Fiber Transport in the Respiratory Airways

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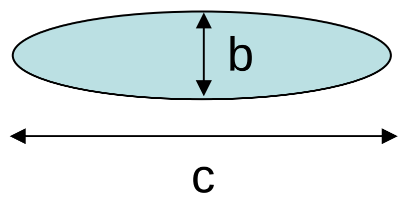
Background

- Health risks associated nanoparticles
- Exposure by inhalation
- Implications of particle shape
- Asbestos fibers and nanotubes
- Transport and deposition properties

Fiber Modeling

- Translational and rotational motion
- Spheres with equivalent diameters vs. fiber orientation
- Fiber Stokes number << 1 → neglect inertia
- Ellipsoid of revolution.
- Fiber aspect ratio, $\beta = c/b$



Coordinate frames

- Two coordinate systems

  - global (x,y,z), fixed in space

  - local (x',y',z'), fixed to fiber

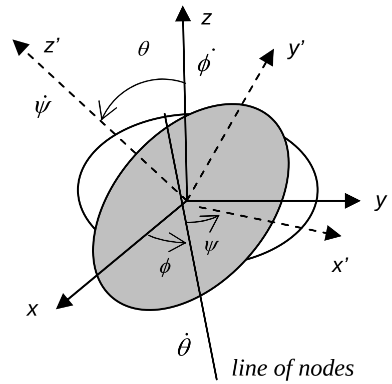
- Rotation matrix *A* transforms from local to global coordinates

  $\mathbf{x'} = A\mathbf{x}$

Fiber orientation & rotation matrix

- Euler angles

$$A = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\phi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\theta\sin\psi \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & \cos\theta\cos\phi\cos\psi - \sin\psi\sin\phi & \sin\theta\cos\psi \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix}$$



- Quaternions

$$A = 2\begin{pmatrix} q_1^2 + q_4^2 - \frac{1}{2} & q_1q_2 + q_3q_4 & q_1q_3 - q_2q_4 \\ q_1q_2 - q_3q_4 & q_2^2 + q_4^2 - \frac{1}{2} & q_2q_3 + q_1q_4 \\ q_1q_3 + q_2q_4 & q_2q_3 - q_1q_4 & q_3^2 + q_4^2 - \frac{1}{2} \end{pmatrix}$$

$$q_1 = \sin\frac{\theta}{2}\cos\frac{\phi-\psi}{2}, \quad q_3 = \cos\frac{\theta}{2}\sin\frac{\phi+\psi}{2},$$

$$q_2 = \sin\frac{\theta}{2}\sin\frac{\phi-\psi}{2}, \quad q_4 = \cos\frac{\theta}{2}\cos\frac{\phi+\psi}{2},$$

$$\sum_n q_n^2 = 1$$

Euler angles	Quaternions
+ Intuitive – Singular terms for certain angles → not suited for rigid motion simulations for fibers undergoing full rotations.	– Abstract + Well-behaved equations of motion + No trigonometric functions in rotation matrix + Numerical drift easily controlled

Equations for fiber translation

$$F_{grav,i} + F_{drag,i} + F_{Br,i} = 0$$

$$F_{grav} = \frac{\pi \rho_f g d_f^3 \beta}{6} \quad \text{in z-dir}$$

$$F_{drag,i} = 3\pi\mu d_{i'} \left(u_i - \frac{dx_i}{dt} \right)$$

$$\frac{d_{\parallel}}{d_f} = \frac{\frac{4}{3}(\beta^2 - 1)}{C_{\parallel}\left[\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}} \ln\left(\beta + \sqrt{\beta^2 - 1}\right) - \beta \right]}, \qquad \frac{d_{\perp}}{d_f} = \frac{\frac{8}{3}(\beta^2 - 1)}{C_{\perp}\left[\frac{2\beta^2 - 3}{\sqrt{\beta^2 - 1}} \ln\left(\beta + \sqrt{\beta^2 - 1}\right) + \beta \right]}.$$

Fiber equation of motion

Non-dimensional variables:

$\mathbf{x}^* = \mathbf{x}/R$, $t^* = tU/R$, $\mathbf{u}^* = \mathbf{u}/U$

$$\begin{bmatrix} \frac{dx^*}{dt^*} \\ \frac{dy^*}{dt^*} \\ \frac{dz^*}{dt^*} \end{bmatrix} = \begin{bmatrix} u^* \\ v^* \\ w^* \end{bmatrix} + \underbrace{A^T \begin{bmatrix} \frac{d_f}{d_\perp} & 0 & 0 \\ 0 & \frac{d_f}{d_\perp} & 0 \\ 0 & 0 & \frac{d_f}{d_\square} \end{bmatrix} A \begin{bmatrix} 0 \\ 0 \\ k \end{bmatrix}}_{\text{Local coordinates}} + A^T \underbrace{\begin{bmatrix} f_{Br,x'}^*(t^*) \\ f_{Br,y'}^*(t^*) \\ f_{Br,z'}^*(t^*) \end{bmatrix}}_{\text{Local coordinates}}, \qquad k = \frac{\rho_f g d_f^2 \beta}{18 \mu U}$$

Components of fiber velocity

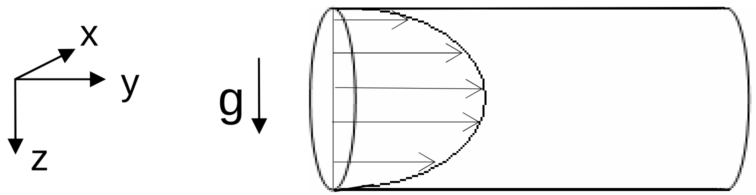
$$\frac{dx^*}{dt^*} = u^* + 4k\left[\left(\frac{d_f}{d_{\parallel}} - \frac{d_f}{d_{\perp}}\right)\left(q_1q_3 + q_2q_4\right)\left(\tfrac{1}{2} - q_1^2 - q_2^2\right)\right] + 2\left[\begin{array}{l} f^*_{Br,x'}\left(q_1^2 + q_4^2 - \tfrac{1}{2}\right) + f^*_{Br,y'}\left(q_1q_2 - q_3q_4\right) \\ + f^*_{Br,z'}\left(q_1q_3 + q_2q_4\right) \end{array}\right]$$

$$\frac{dy^*}{dt^*} = v^* - 4k\left[\left(\frac{d_f}{d_{\parallel}} - \frac{d_f}{d_{\perp}}\right)\left(q_1q_4 - q_2q_3\right)\left(\tfrac{1}{2} - q_1^2 - q_2^2\right)\right] + 2\left[\begin{array}{l} f^*_{Br,x'}\left(q_1q_2 + q_3q_4\right) + f^*_{Br,y'}\left(q_2^2 + q_4^2 - \tfrac{1}{2}\right) \\ + f^*_{Br,z'}\left(q_2q_3 - q_1q_4\right) \end{array}\right]$$

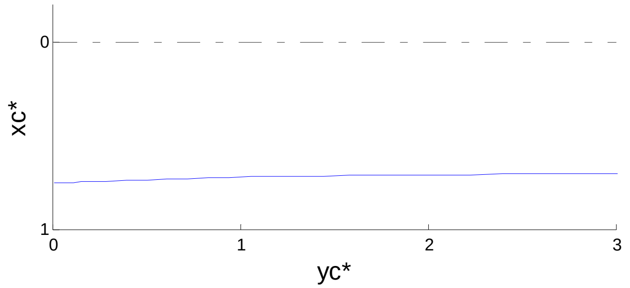
$$\frac{dz^*}{dt^*} = w^* + 4k\left[\frac{d_f}{d_{\parallel}}\left(\tfrac{1}{2} - q_1^2 - q_2^2\right)^2 + \frac{d_f}{d_{\perp}}\left(q_1^2 + q_2^2\right)\left(q_3^2 + q_4^2\right)\right] + 2\left[\begin{array}{l} f^*_{Br,x'}\left(q_1q_3 - q_2q_4\right) + f^*_{Br,y'}\left(q_2q_3 + q_1q_4\right) \\ + f^*_{Br,z'}\left(\tfrac{1}{2} - q_1^2 - q_2^2\right) \end{array}\right]$$

Solved using MATLAB

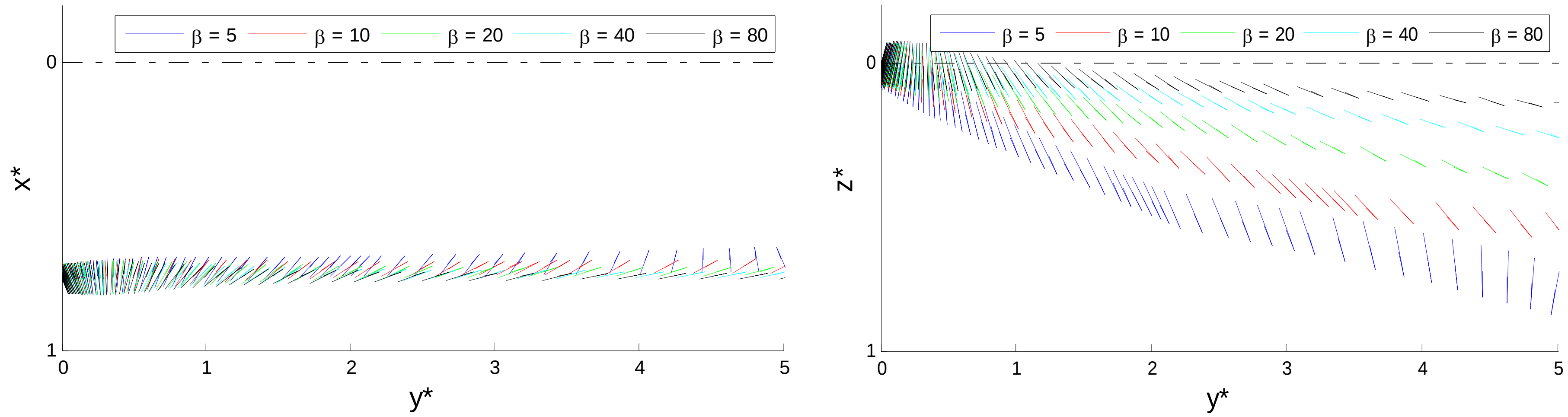
Results



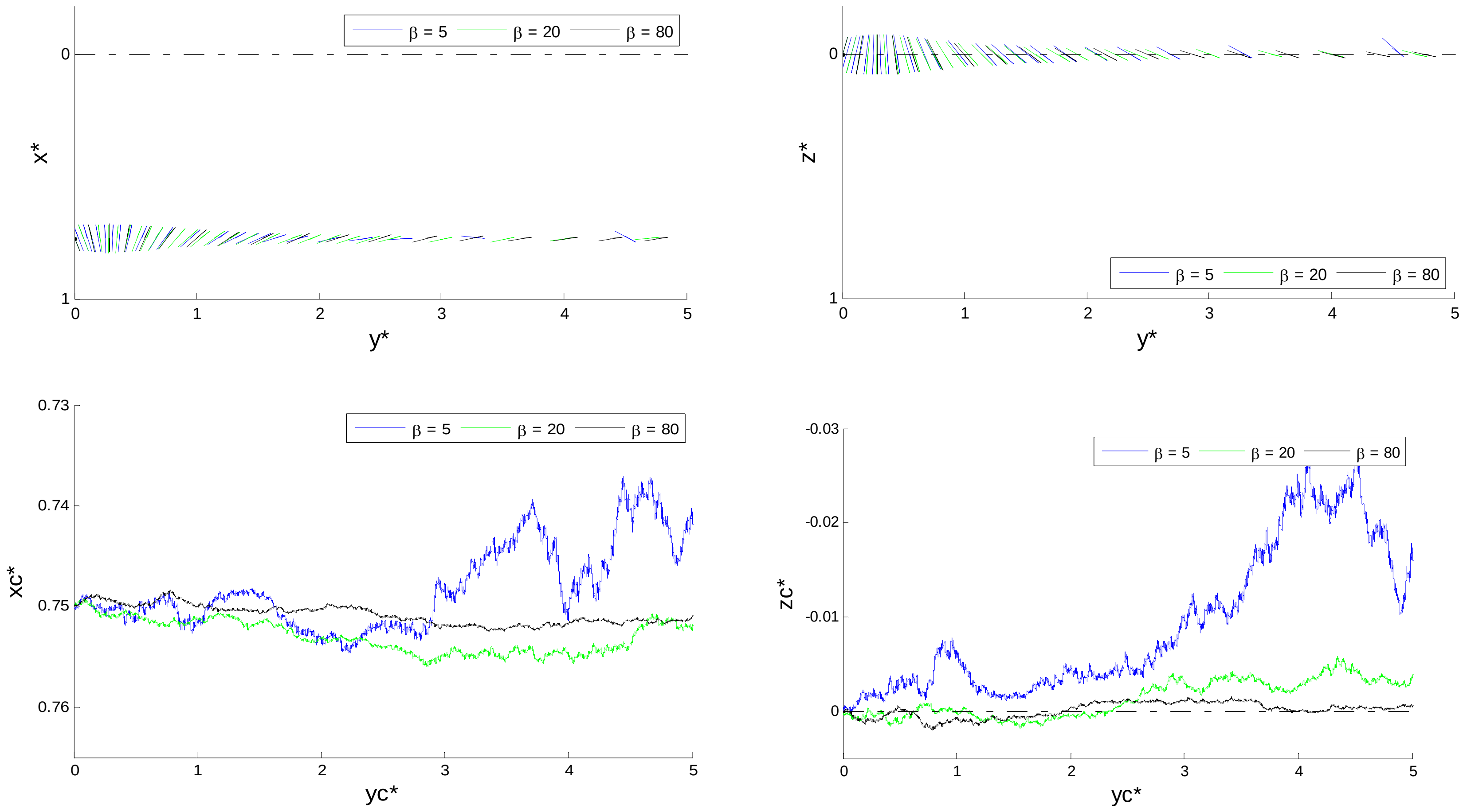
- Small drift motion



Microfibers



Nanofibers



Thank you

Questions?