aerodynamic_Stober} = d_{ve}\sqrt{\frac{\rho}{\rho_0 \kappa}},$$

$$K_{\hat{x}\hat{x}} = K_{\hat{y}\hat{y}} = \frac{16(\beta^2 - 1)}{[(2\beta^2 - 3)\ln(\beta + \sqrt{\beta^2 - 1})/\sqrt{\beta^2 - 1}] + \beta},$$

$$K_{\hat{z}\hat{z}} = \frac{8(\beta^2 - 1)}{[(2\beta^2 - 1)\ln(\beta + \sqrt{\beta^2 - 1})/\sqrt{\beta^2 - 1}] - \beta},$$

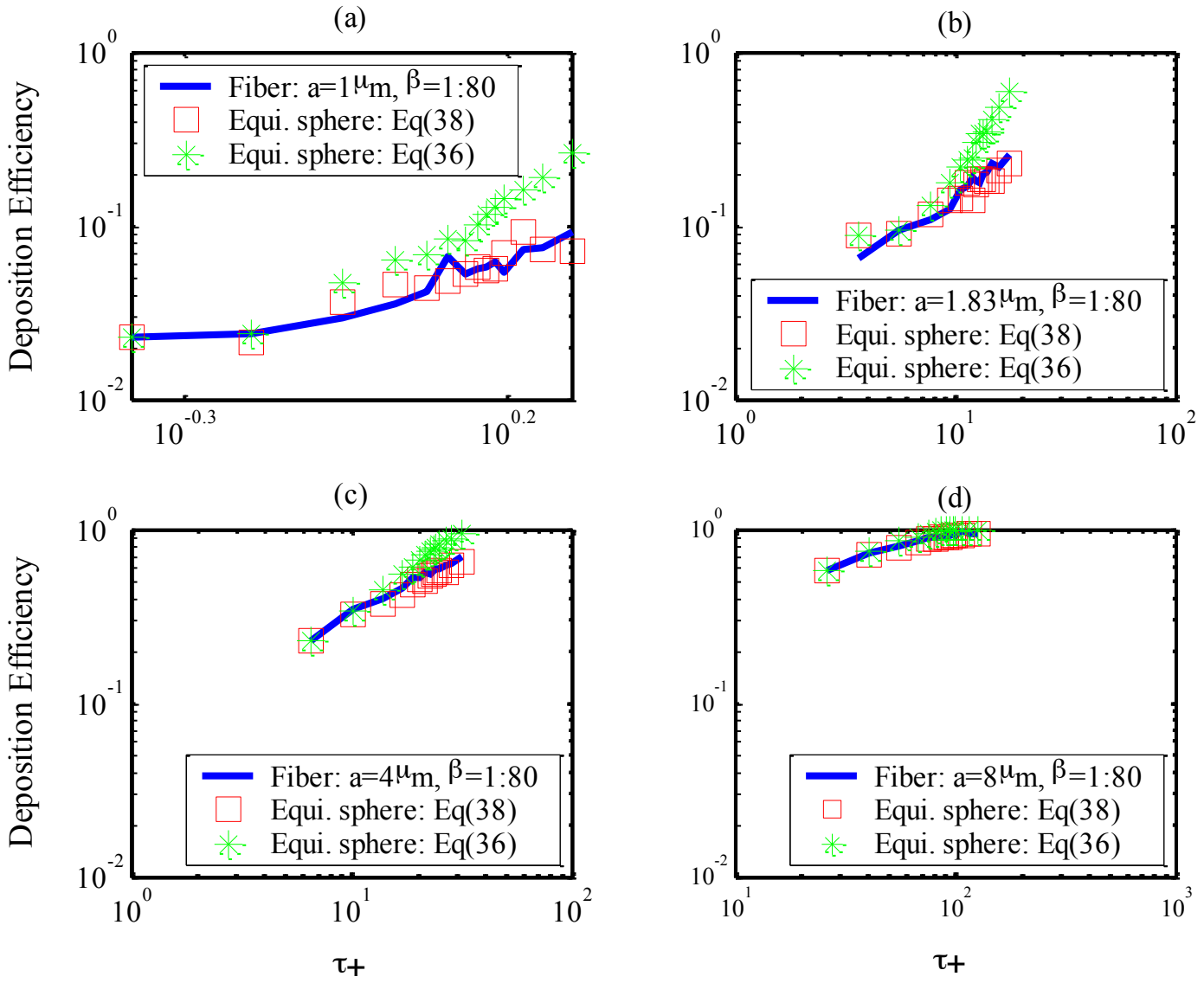
$$\kappa_{\perp} = \frac{\frac{8}{3}(\beta^2 - 1)\beta^{-\frac{1}{3}}}{\frac{2\beta^2 - 3}{\sqrt{\beta^2 - 1}}\ln(\beta + \sqrt{\beta^2 - 1}) + \beta},$$

$$\kappa_{\parallel} = \frac{\frac{4}{3}(\beta^2 - 1)\beta^{-\frac{1}{3}}}{\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}}\ln(\beta + \sqrt{\beta^2 - 1}) - \beta},$$

$$\kappa_r = \frac{3\kappa_{\perp}\kappa_{\parallel}}{\kappa_{\perp} + 2\kappa_{\parallel}}$$

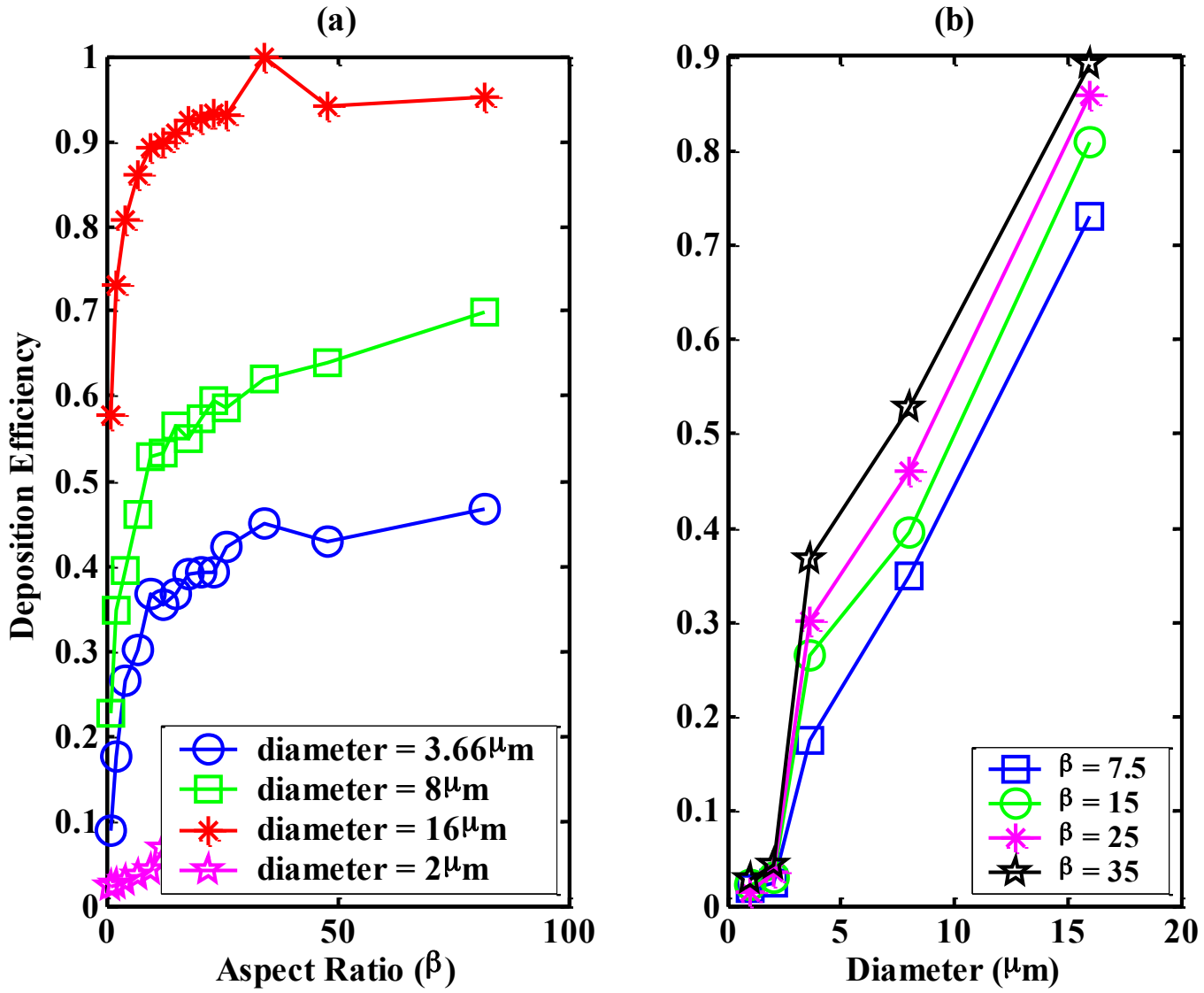
Comparison with Equivalent Spheres

Clarkson University



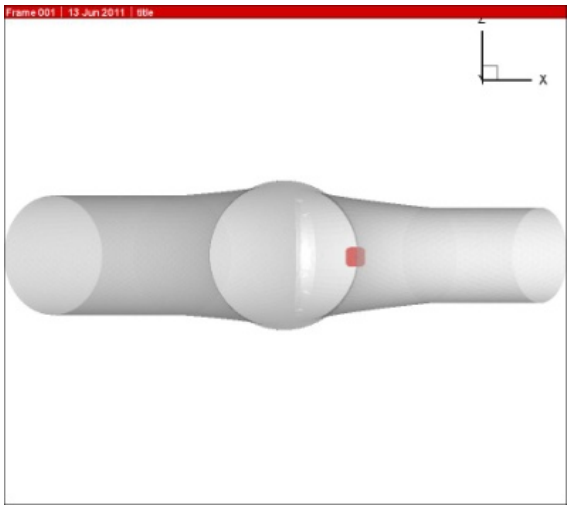
Fiber Deposition

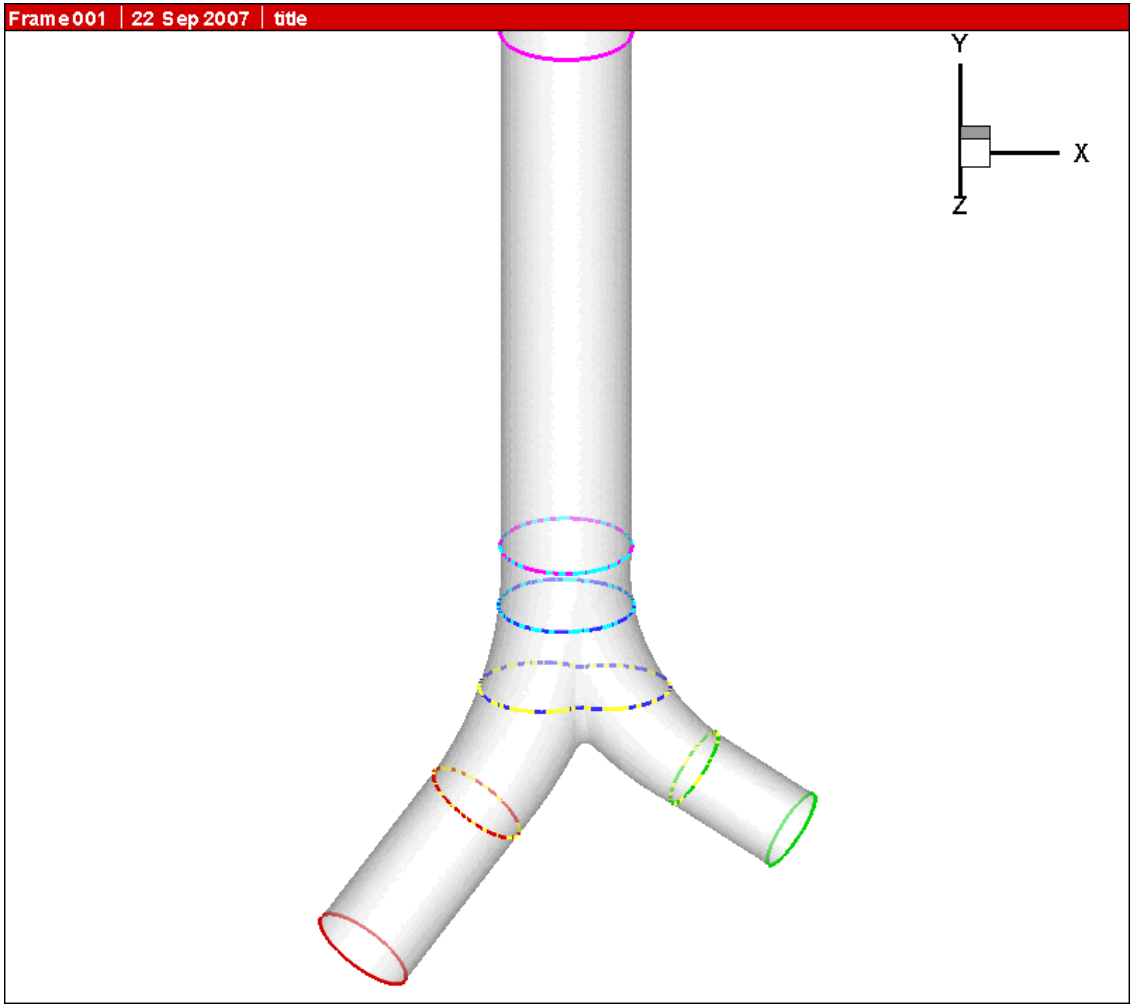
Clarkson University



Fiber Transport and Deposition

Clarkson University

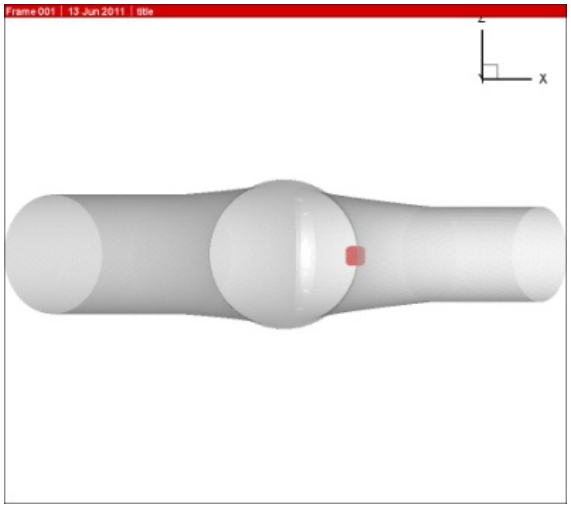


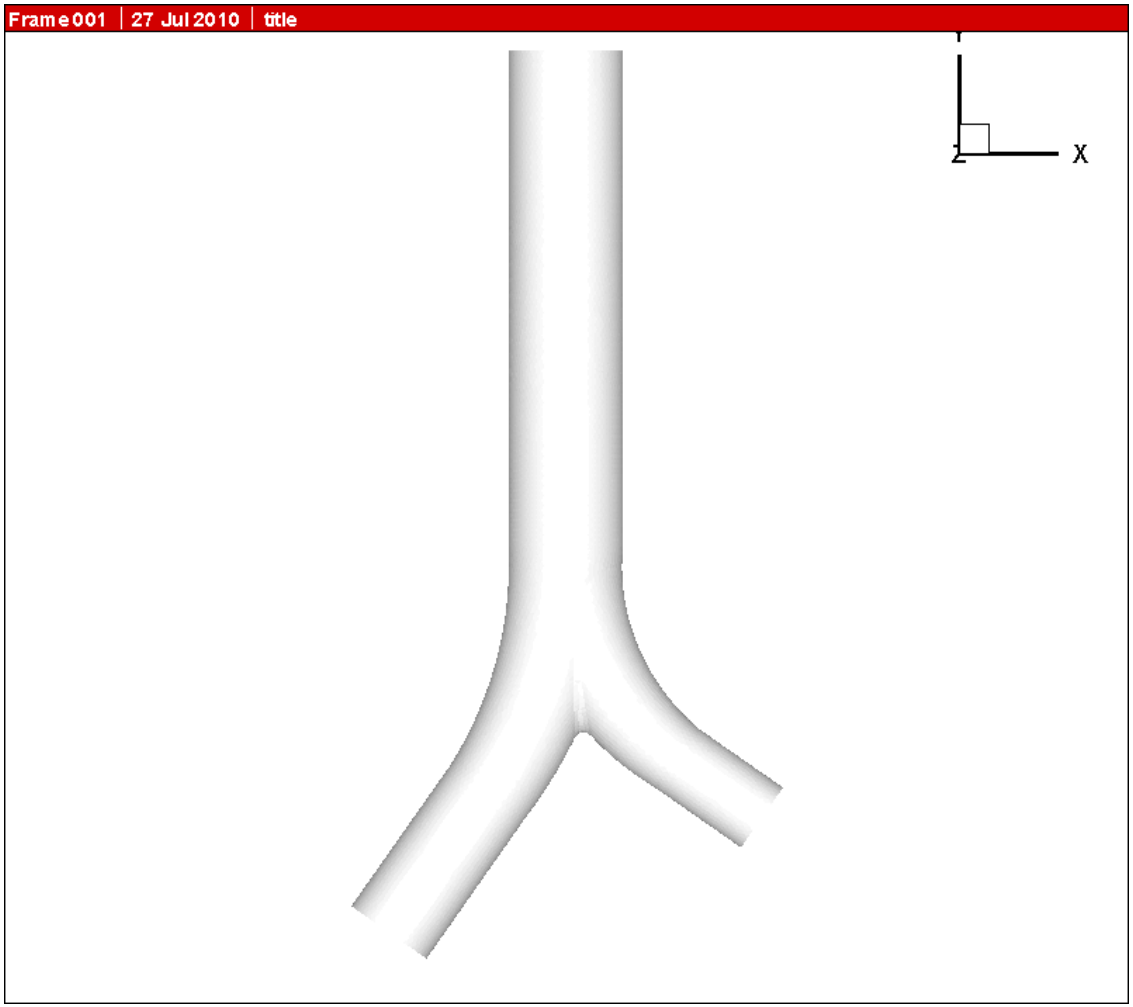


d = 3.66 µm, aspect ratio = 15, length = 55 µm

Fiber Transport and Deposition

Clarkson University

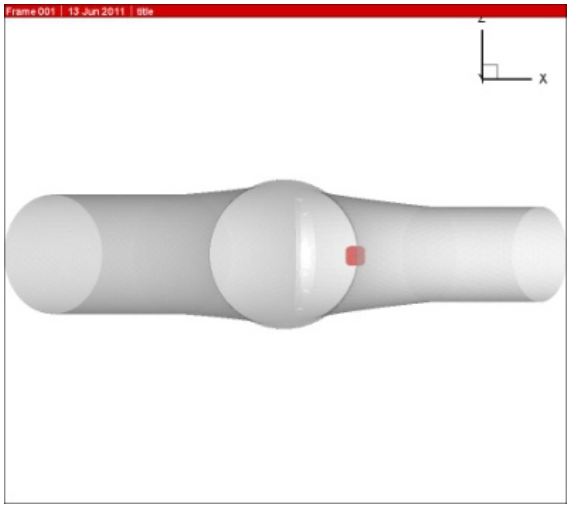


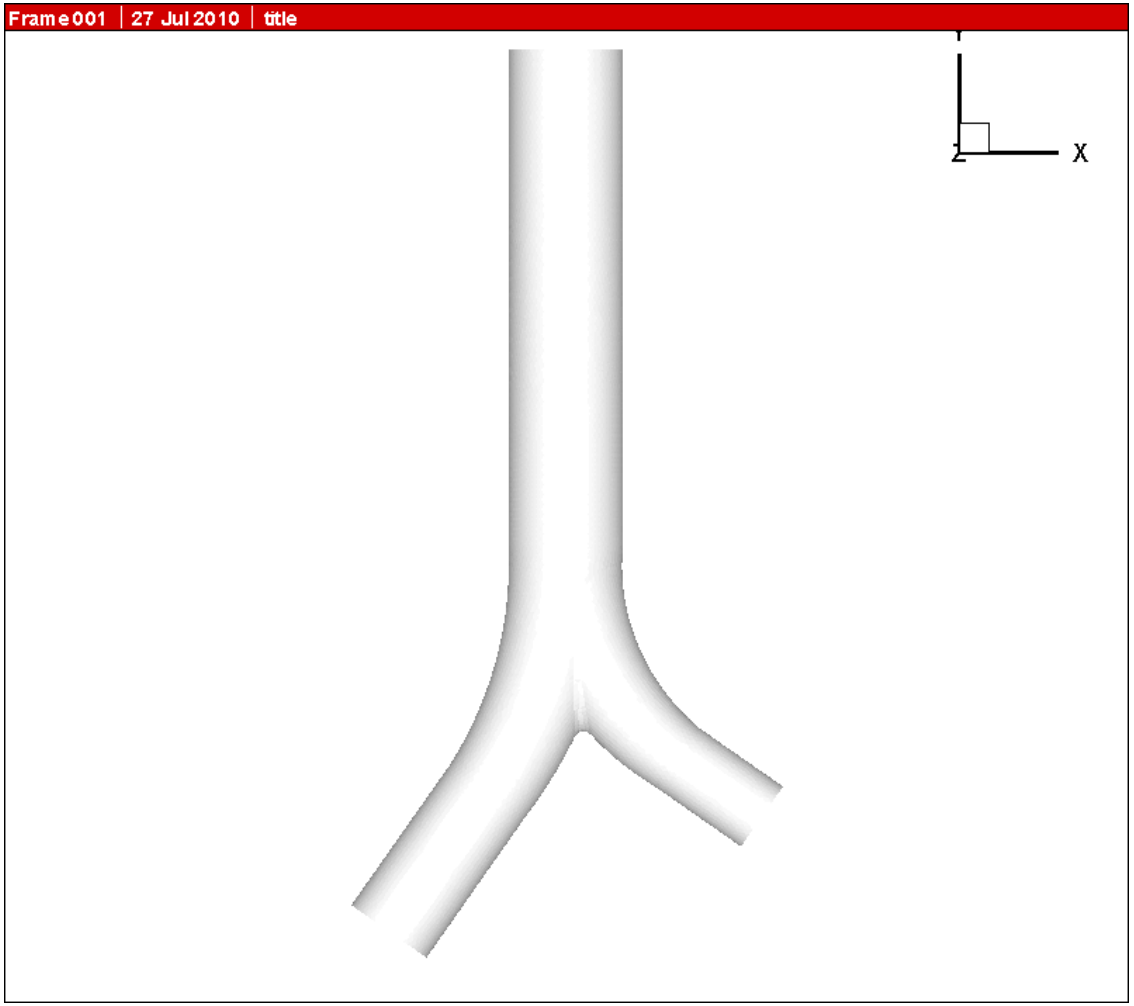


d = 0.1 µm, aspect ratio = 12,
length = 1.2 µm

Fiber Transport and Deposition

Clarkson University





d = 0.1 µm, aspect ratio = 4, length = 0.4 µm

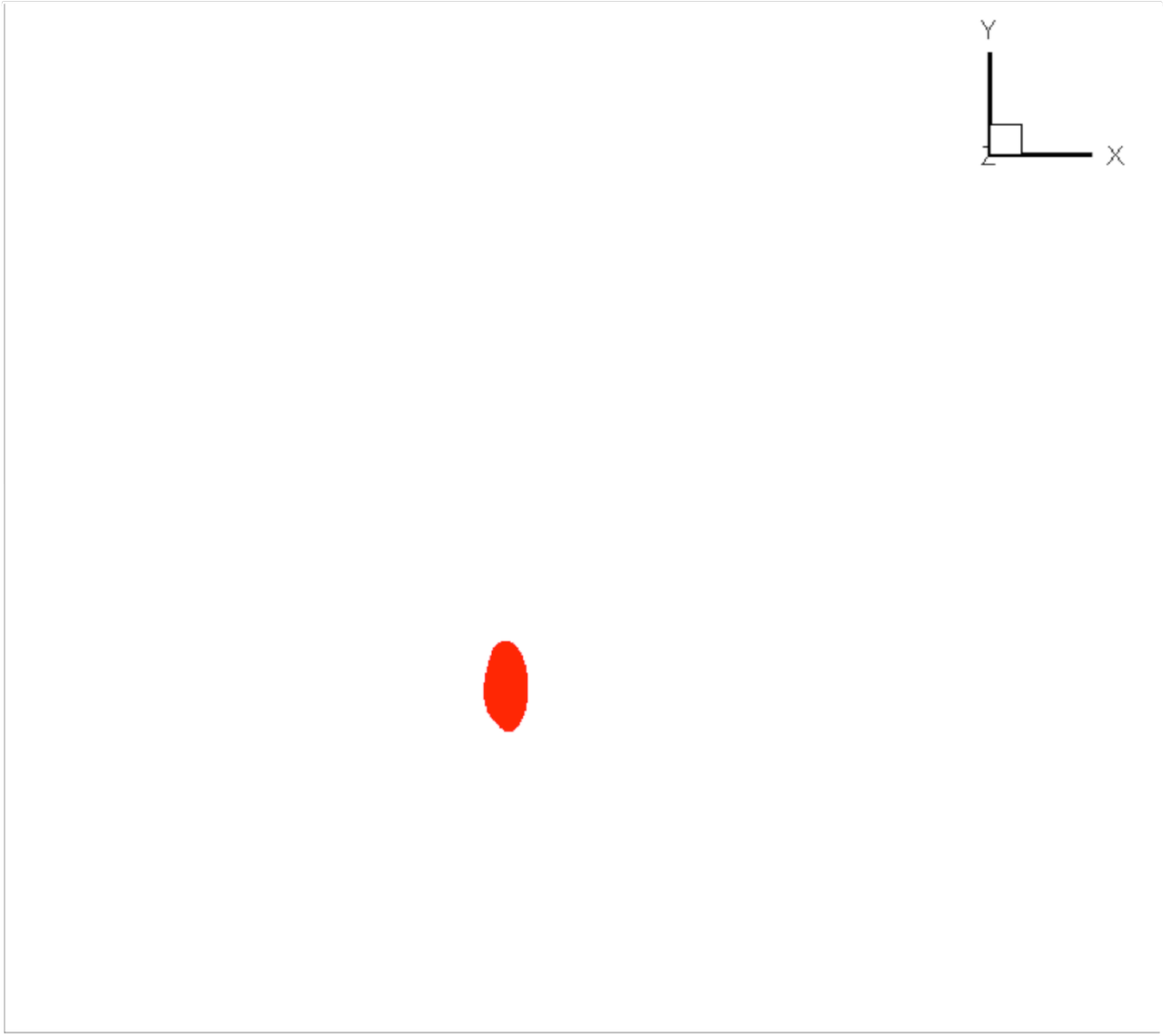
Remarks

Clarkson University

- For fiber sizes considered (a=1.83 μm, aspect ratio from 1 to 80), the motion is dominated by its inertia.
- Highly localized deposition occurs near the carina ridge bifurcation.
- Turbulence near wall correction is importance in the study of fiber deposition in human lung where turbulence is present.
- The equivalent Stokes number sphere of Fan and Ahmadi (1995) provides a good approximation for fiber deposition in the human tracheobronchial airways
- The simulated deposition efficiency agrees well with the experimental data

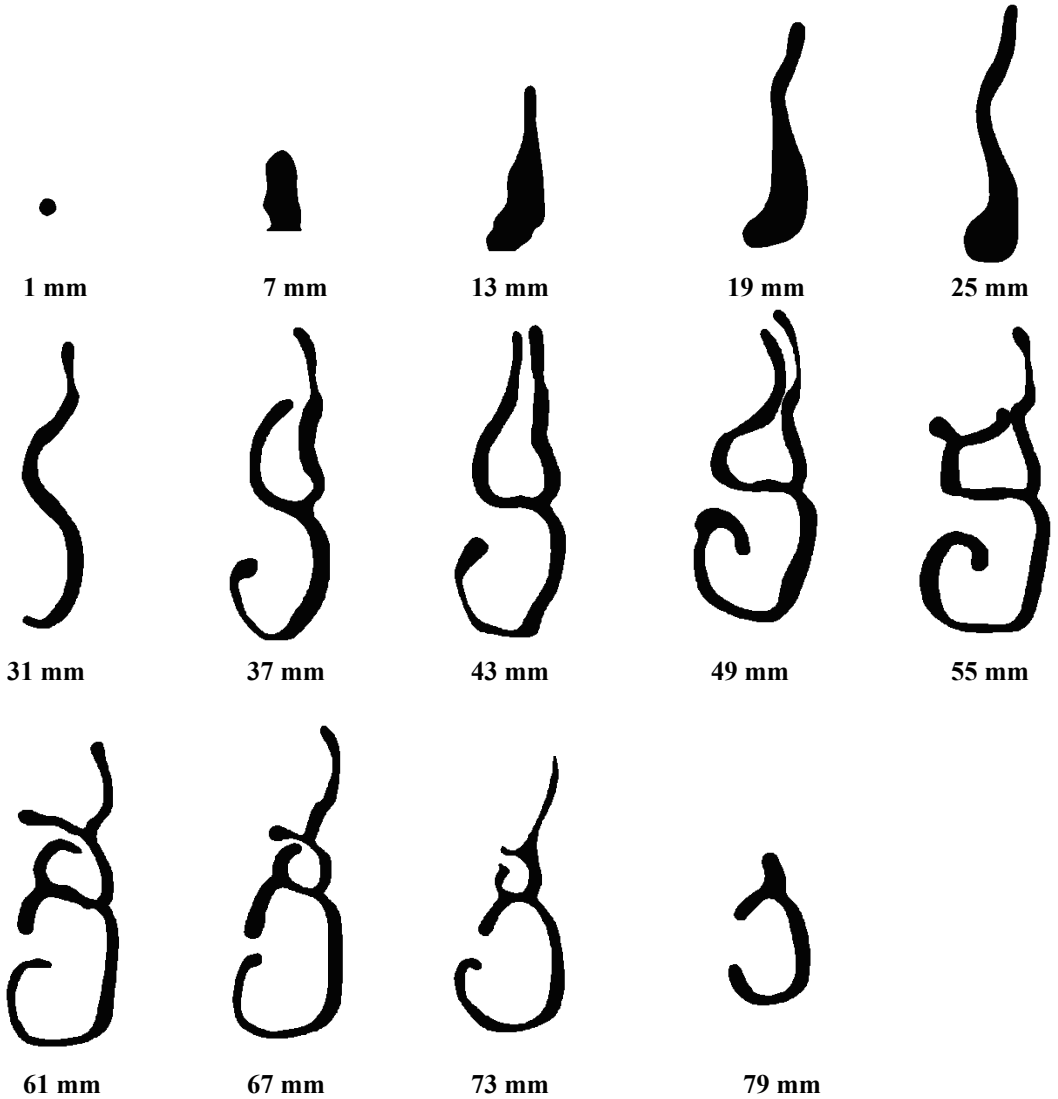
Airflow in the Nasal Cavity

Clarkson University



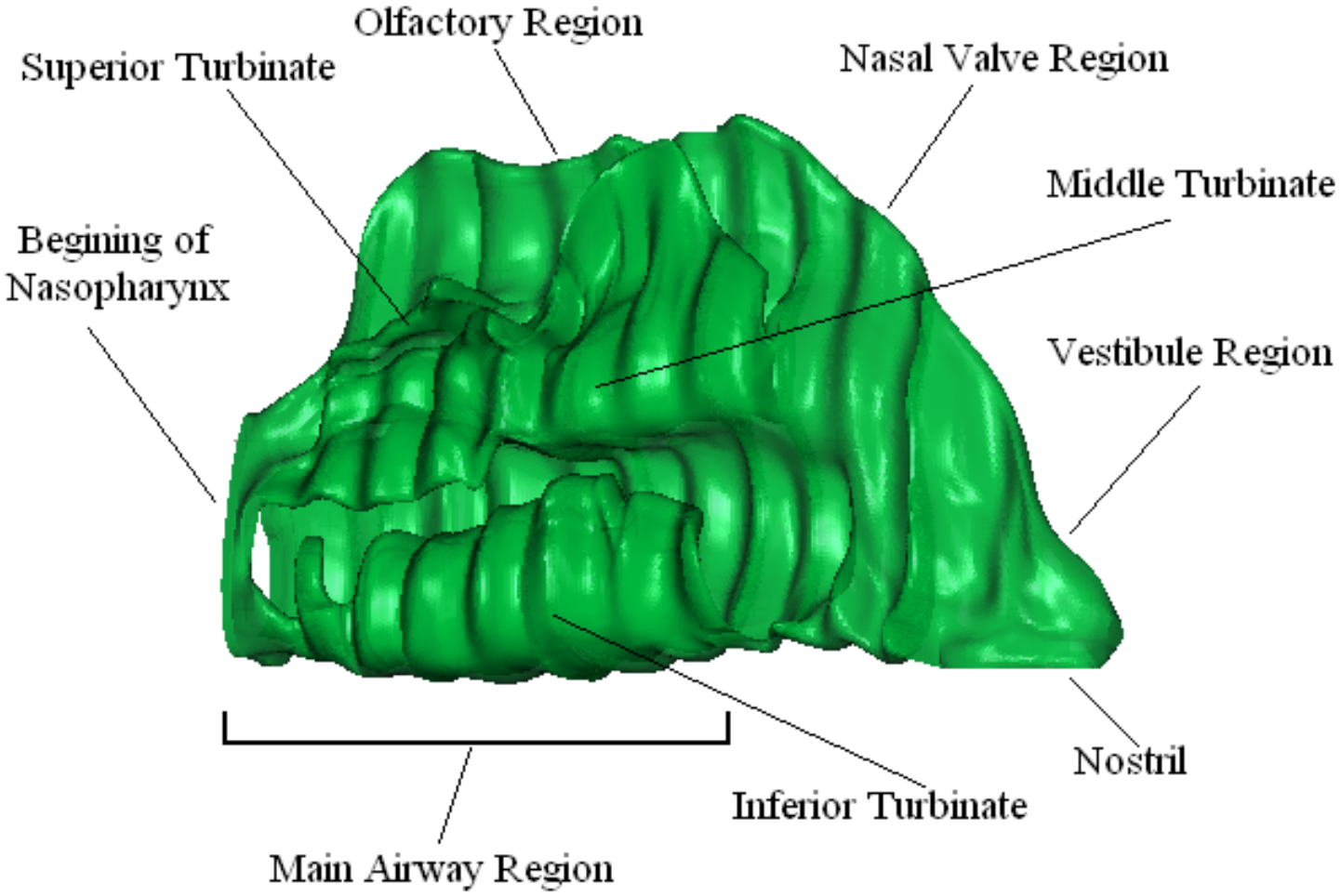
Nasal Cavity Coronal Sections

Clarkson University



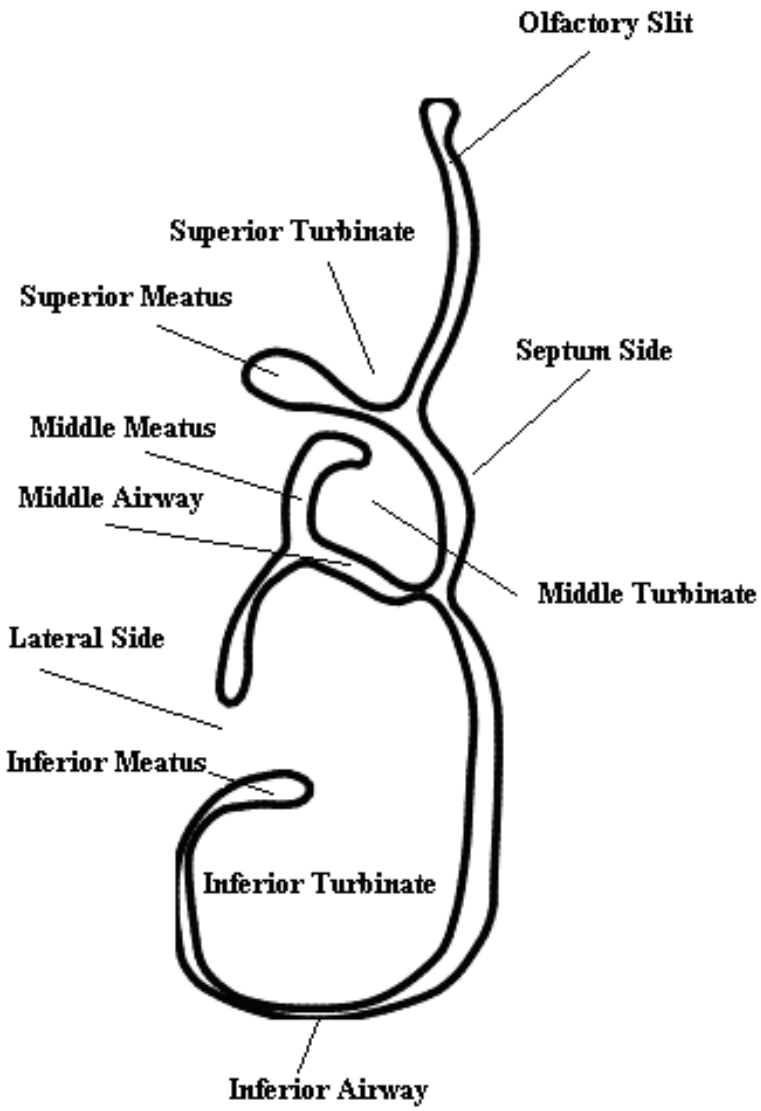
Nasal Model

Clarkson University



Nasal Anatomy- Main Airway Region

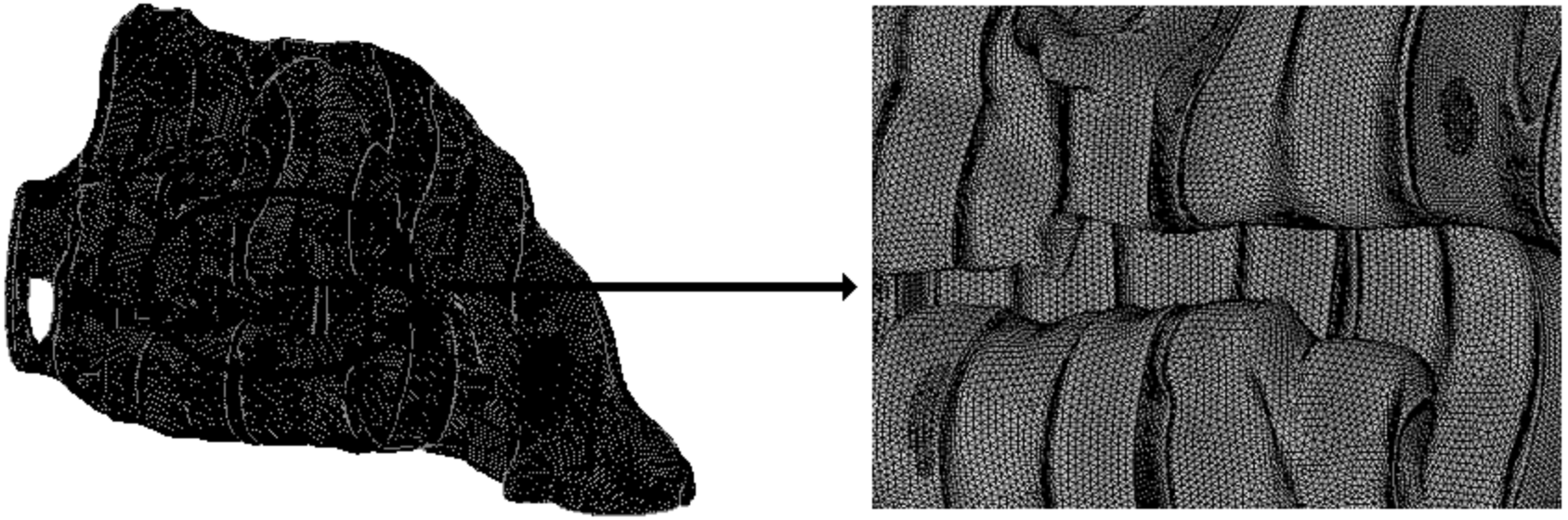
Clarkson University



Computational Grid

Clarkson University

800, 000 CELLS



Airflow in the Nasal Cavity

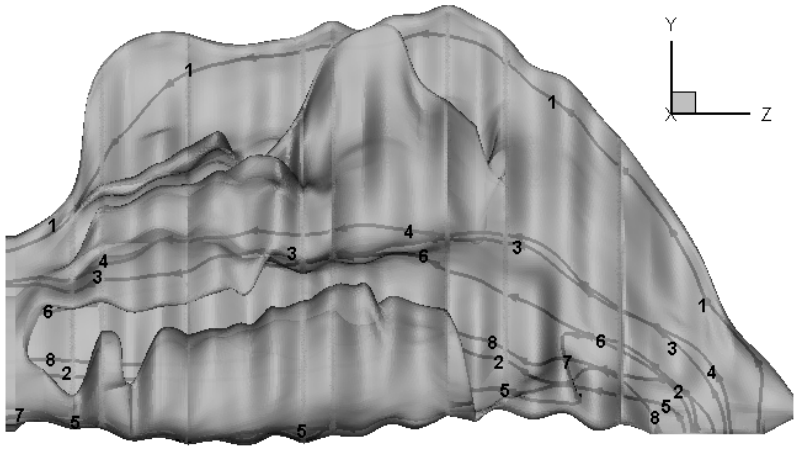
Clarkson University

NIOSH

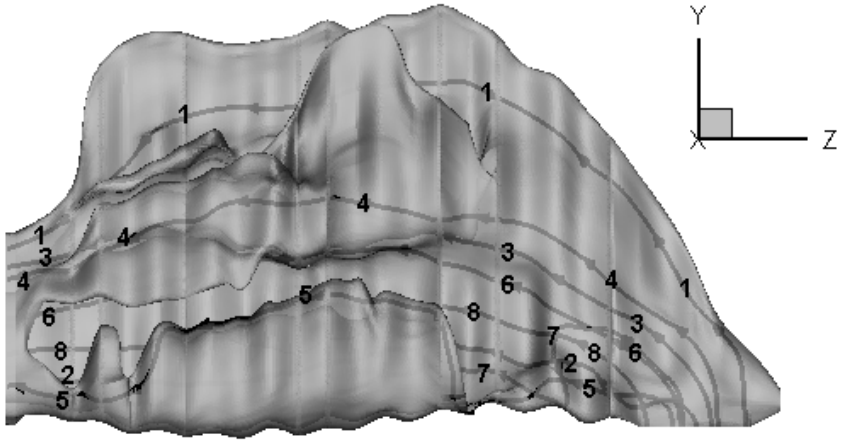
Velocity magnitude contours in the nose.

Stream Traces

Clarkson University



4 L/min

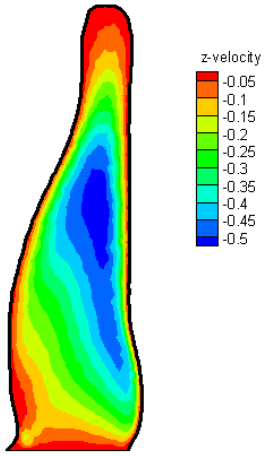


14 L/min

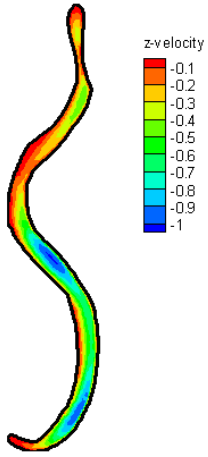
Axial Velocity at Different Sections

Clarkson University

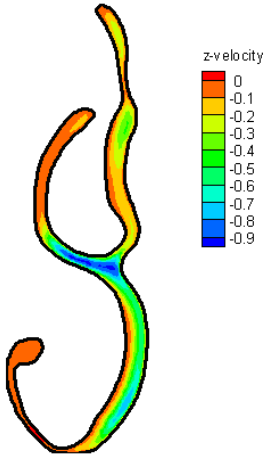
4 L/min



Vestibule

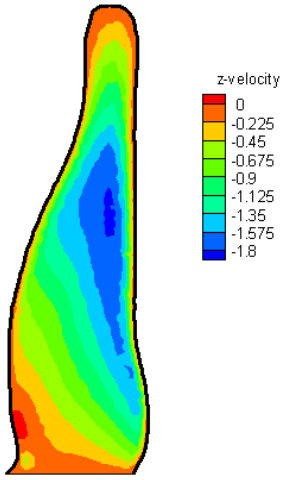


Nasal valve

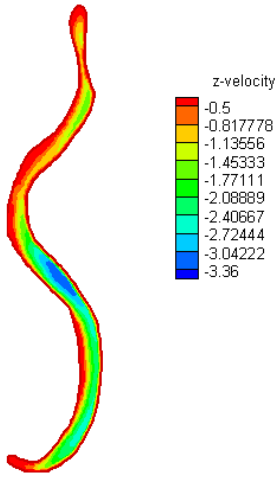


Main airway

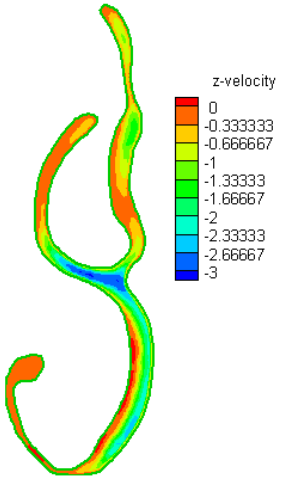
14 L/min



Vestibule



Nasal valve

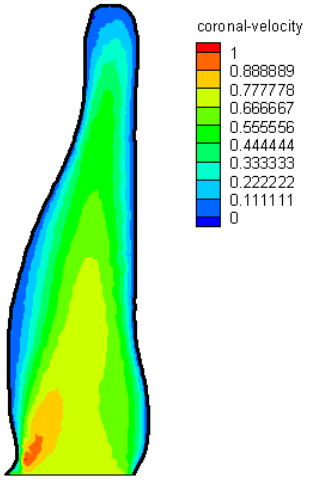


Main airway

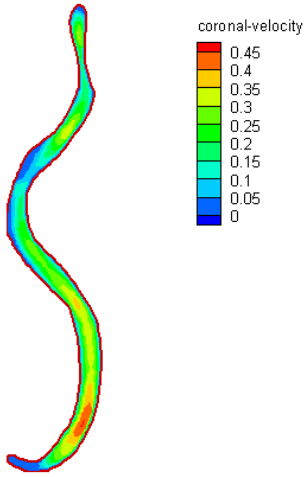
Coronal Velocity at Different Sections

Clarkson University

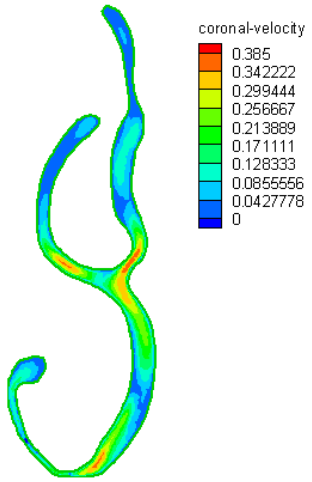
4 L/min



Vestibule

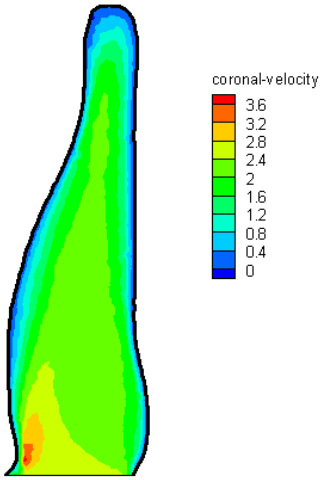


Nasal valve

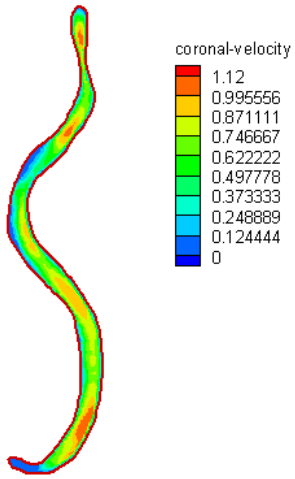


Main airway

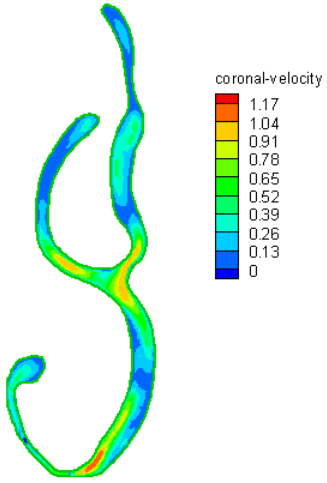
14 L/min



Vestibule



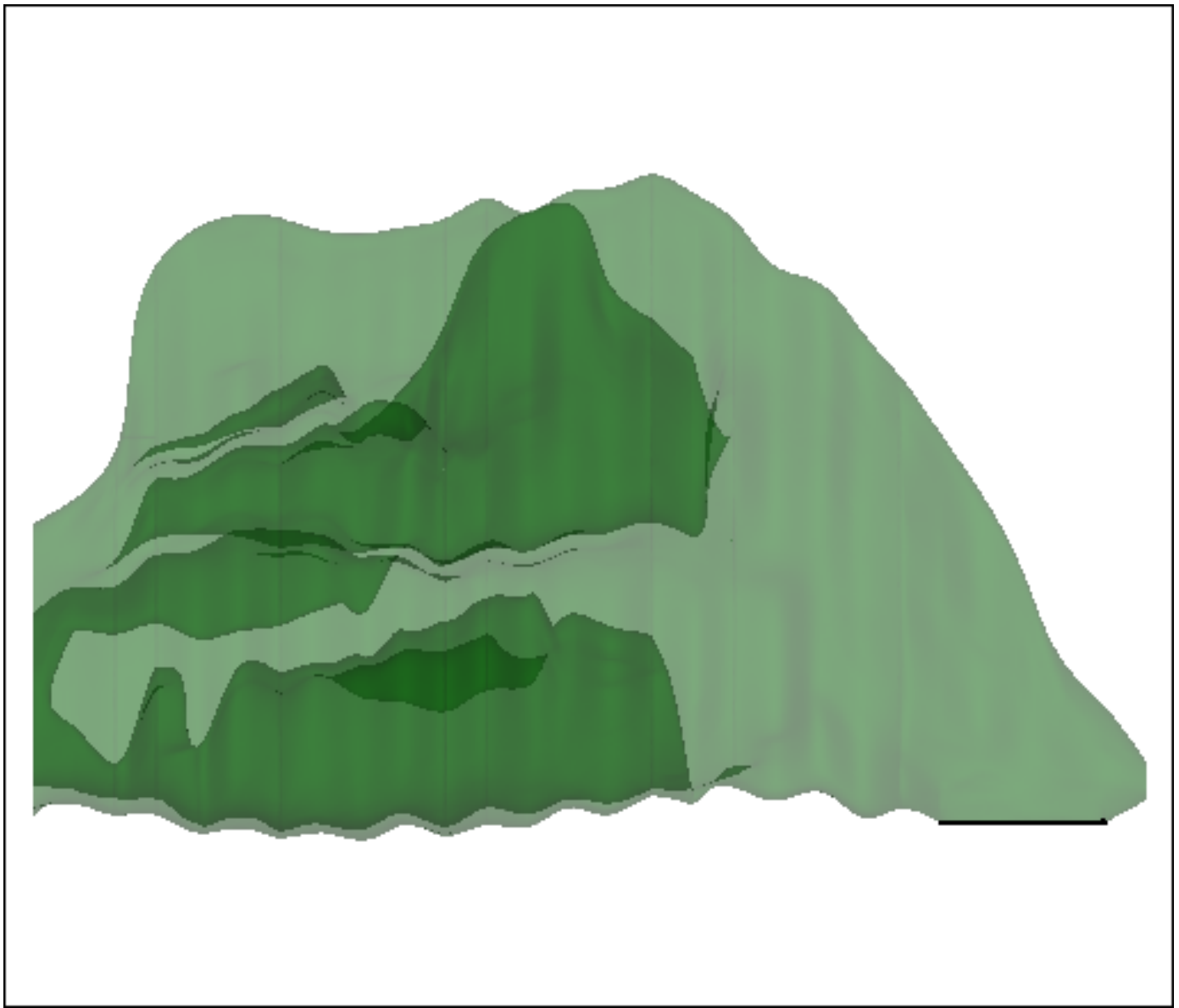
Nasal valve



Main airway

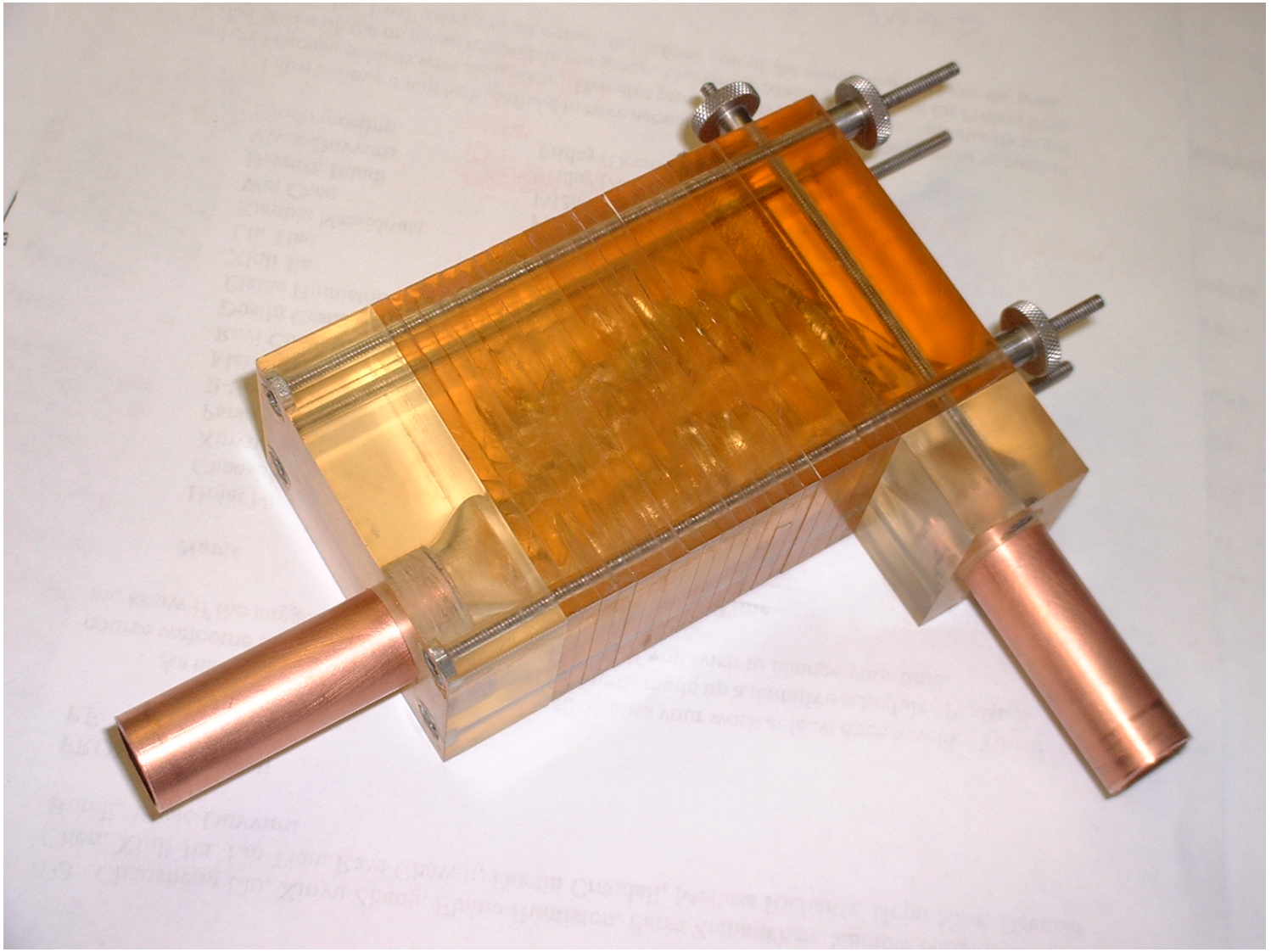
Nasal Deposition

Clarkson University



NASAL MODEL

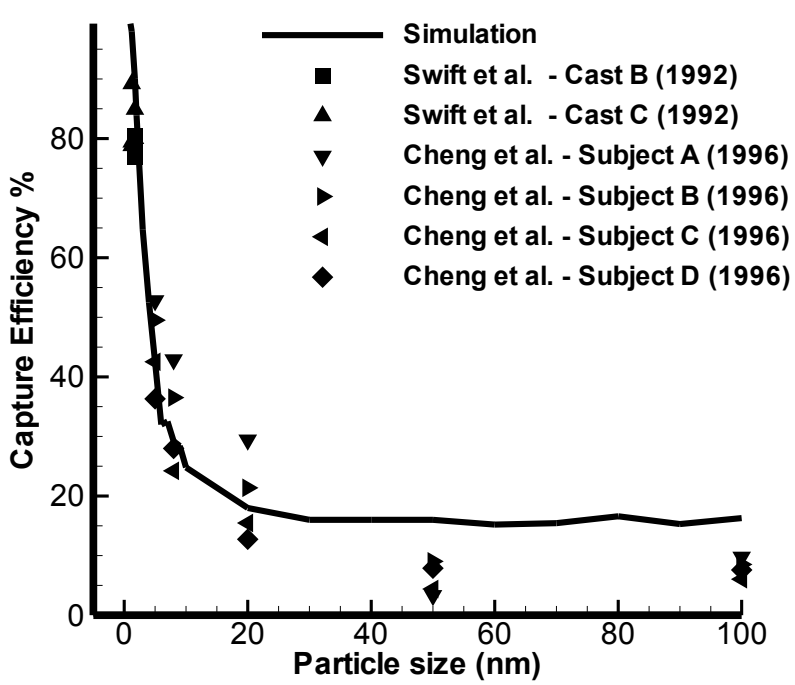
Clarkson University



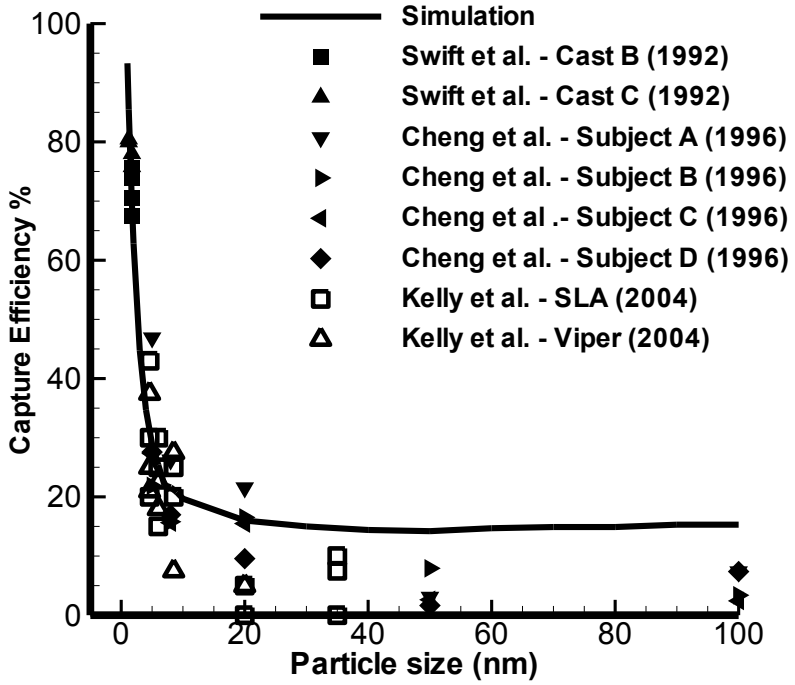
Comparison of Captrue Efficiency with Experimental Data

Clarkson University

Ultra fine Particles



4 L/min

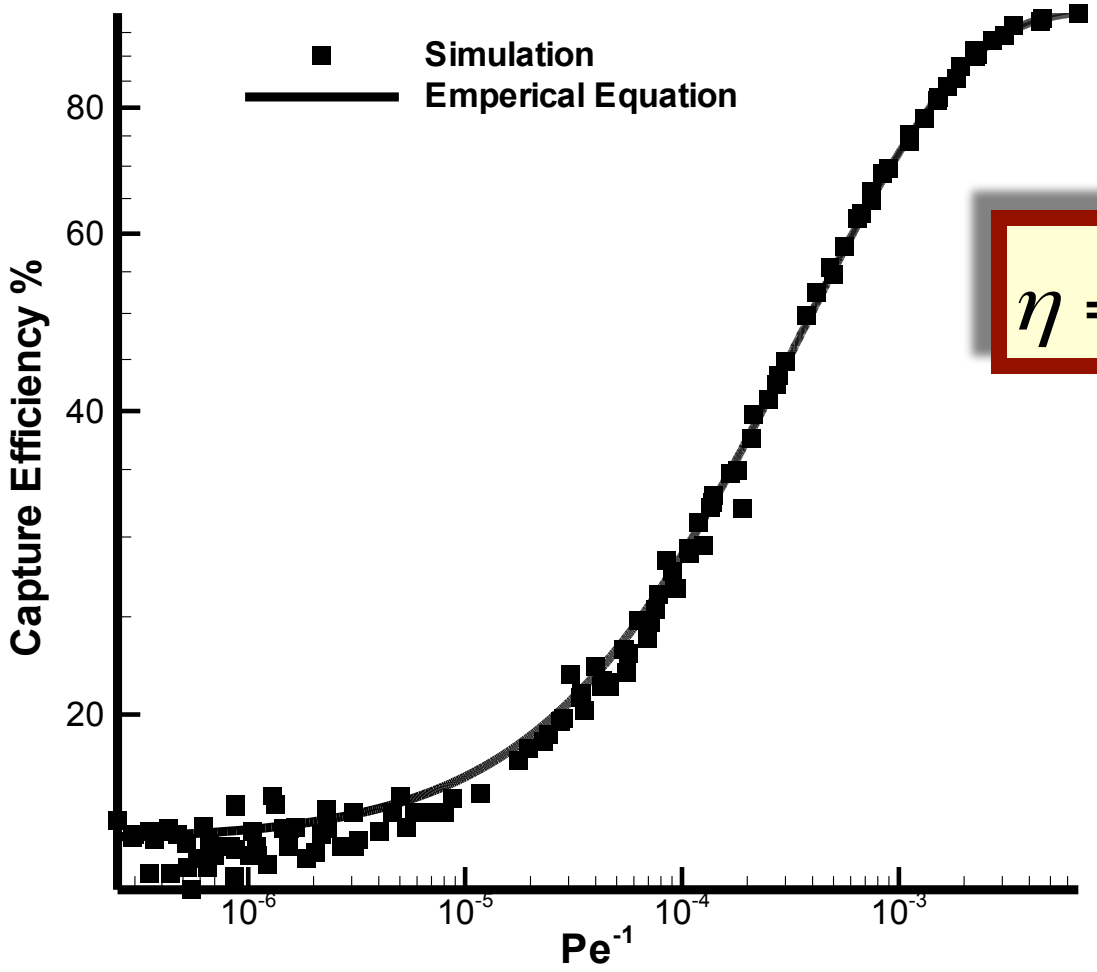


10 L/min

Nosal Captrue Efficiency Versus Peclet Number

Clarkson University

Ultra fine Particles

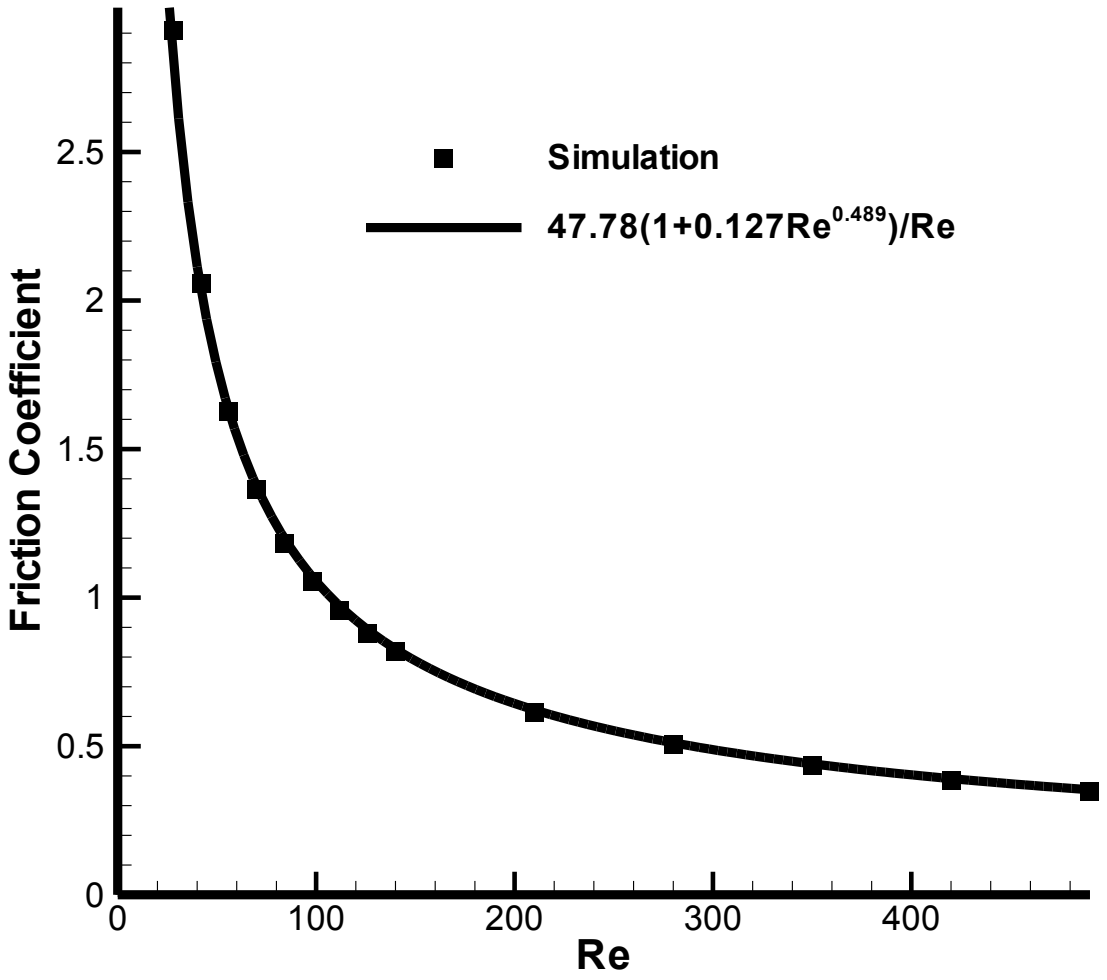


$$\eta = 100(1 - 0.85e^{-280Pe^{-0.8}})$$

$$Pe = \frac{Q}{DL}$$

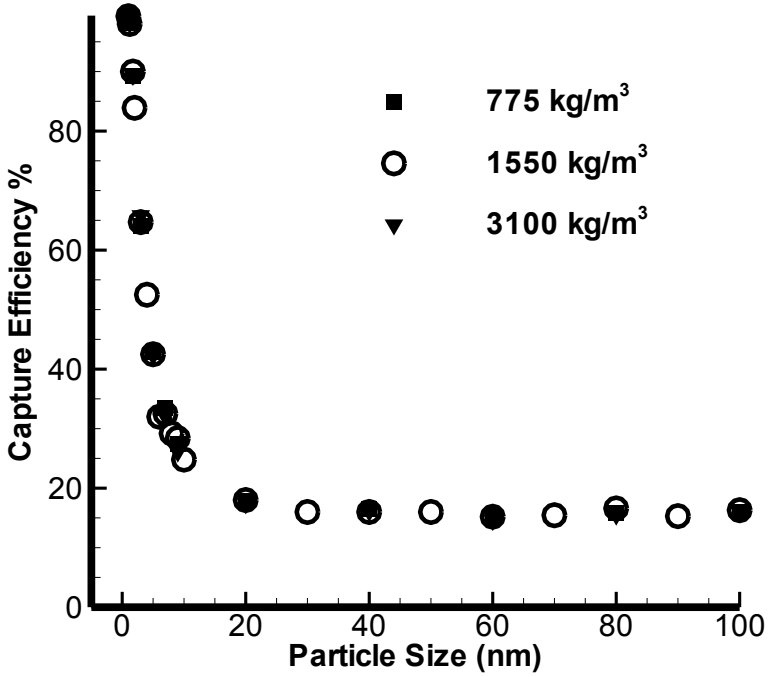
Nasal Cavity Friction Coefficient

Clarkson University

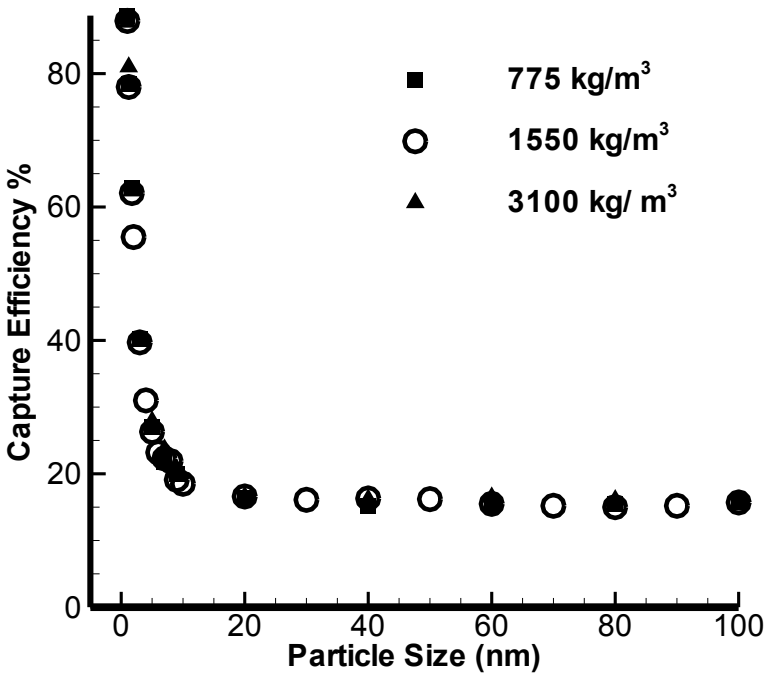


Effect of Particle Density

Clarkson University



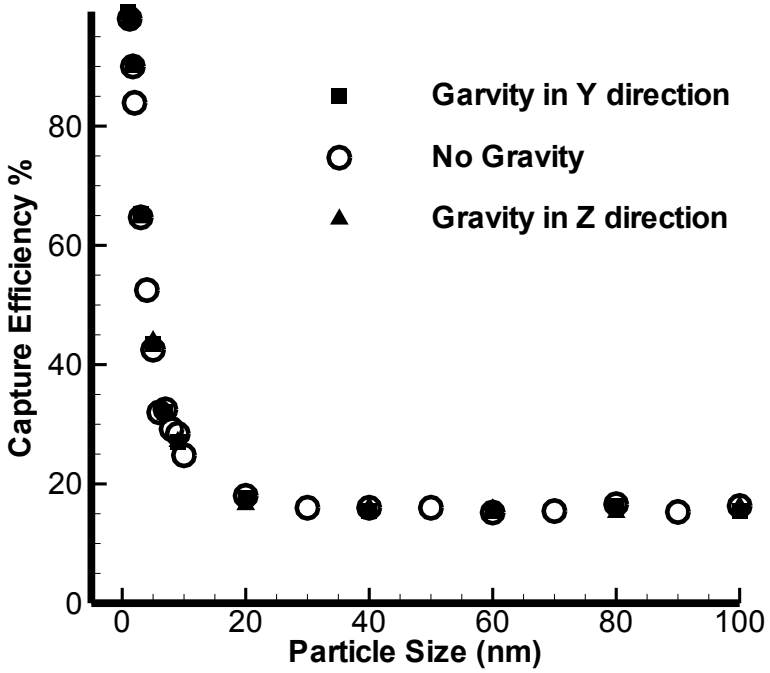
4 L/min



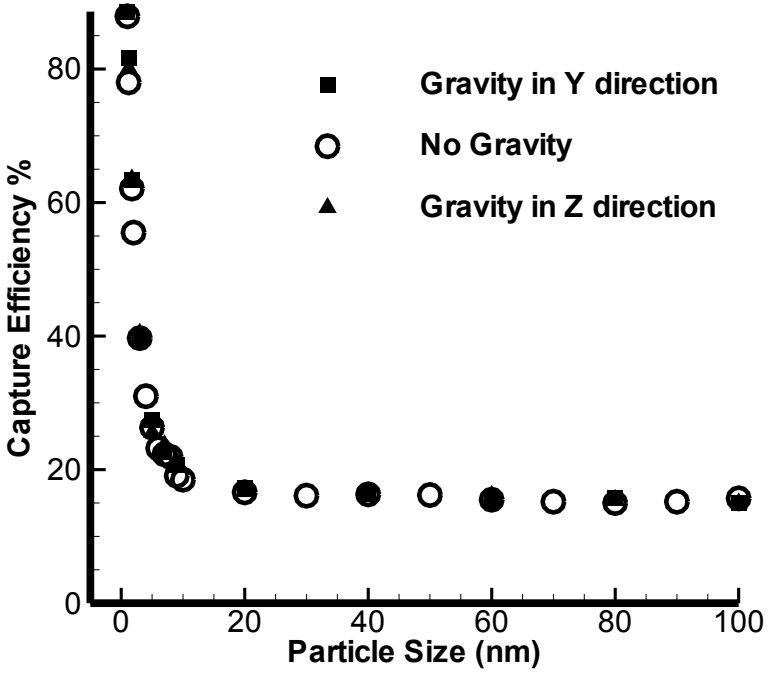
14 L/min

Effect of Gravity

Clarkson University



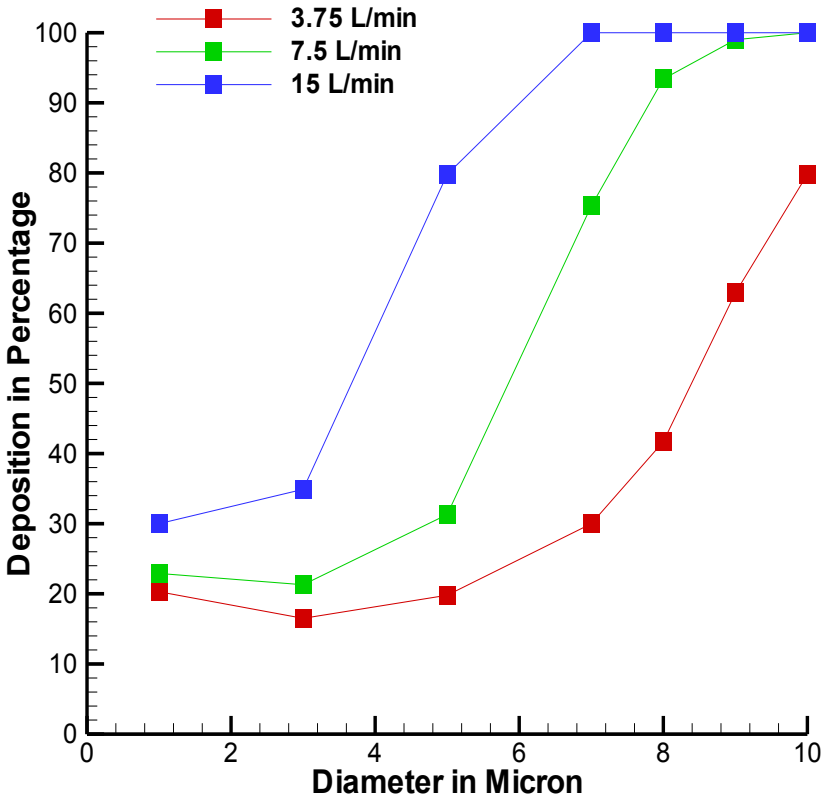
4 L/min

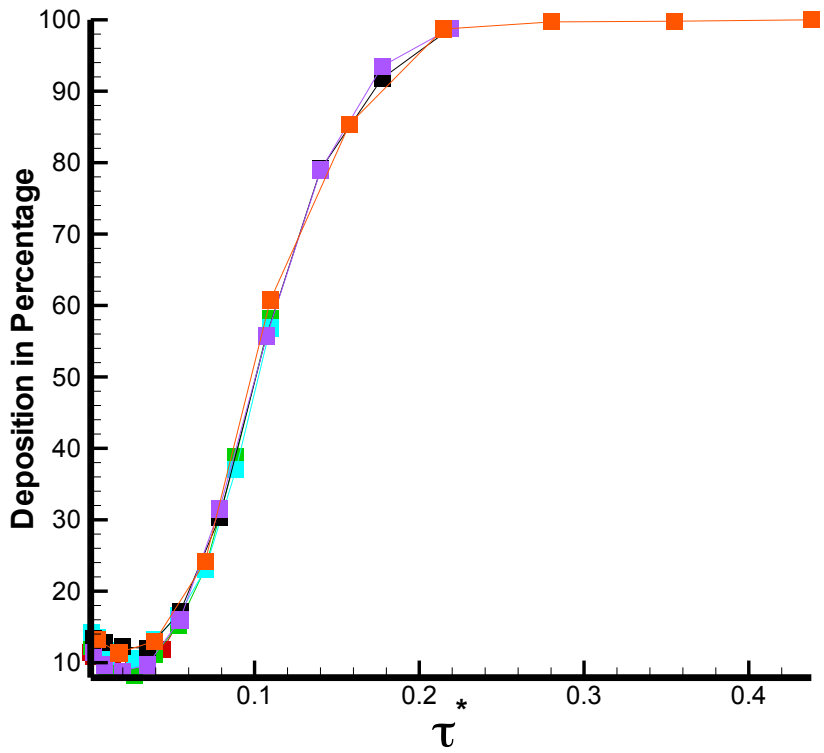


14 L/min

Nose Deposition

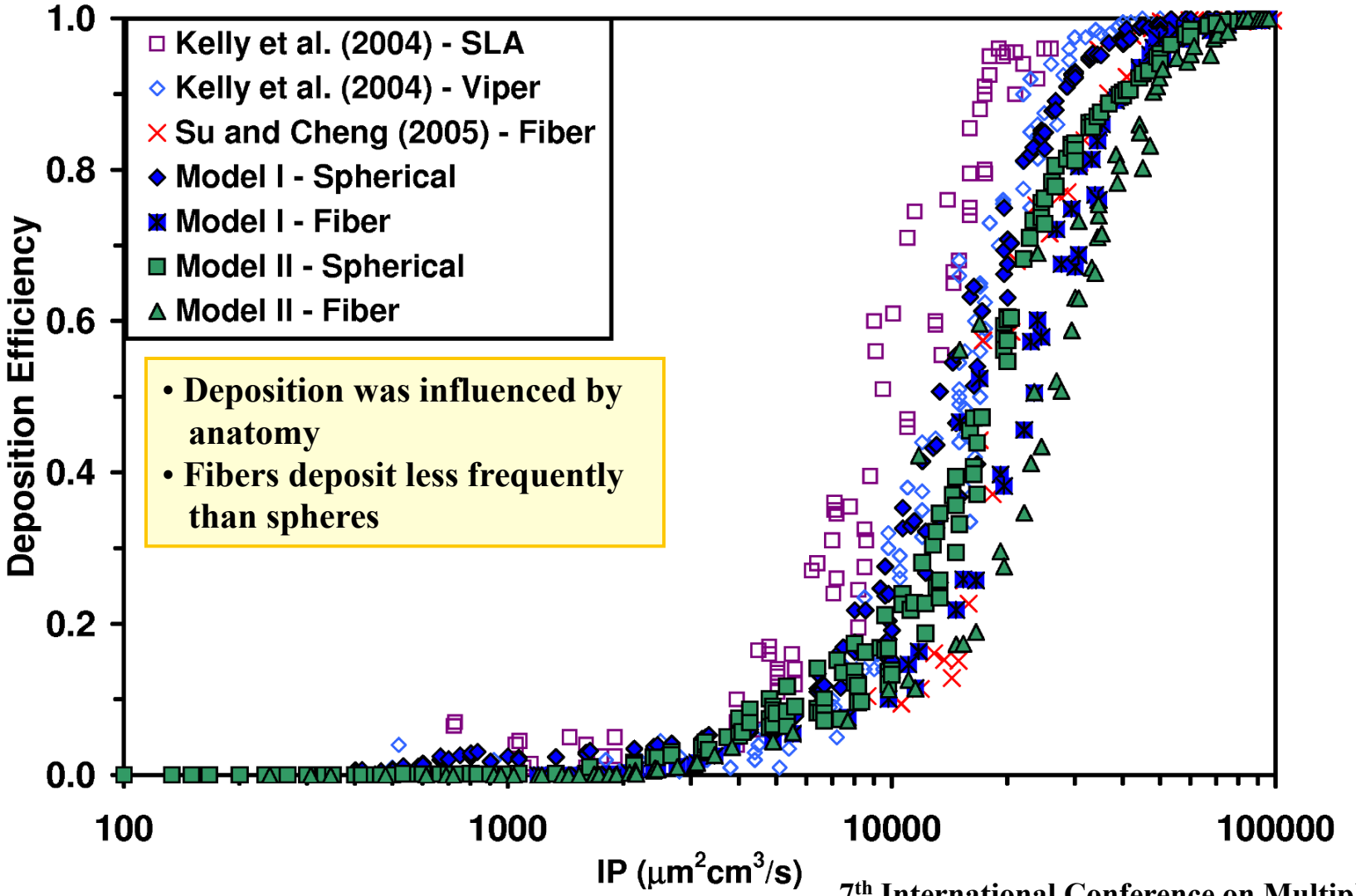
Clarkson University



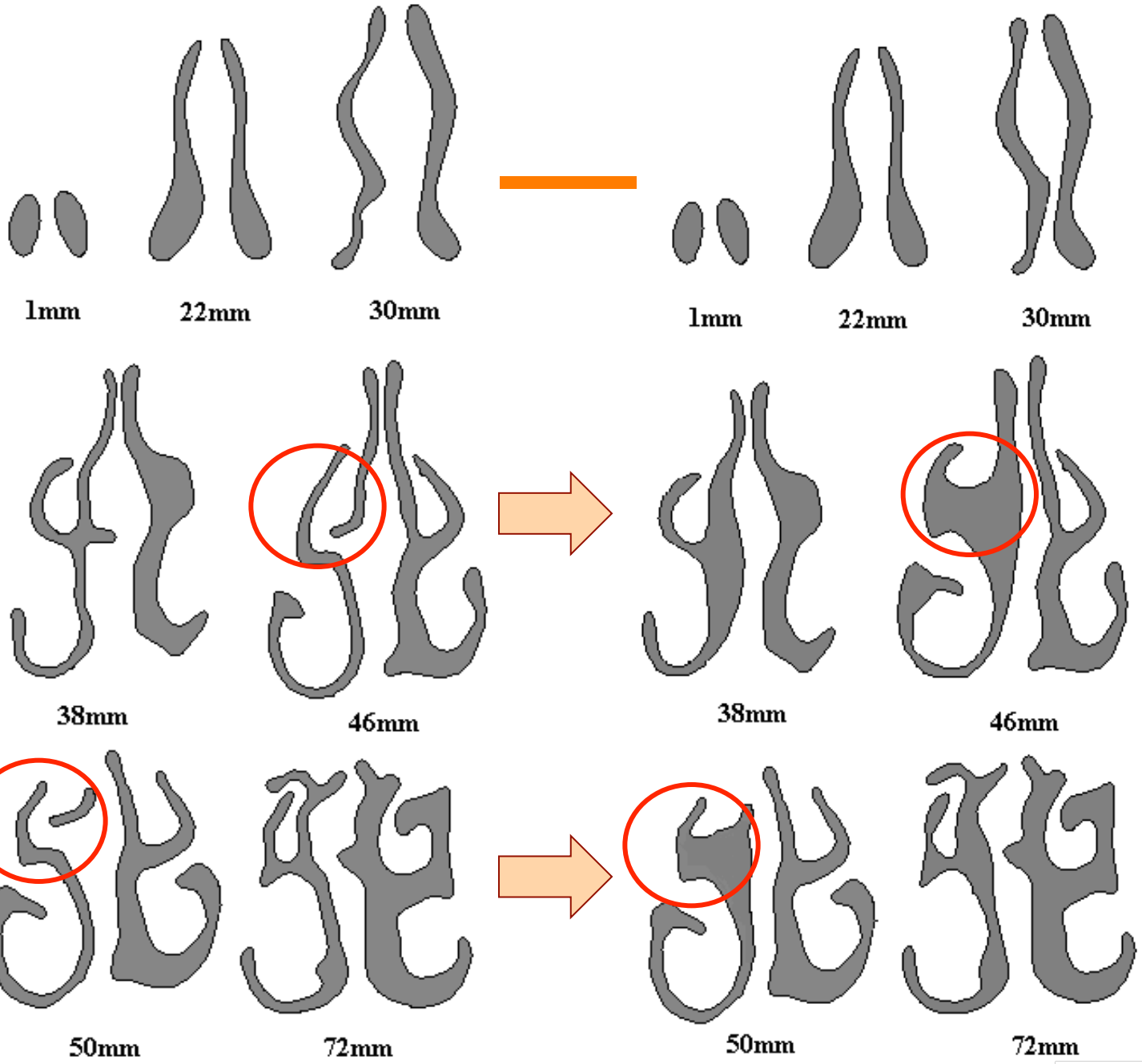


Deposition Efficiency

Clarkson University



Clarkson University



Before Septoplasty

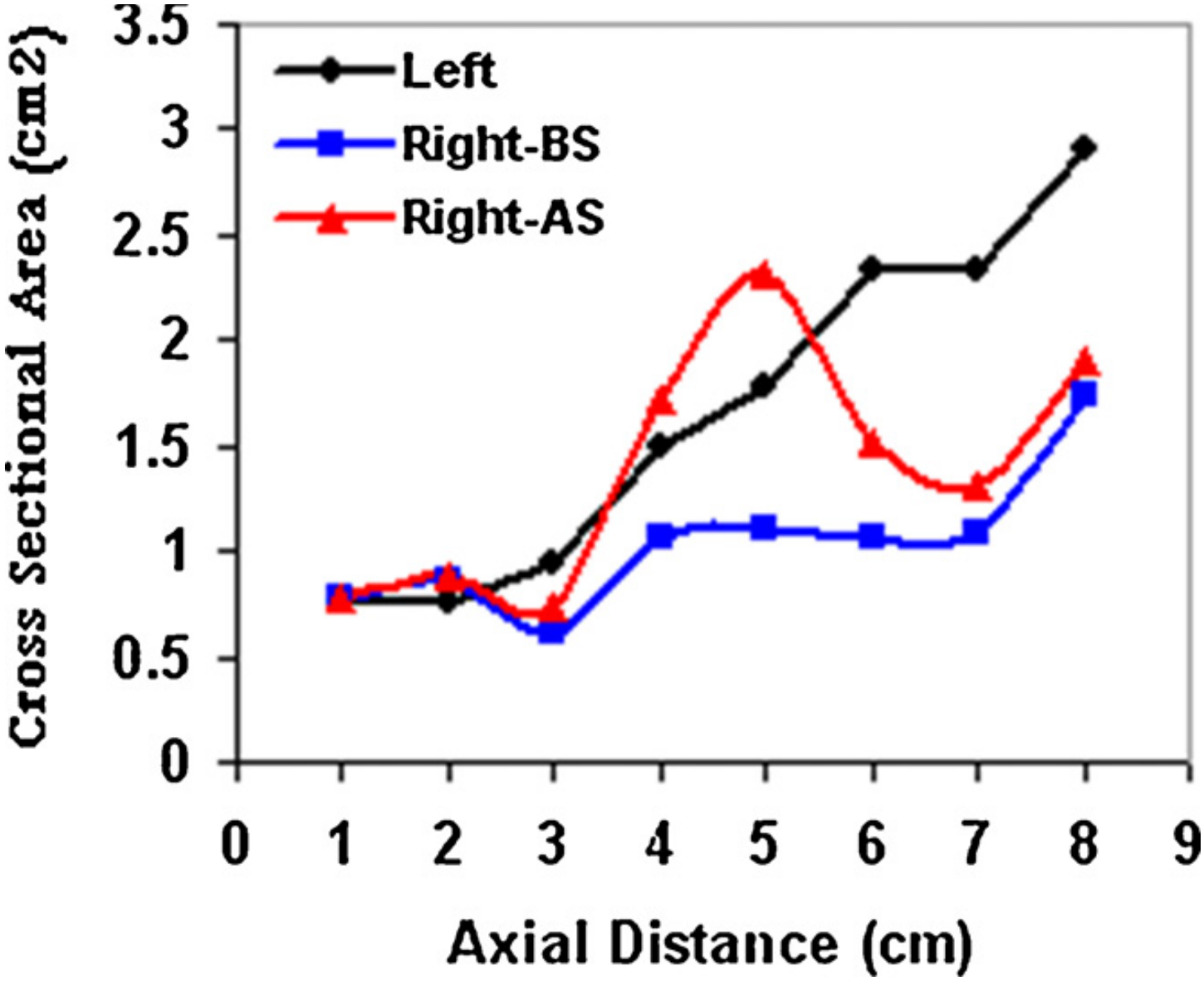
After Septoplasty

Moghadas et al. (2011)

Abouali et al. (2012)

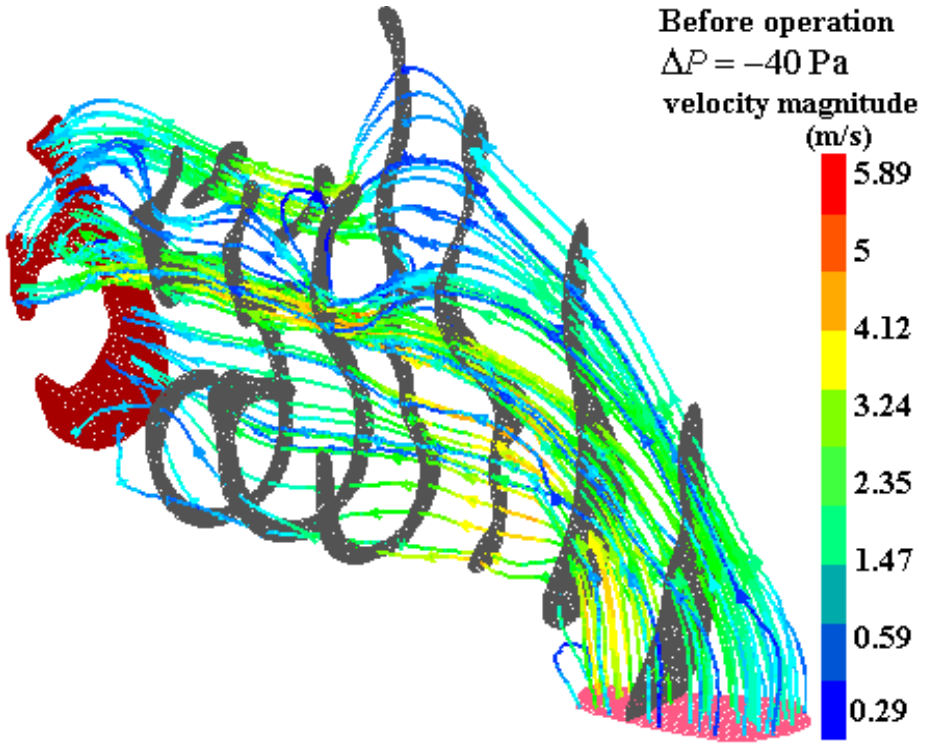
Passage Cross Section Areas

Clarkson University

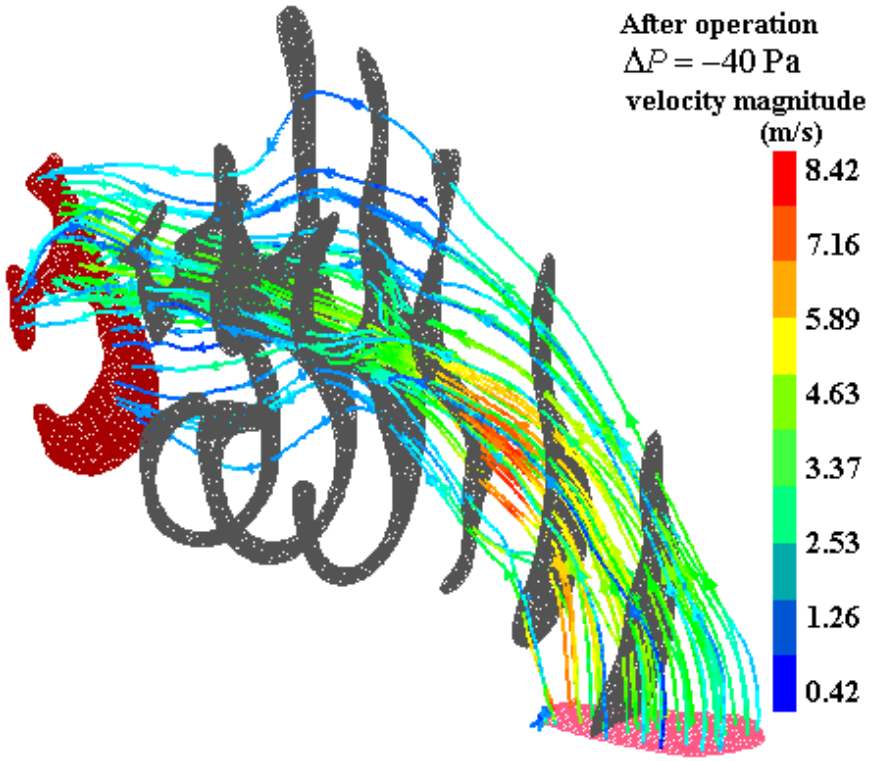


Flow Pattern

Clarkson University



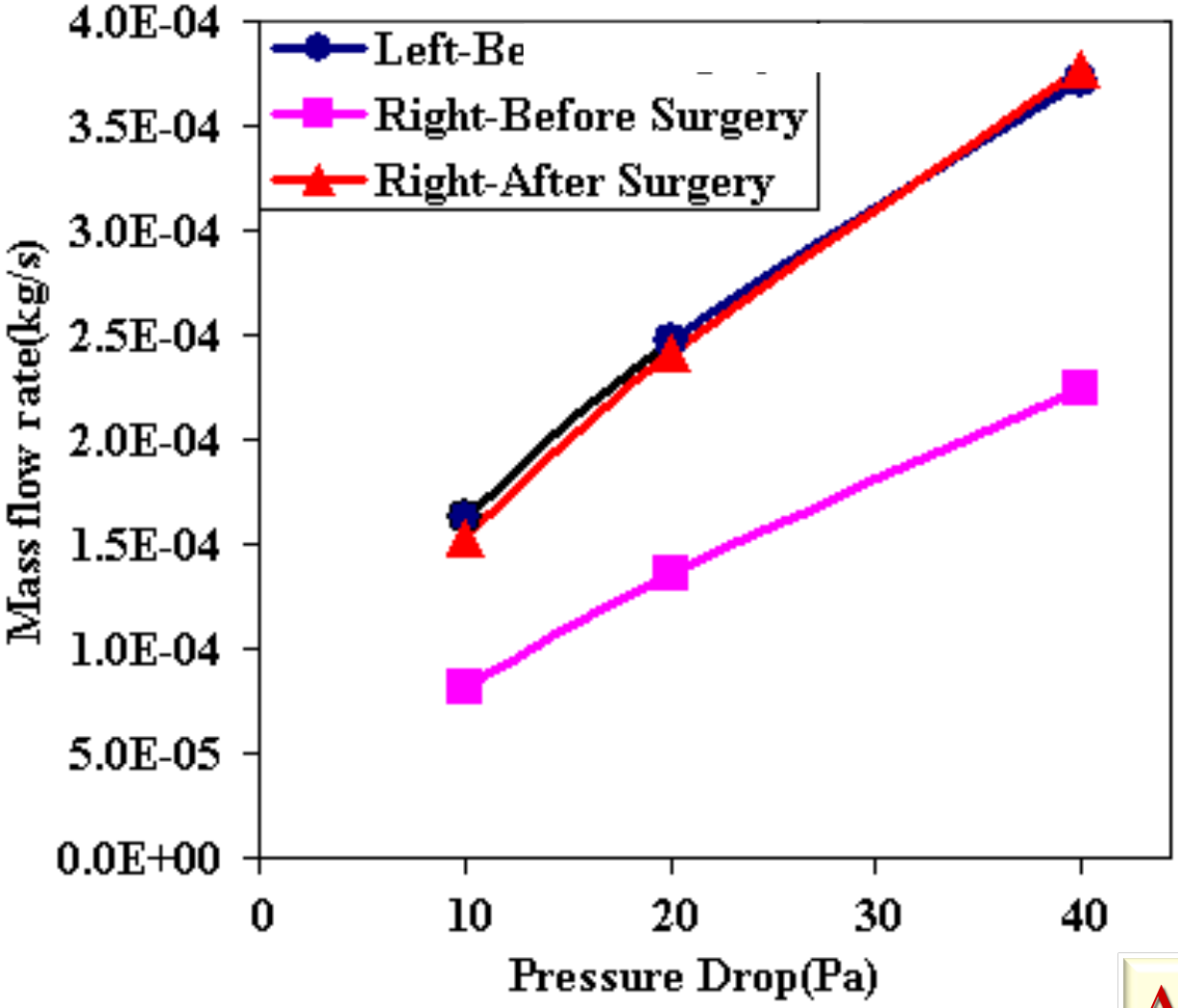
Before Operation



After Operation

Flow Rate-Pressure Drop

Clarkson University



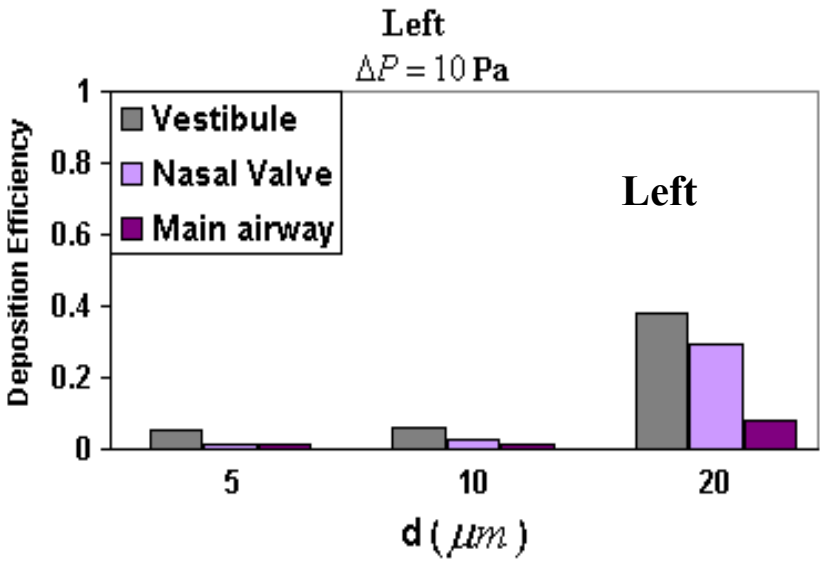
Moghadas et al. (2011)

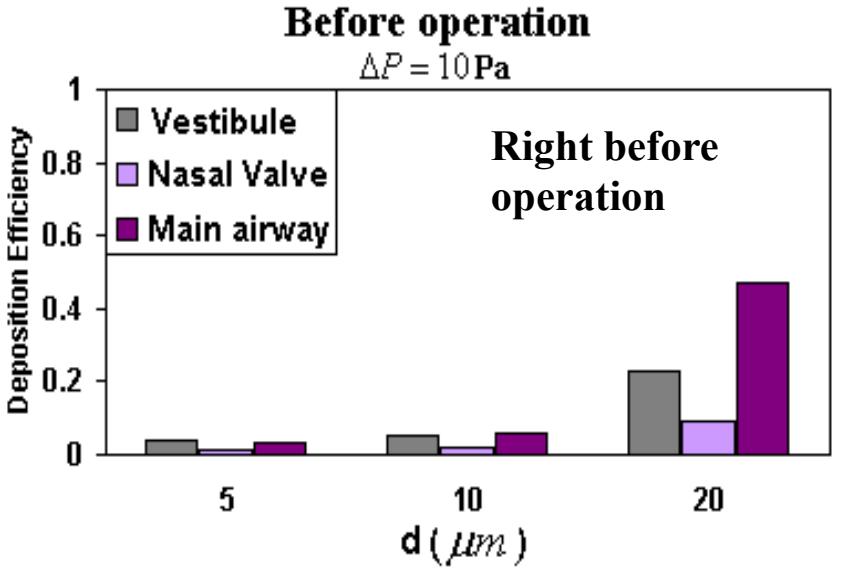
Abouali et al. (2012)

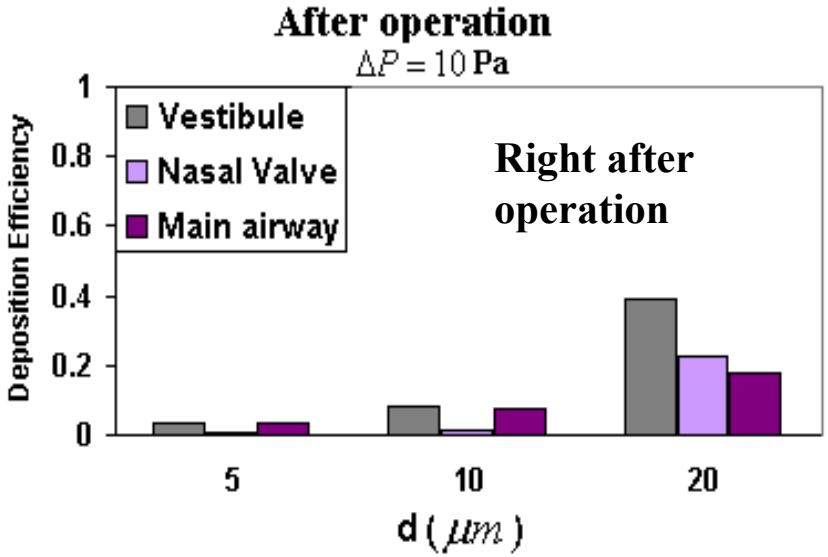
Regional Deposition

Clarkson University

Micro-Particles







Sample Trajectories

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Upper Airways

d=20 micron
7.5 L/min

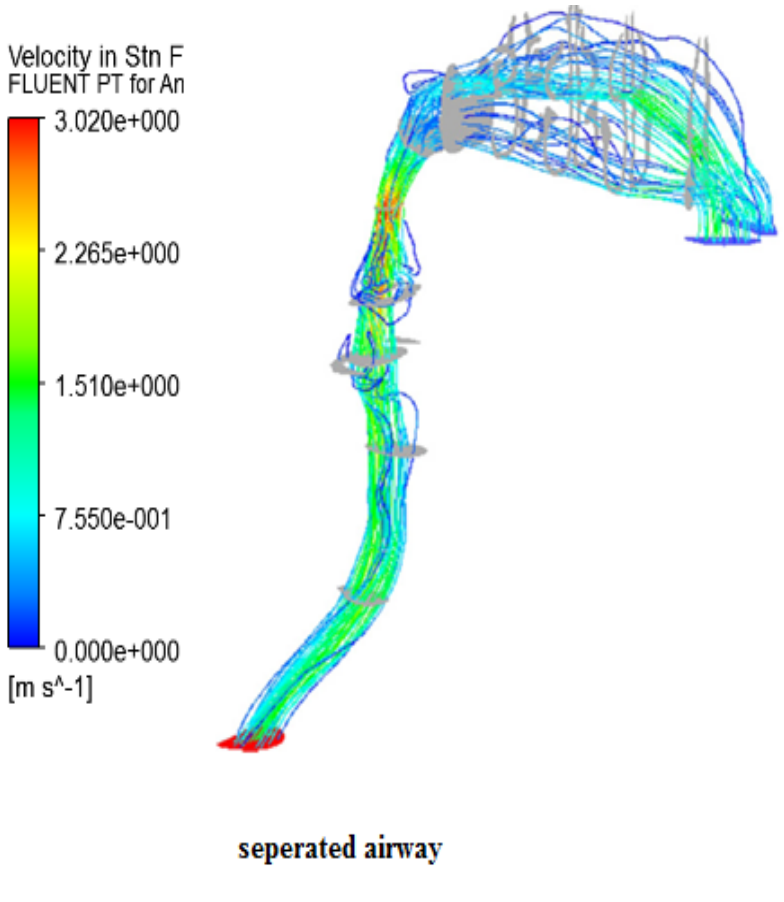
Ghahramani et al. (2013)

Upper Airways in Mannequin

Clarkson University

Comparison of Airflow Fields

Clarkson University



seperated airway

connected airway

Effect of Thermal Plume and facial features

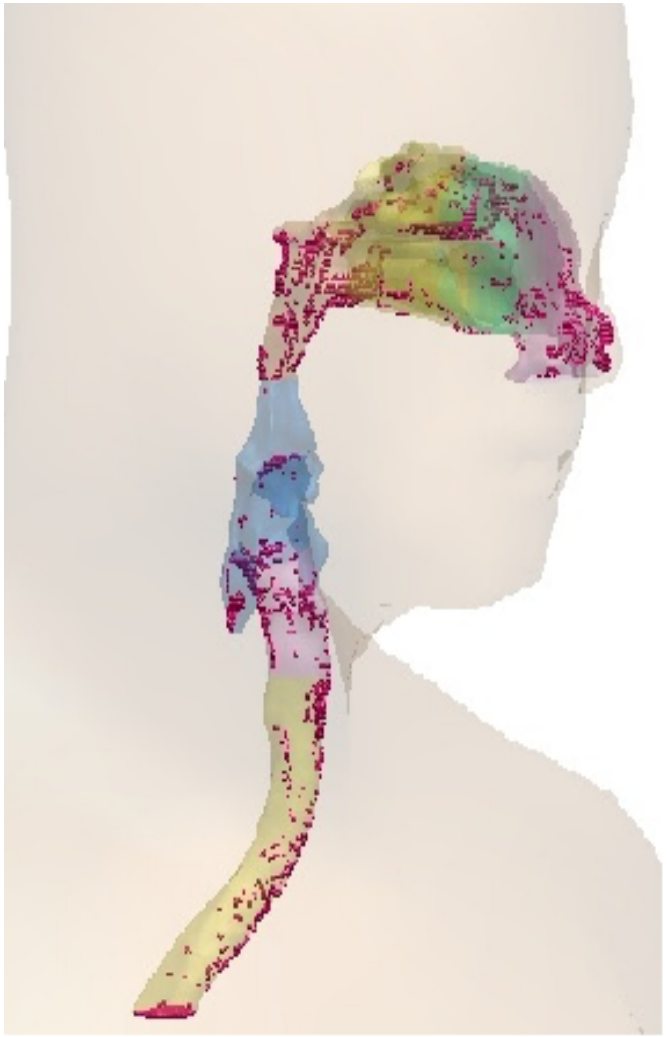
Q=7 L/min

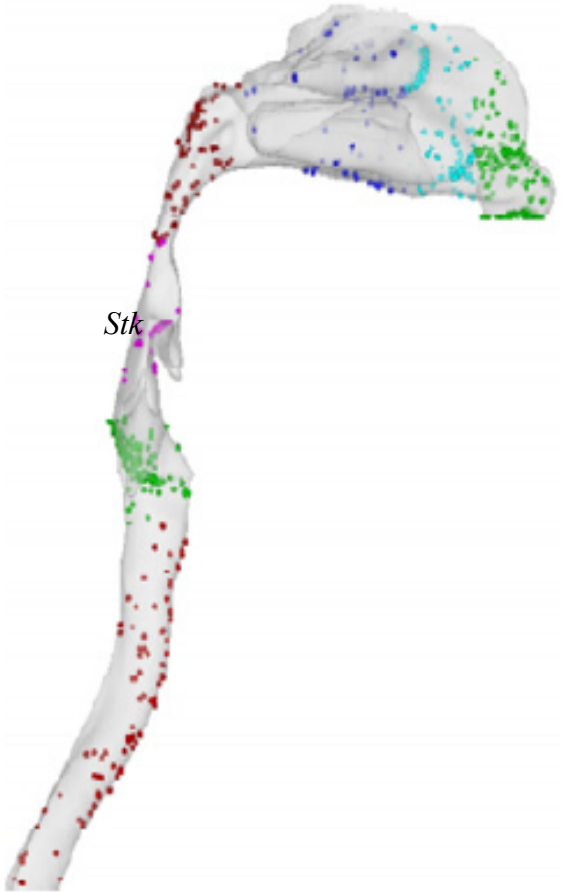
The stream lines of the airflow (colored by velocity magnitude

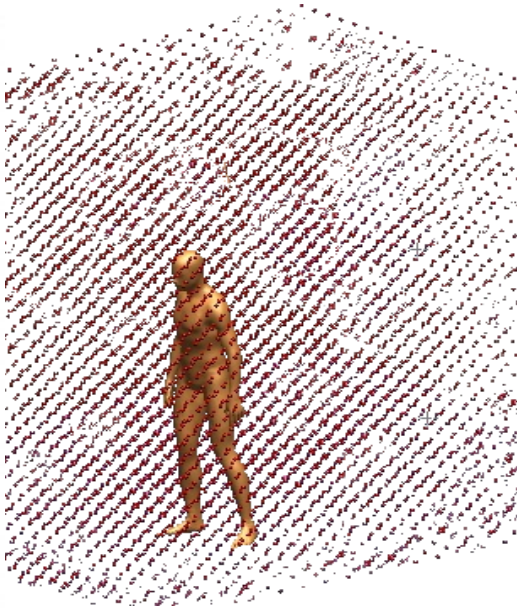
Ghahramani et al. (2013)

Comparison of Regional Deposition

Clarkson University



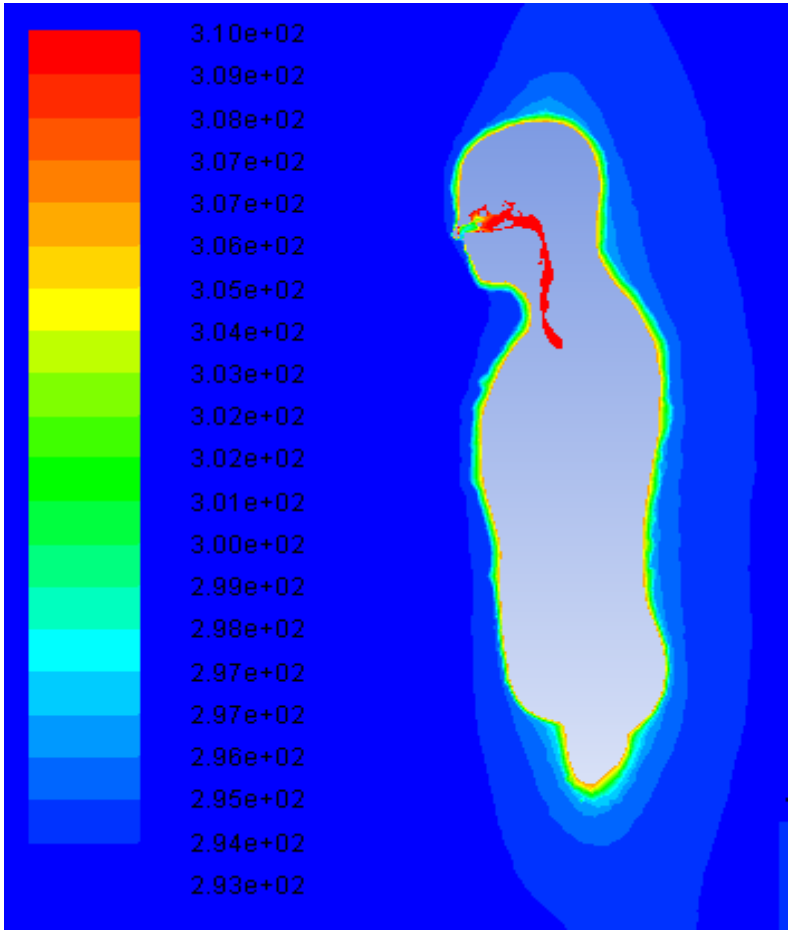




Regional deposition for 10µm particles with breathing rate of 7 L/min.

Temperature Contours

Clarkson University



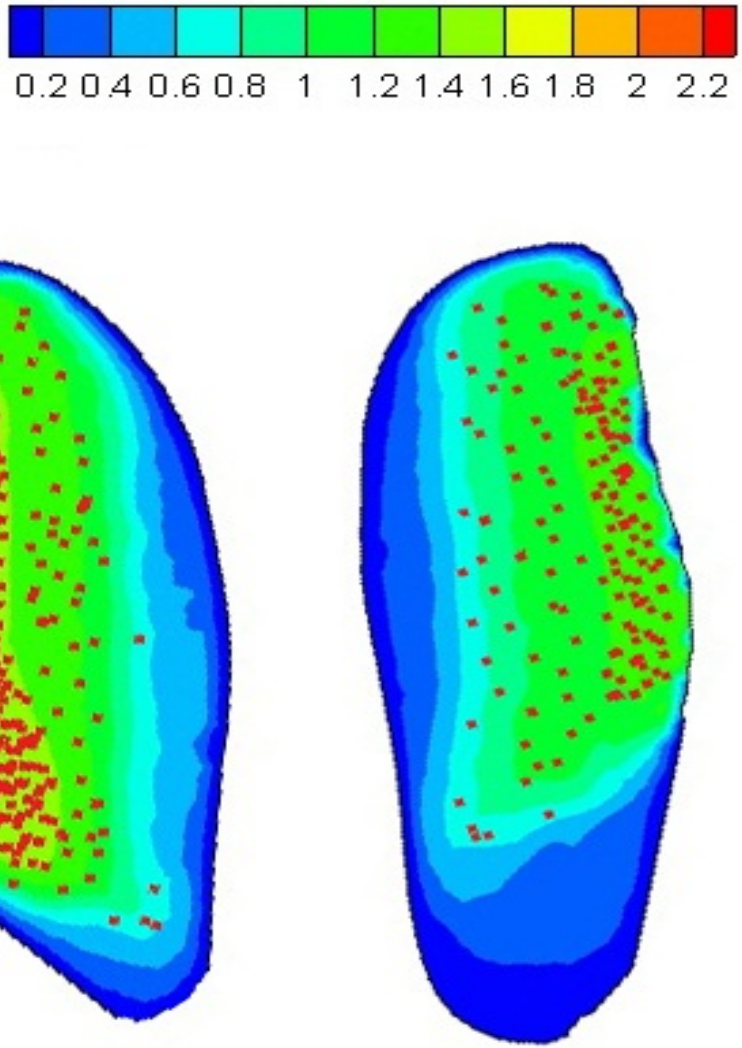
Air temperature =20°C

Mannequin surface temperature = 34°C

Ghahramani et al. (2013)

Particle Concentration at Nostril

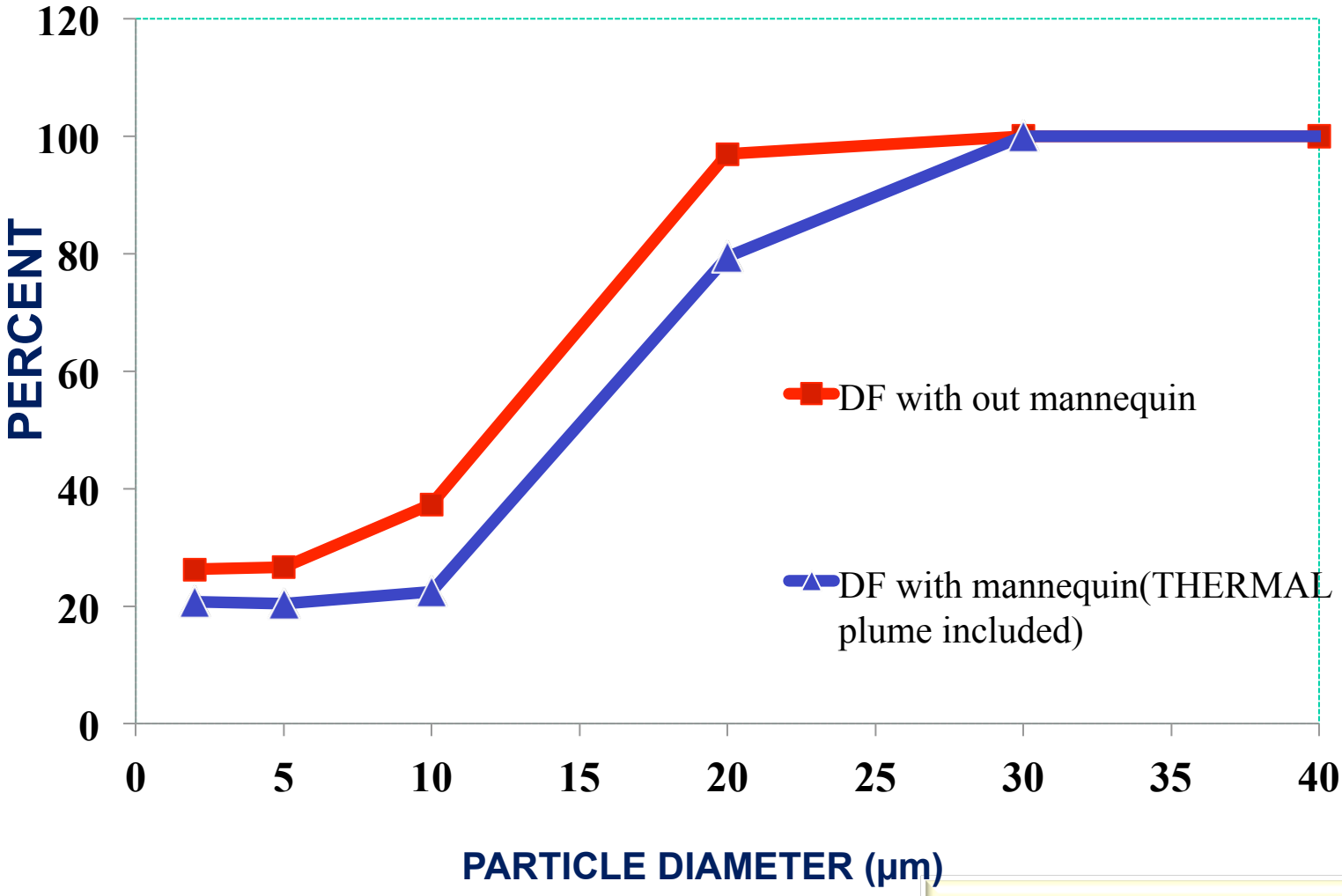
Clarkson University



Ghahramani et al. (2013)

Total Deposition Fraction

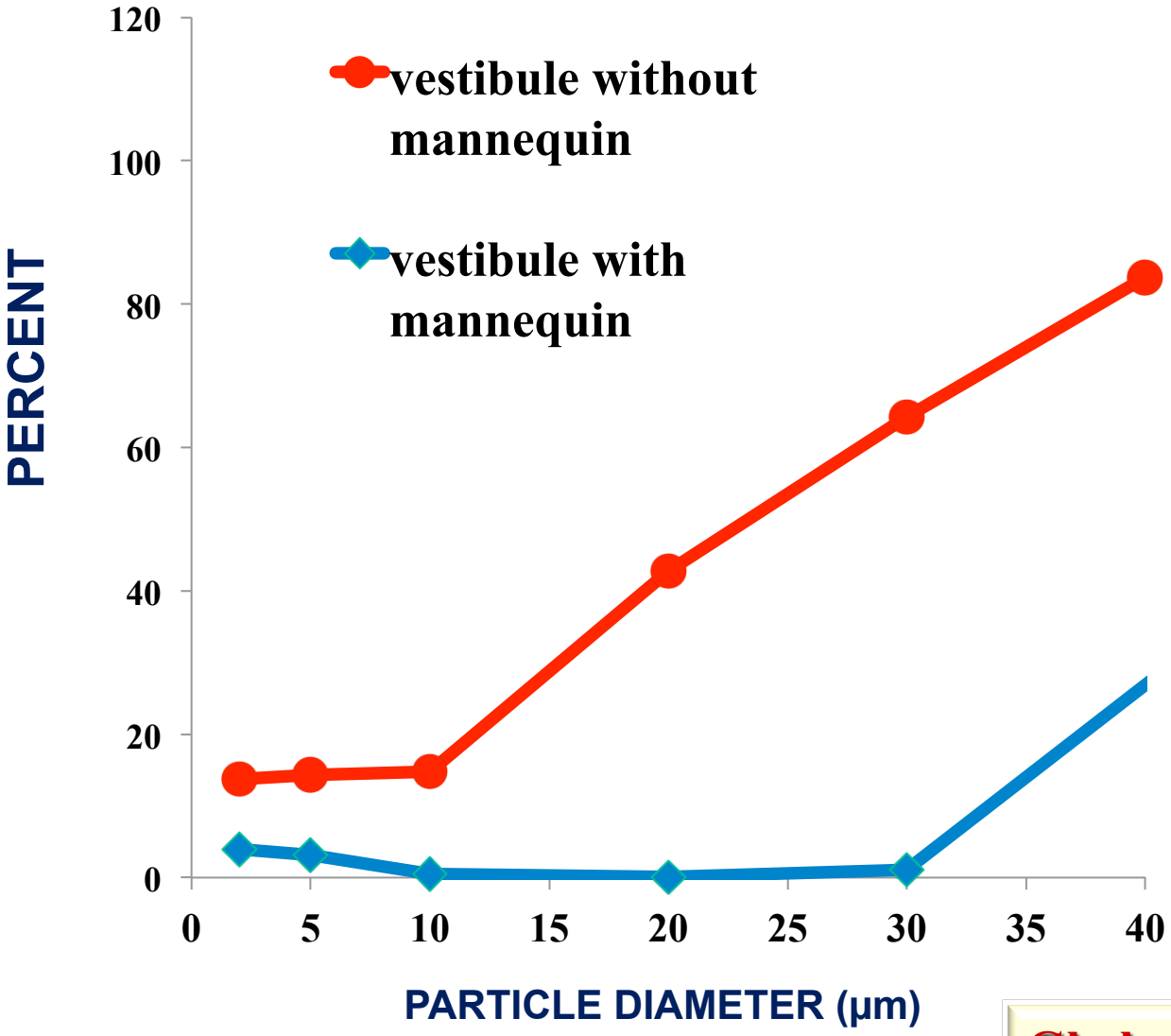
Clarkson University

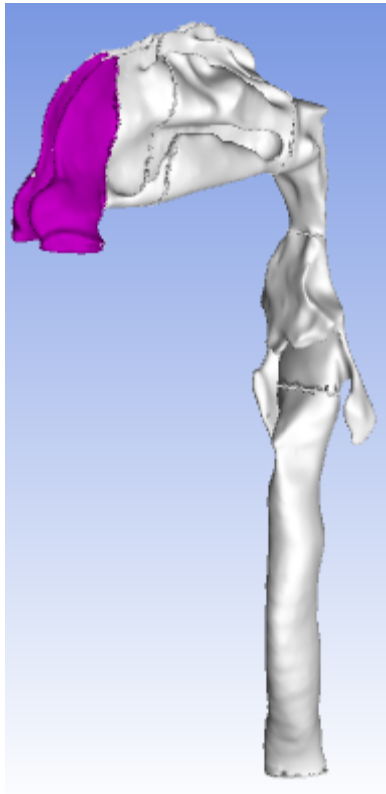


Ghahramani et al. (2013)

Deposition - Vestibule

Clarkson University

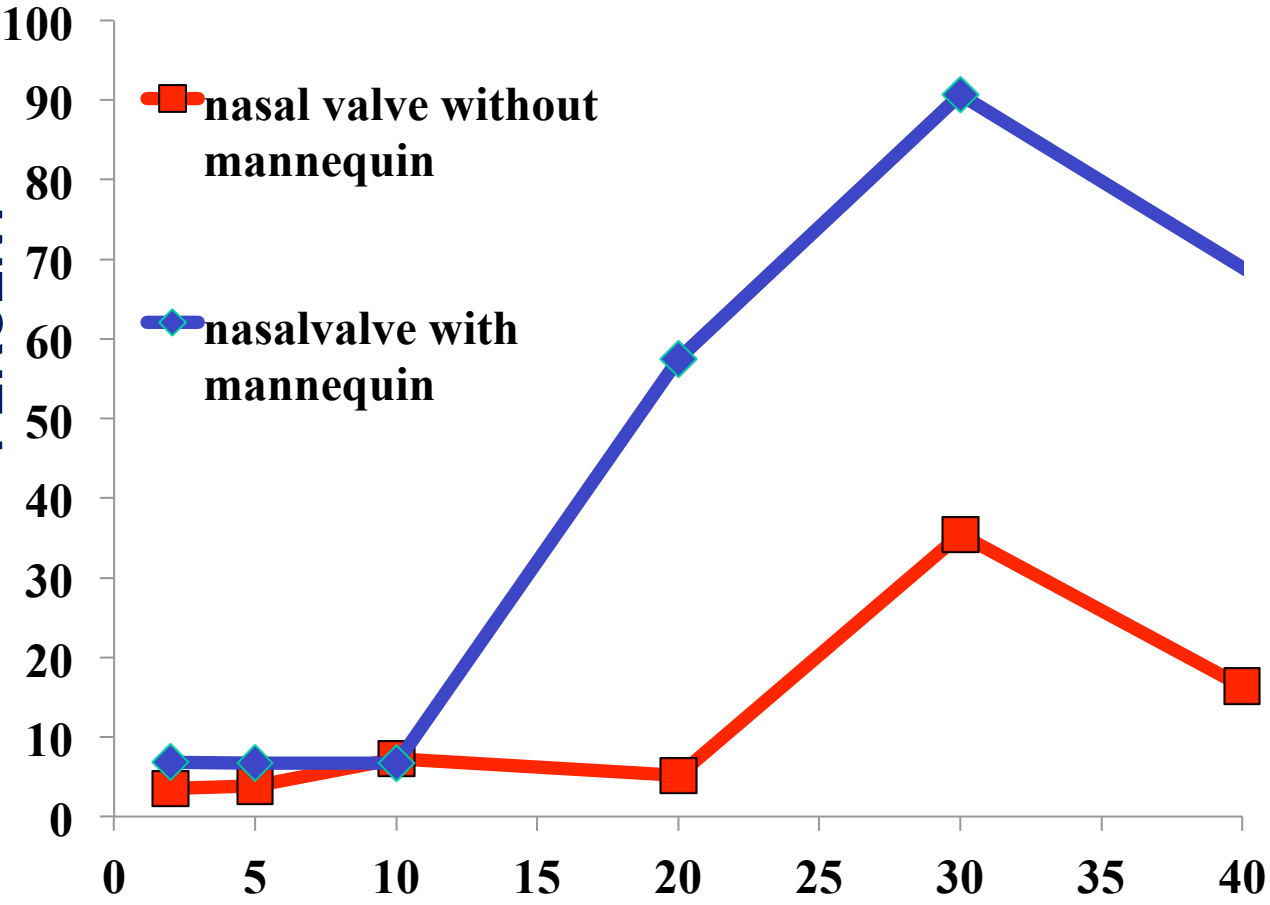


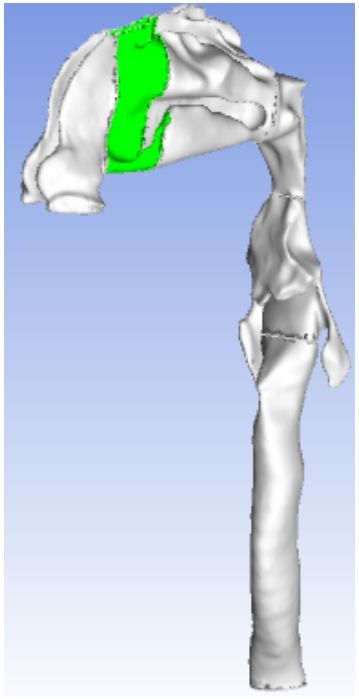


Ghahramani et al. (2013)

Deposition – Nasal Valve

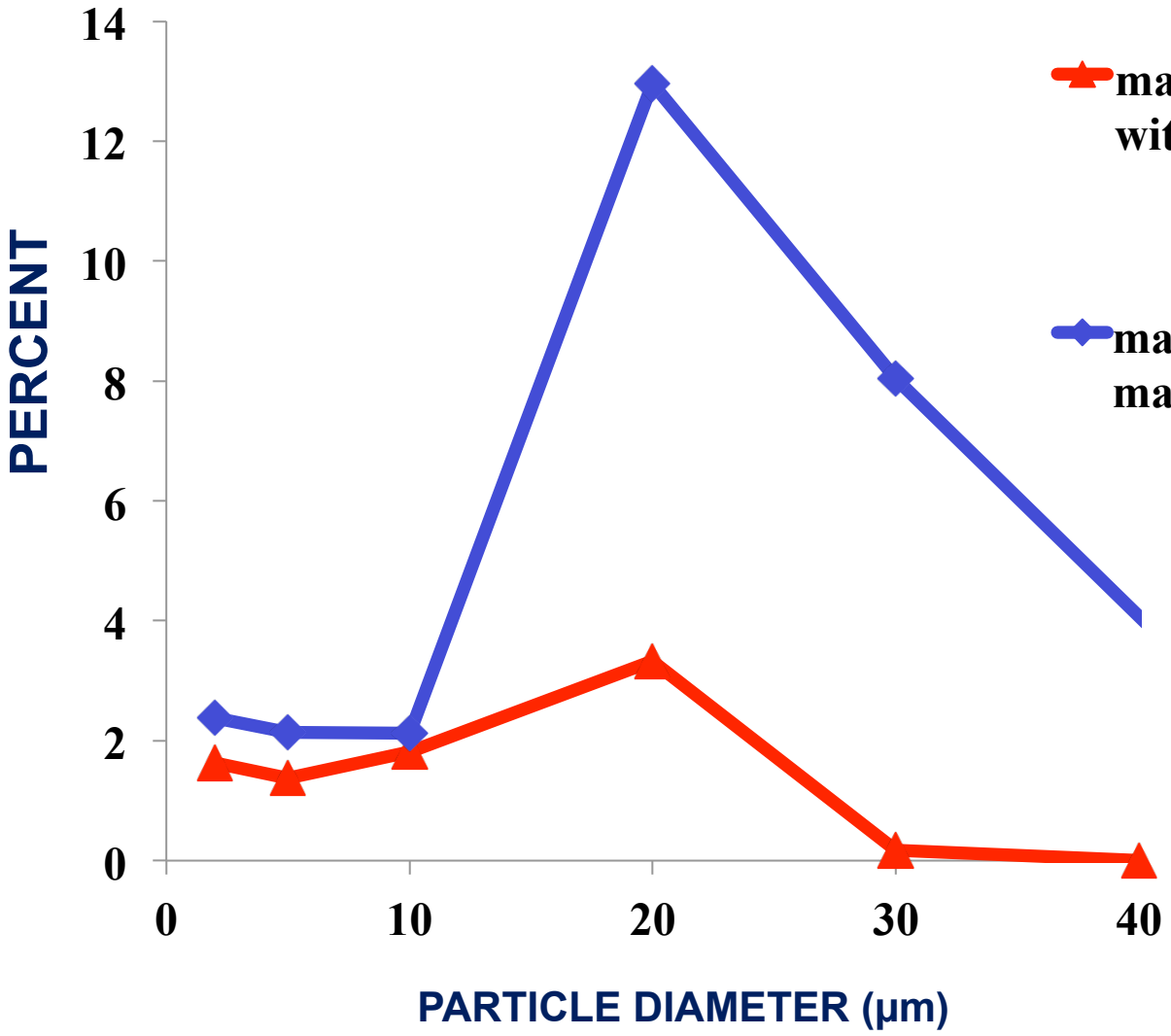
Clarkson University

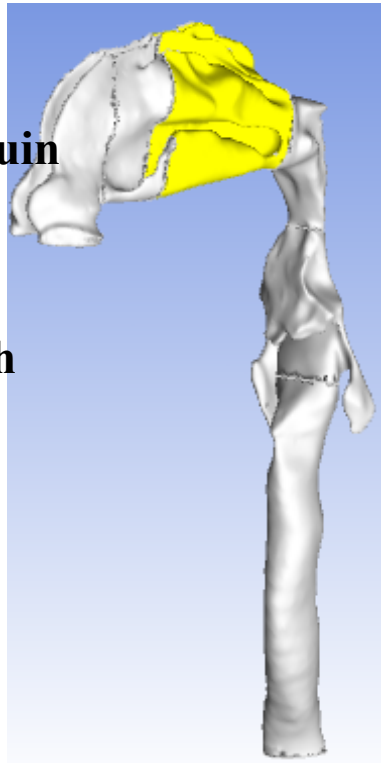




Deposition – Main Airways

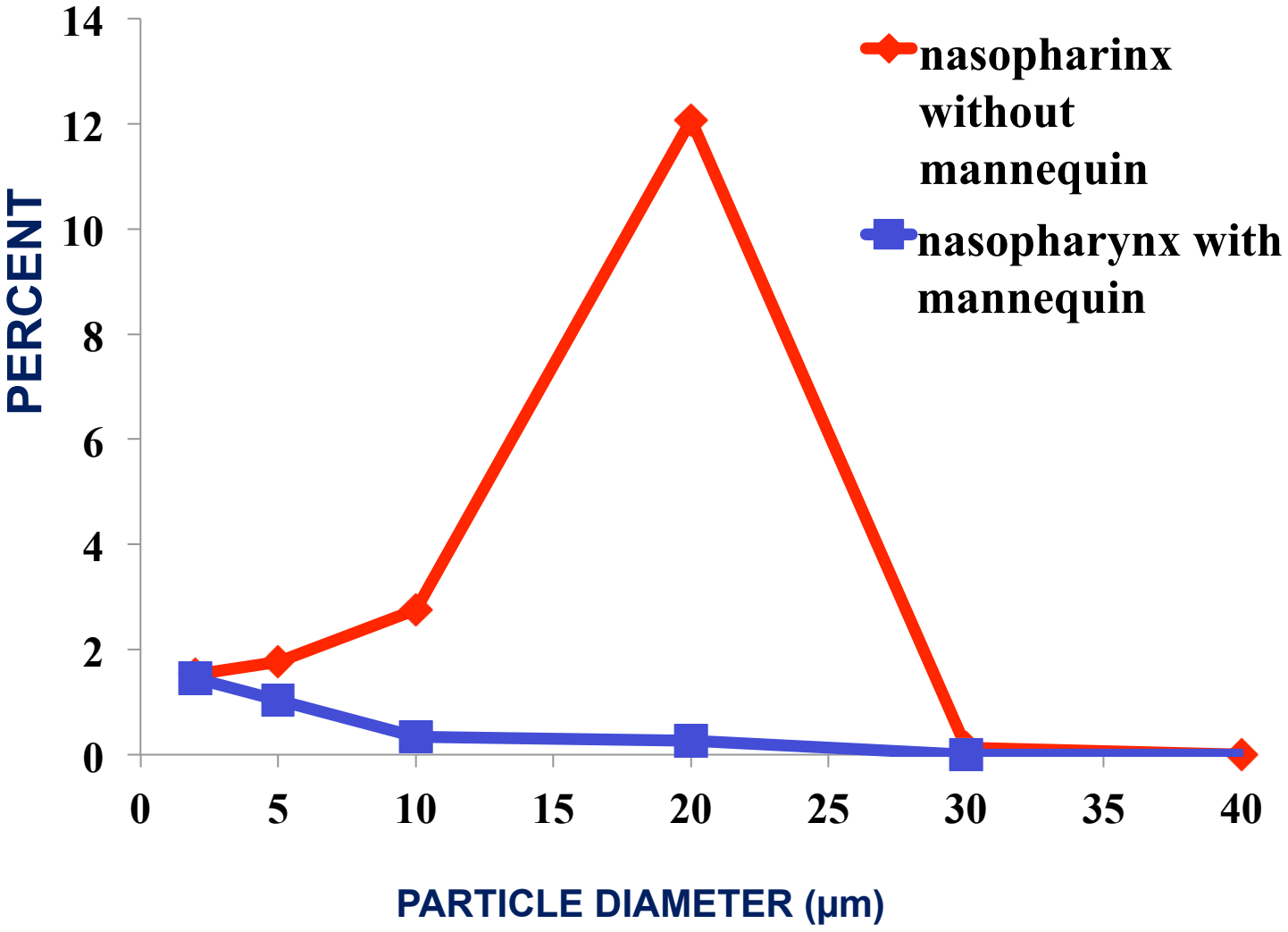
Clarkson University

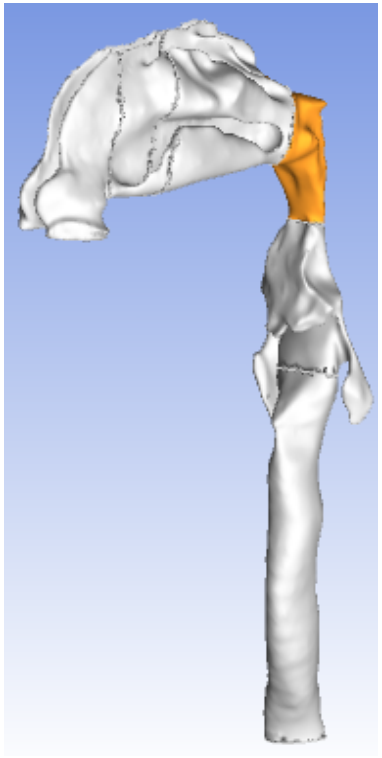




Deposition – Nasopharynx

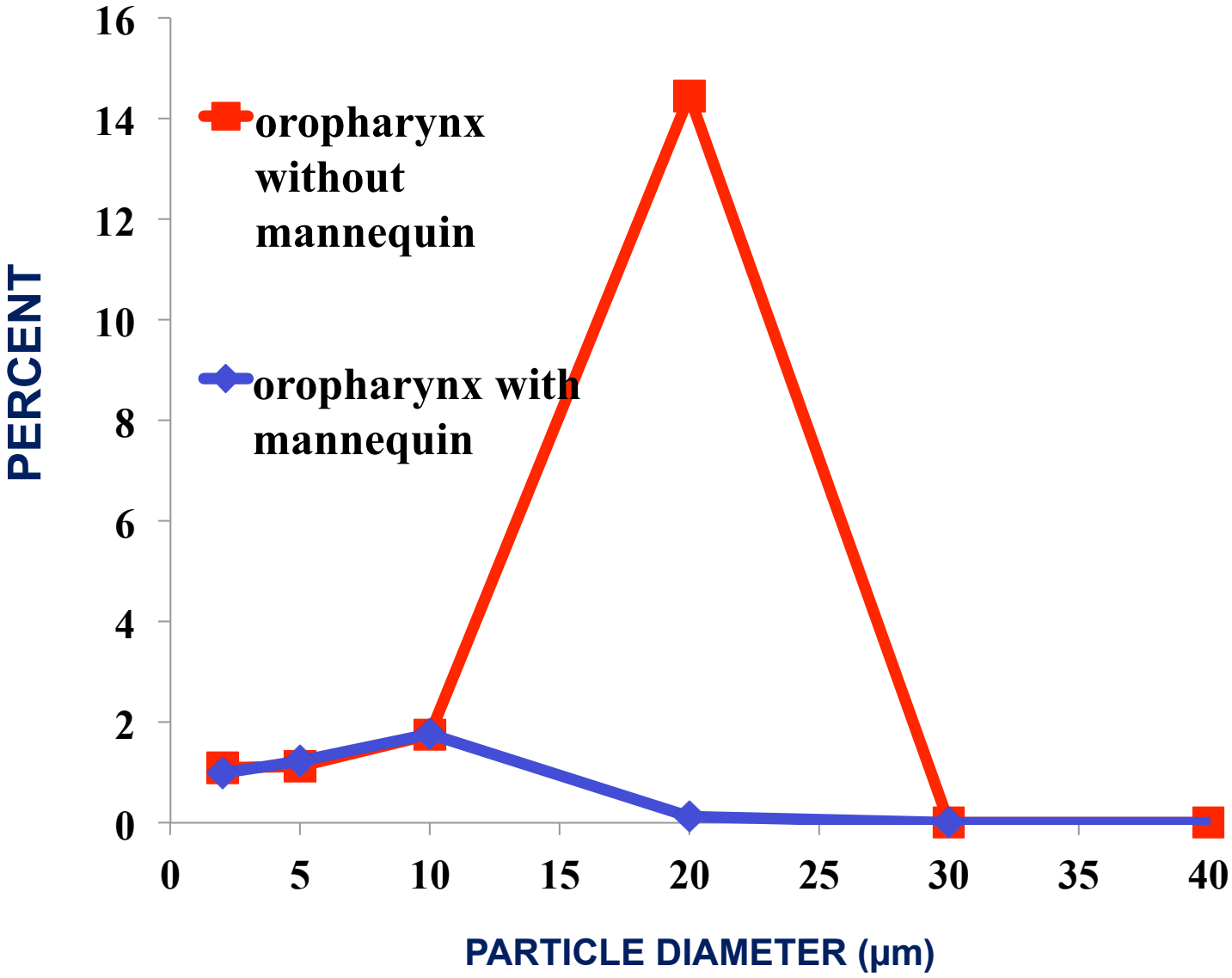
Clarkson University

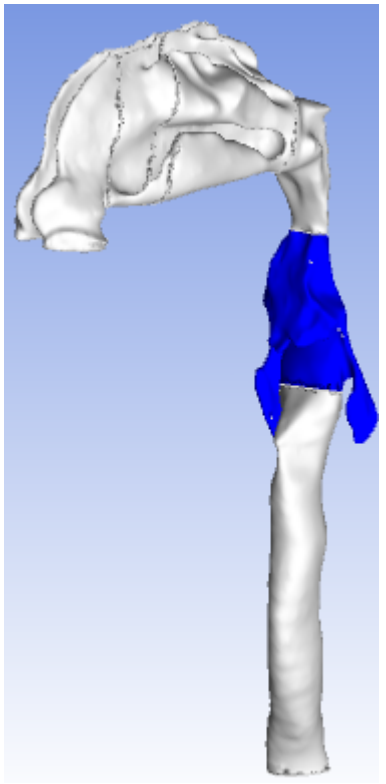




Deposition – Oropharynx

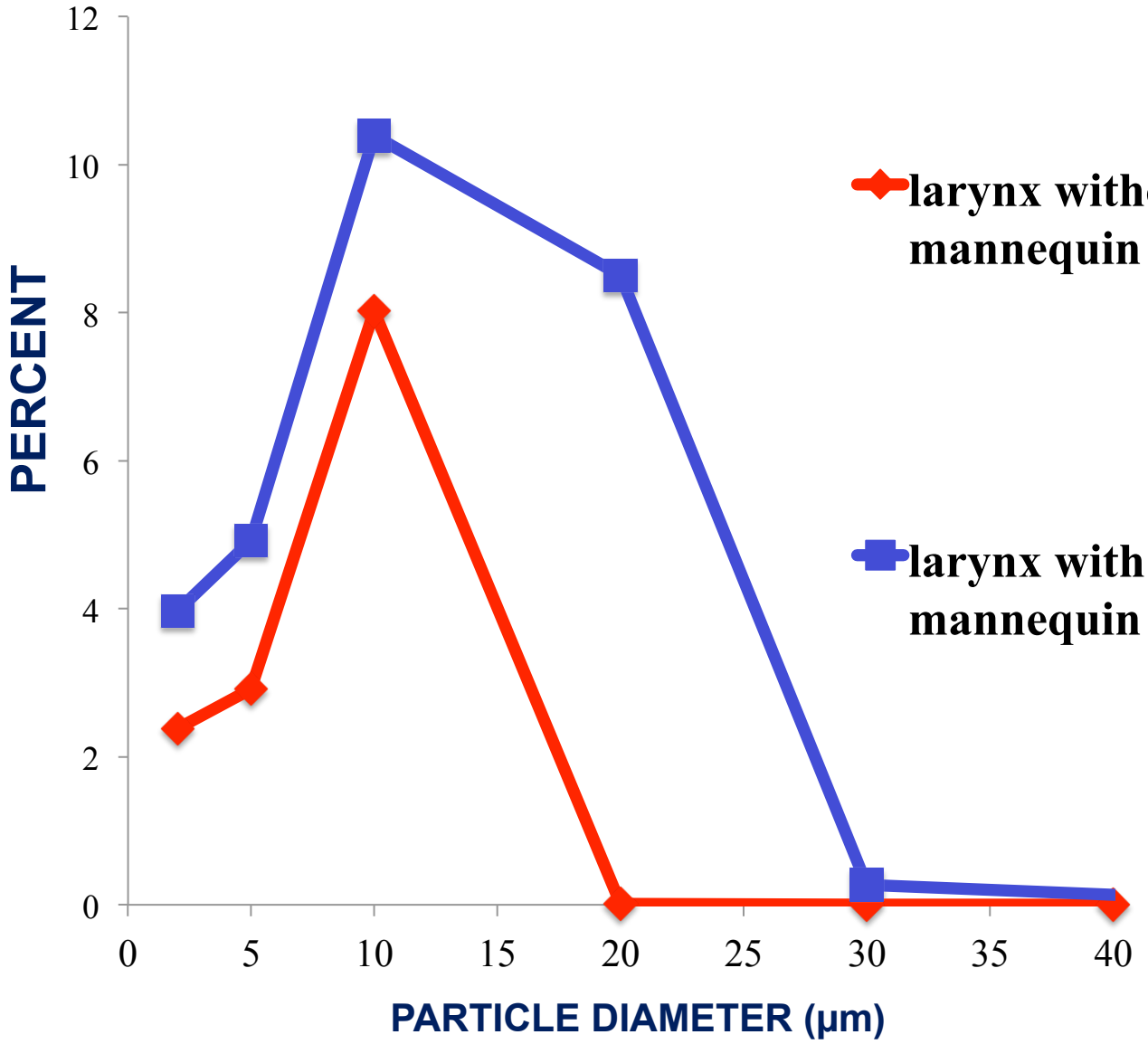
Clarkson University

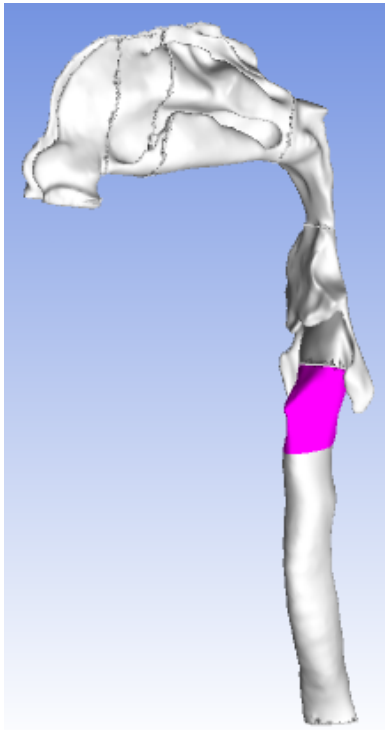




Deposition – Larynx

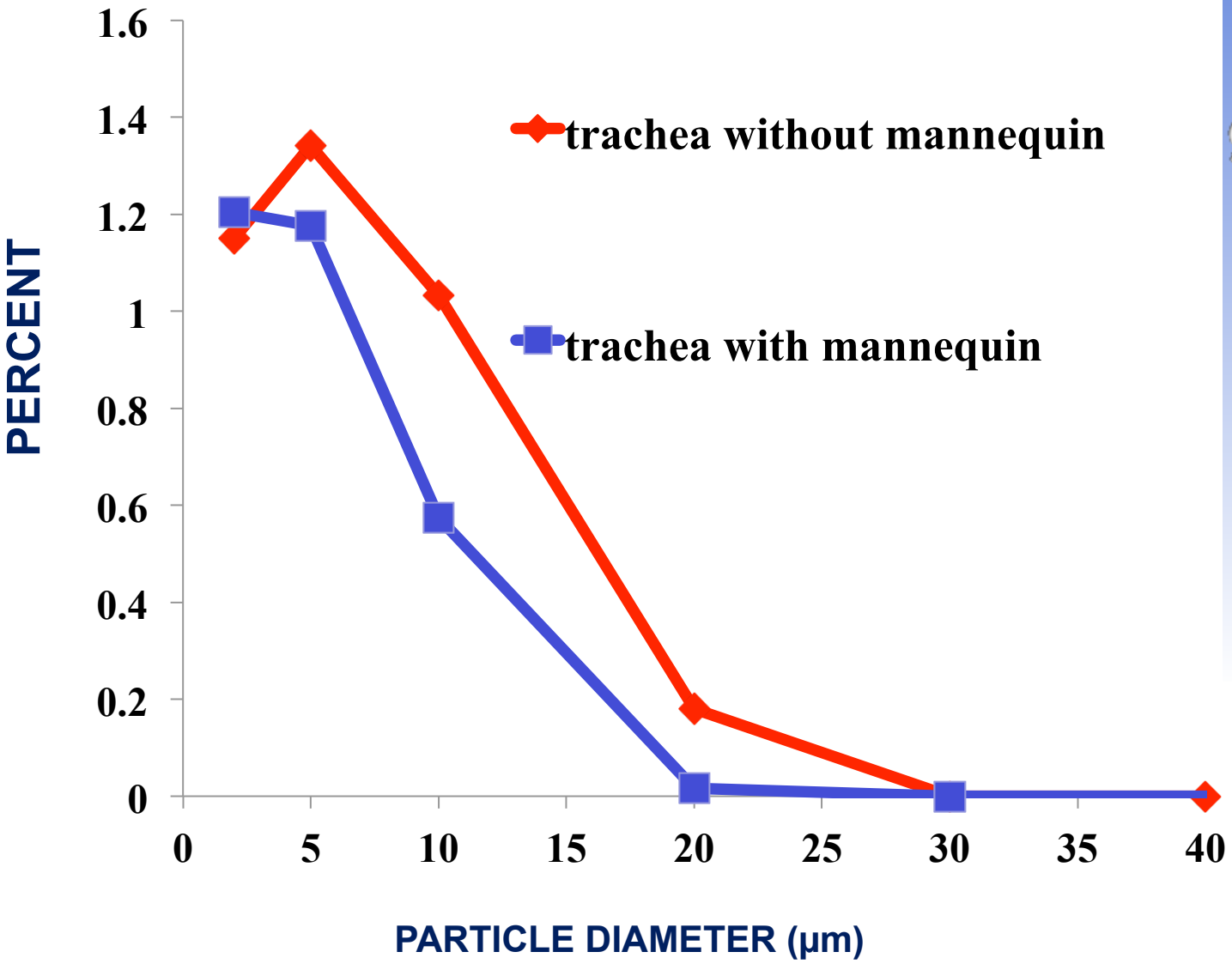
Clarkson University

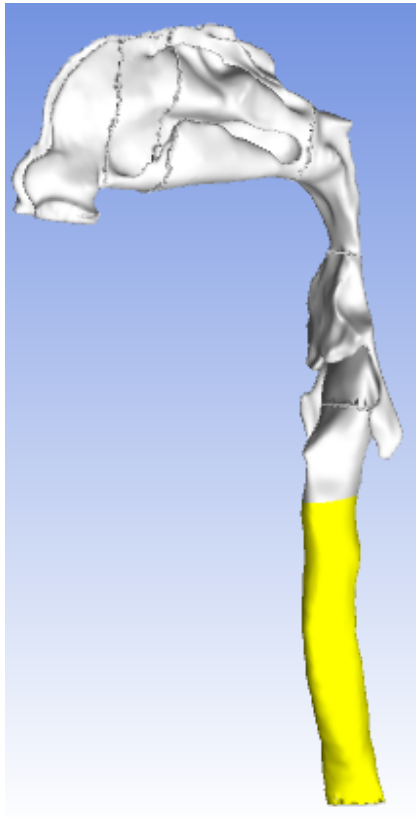




Deposition – Trachea

Clarkson University





Conclusions

Clarkson University

- Use of computational modeling of multiphase flows provides a better understanding of particles and fibers deposition in human airways.
- Fibers stay parallel to the flow most of the time with rapid rotation in shear fields.
- Computational modeling could helps in performing vertual surgeries.

Collaborators

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- Dr. Emdad *
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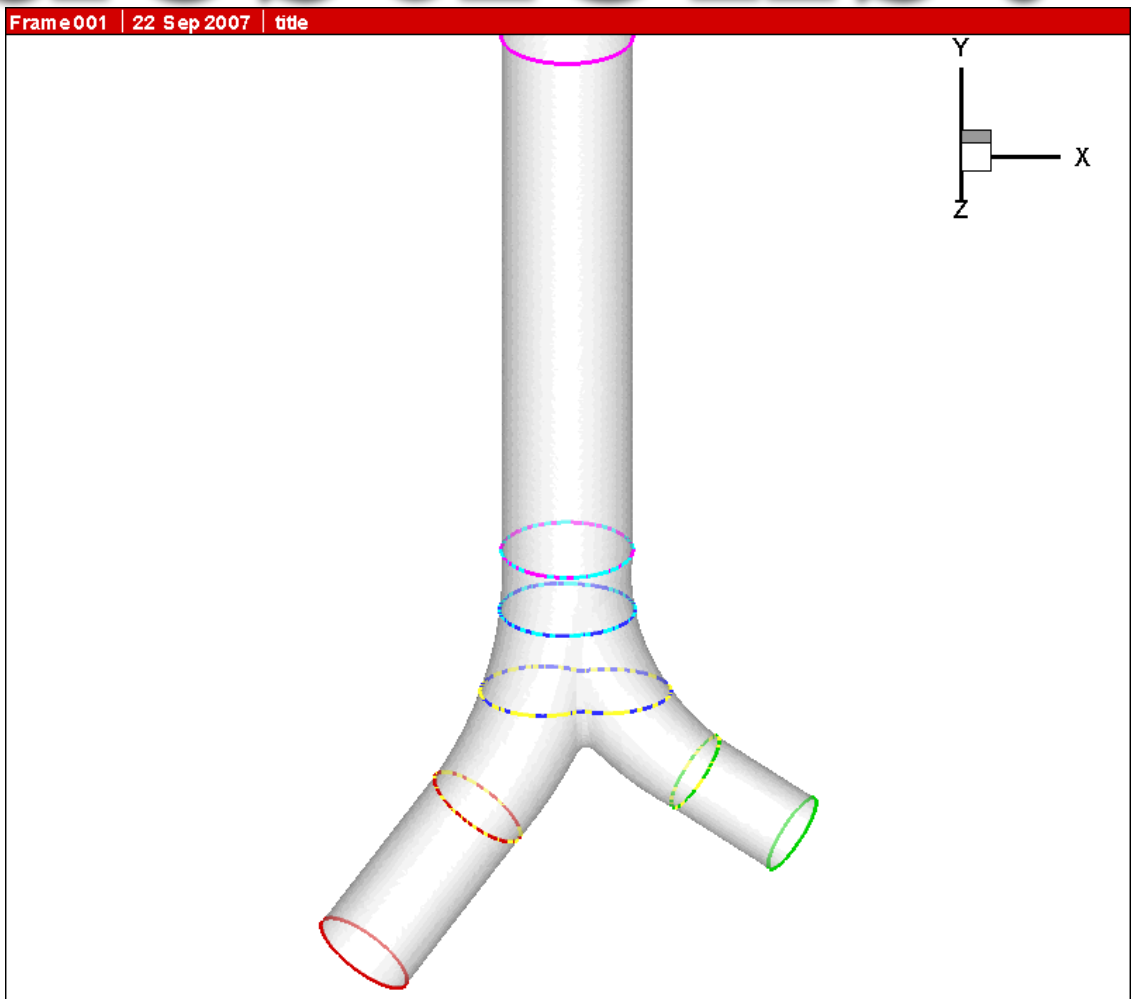
- Dr. Mazocca
- Dr. Basirat *
- Dr. Saidi *
- Dr. Helenbrook
- Dr. Kiato
- Dr. Firoozabadi *
- Dr. Yaghoubi *
- Dr. Fazelzadeh *

Thank You!
Questions?

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