Air filtration simulation with focus on slip effects

Liping Cheng,
Dirk Kehrwald,
Arnulf Latz,
Stefan Rief,
Kilian Schmidt and
Andreas Wiegmann

= Fraunhofer Institute for Industrial Mathematics
What’s new?

Filtration community is interested in slip effects due to very small scales:

- Nano particles
- Nano fibers

*Our earlier description* [Latz & Wiegmann, Filtech 2003] *was not valid for these regimes*

- For particles, implemented *Cunningham correction*
- For fibers, *fractional slip* replaces no-slip boundary conditions
What’s not so new?

‘Physicists’ model produces individual contributions of standard modeled effects:

- Interception
- Inertial Impaction
- Brownian Motion (Diffusion: Smoluchowski-Einstein-Langevin)
- Sieving (not today)

... but we never explained it that well!

Outline:

I. Mathematical models  II. Results  III. Discussion
No slip vs fractional slip

\[-\mu \Delta \vec{u} + \nabla p = 0 \text{ (momentum balance)}\]
\[\nabla \cdot \vec{u} = 0 \text{ (mass conservation)}\]
\[\vec{u} = 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)}\]
\[P_{in} = P_{out} + c \text{ (pressure drop is given)}\]

\[\mu \text{ : fluid viscosity,}\]
\[\vec{u} \text{ : velocity, periodic,}\]
\[p \text{ : pressure, periodic up to pressure drop in flow direction.}\]

\[-\mu \Delta \vec{u} + \nabla p = 0 \text{ (momentum balance)}\]
\[\nabla \cdot \vec{u} = 0 \text{ (mass conservation)}\]
\[n \cdot \vec{u} = 0 \text{ on } \Gamma \text{ (no flow into fibers)}\]
\[\vec{t} \cdot \vec{u} = -\lambda n \cdot \nabla (\vec{u} \cdot \vec{t}) \text{ on } \Gamma \text{ (slip flow along fibers)}\]
\[P_{in} = P_{out} + c \text{ (pressure drop is given)}\]

\[n \text{ : normal direction to the fiber surface,}\]
\[\lambda \text{ : slip length,}\]
\[\vec{t} \text{ : any tangential direction with } \vec{t} \cdot n = 0.\]
Particle motion

\[ d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) \, dt + \sigma \times d\vec{W}(t), \]
\[ d\vec{x} = \vec{v}(\vec{x}(t)) \, dt, \]
\[ \sigma^2 = \frac{2k_b T \gamma}{m}, \]
\[ \gamma = 6\pi \rho \mu \frac{R}{m}, \]
\[ \langle dW_i(t), dW_j(t) \rangle = \delta_{ij} \, dt. \]

\( \vec{u} \) : fluid velocity
\( \vec{v} \) : particle velocity
\( t \) : time
\( T \) : temperature
\( \gamma \) : friction coefficient
\( R \) : particle radius
\( \rho \) : fluid density
\( \mu \) : fluid viscosity
\( \vec{W} \) : Wiener Measure (3d)
\( k_b \) : Boltzmann constant
\( m \) : particle mass
\( Kn \) : Knudsen number

[Latz & Wiegmann, Filtech 2003]
Interception

\[ d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) \, dt + \sigma \times d\vec{W}(t), \]
\[ d\vec{x} = \vec{v}(\vec{x}(t)) \, dt, \]
\[ \sigma^2 = \frac{2k_B T \gamma}{m}, \]
\[ \gamma = 6\pi\rho\mu \frac{R}{m}, \]
\[ \langle dW_i(t), dW_j(t) \rangle = \delta_{ij} \, dt. \]

\[ m \to 0, \sigma = 0 \]
\[ \Rightarrow \vec{v} = \vec{u} \]
\[ \Rightarrow d\vec{x} = \vec{u}(\vec{x}(t)) \, dt. \]

\( \vec{u} \): fluid velocity
\( \vec{v} \): particle velocity
\( t \): time
\( T \): temperature
\( \gamma \): friction coefficient
\( R \): particle radius
\( \rho \): fluid density
\( \mu \): fluid viscosity
\( \vec{w} \): Wiener Measure (3d)
\( k_b \): Boltzmann constant
\( m \): particle mass
\( Kn \): Knudsen number

Disable diffusion and let mass tend to zero (keeping all other parameters fixed), the particle velocity tends to the fluid velocity.
Interception

\[ d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) \, dt + \sigma \times d\vec{W}(t), \]
\[ d\vec{x} = \vec{v}(\vec{x}(t)) \, dt, \]

\( \vec{u} \) : fluid velocity
\( \vec{v} \) : particle velocity
\( t \) : time
\( T \) : temperature

\( \gamma \) : Wiener Measure (3d)
\( \sigma \) : Boltzmann constant
\( \rho \) : particle mass
\( R \) : fluid density
\( \gamma \) : fluid viscosity
\( \mu \) : friction coefficient
\( b \) : particle radius
\( K_n \) : Knudsen number

Disable diffusion and let mass tend to zero (keeping all other parameters fixed), the particle velocity tends to the fluid velocity.

\[ m \to 0, \sigma = 0 \]
\[ \Rightarrow \vec{v} = \vec{u} \]
\[ \Rightarrow d\vec{x} = \vec{u}(\vec{x}(t)) \, dt. \]
Inertial Impaction

\[
d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) \, dt + \sigma \times d\vec{W}(t),
\]
\[
d\vec{x} = \vec{v}(\vec{x}(t)) \, dt,
\]
\[
\sigma^2 = \frac{2k_b T \gamma}{m},
\]
\[
\gamma = 6\pi \rho \mu \frac{R}{m},
\]
\[
\langle dW_i(t), dW_j(t) \rangle = \delta_{ij} \, dt.
\]

By only switching off diffusion, the effect of inertial impaction is the difference between this simulation and the one for vanishing mass (interception).
Inertial Impaction

\[ d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) \, dt + \sigma \times d\vec{W}(t), \]
\[ d\vec{x} = \vec{v}(\vec{x}(t)) \, dt, \]

\(\vec{u}\) : fluid velocity
\(\vec{v}\) : particle velocity
\(t\) : time
\(T\) : temperature

\(\kappa_b\) : Boltzmann constant
\(m\) : particle mass
\(Kn\) : Knudsen number

\(\sigma = 0\).

By only switching off diffusion, the effect of inertial impaction is the difference between this simulation and the one for vanishing mass (interception).
Particle Motion including Cunningham correction

\[ d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) dt + \sigma \times d\vec{W}(t), \]
\[ d\vec{x} = \vec{v}(\vec{x}(t)) dt, \]
\[ \sigma^2 = \frac{2k_B T \gamma}{m}, \]
\[ \gamma = 6\pi \rho \mu \frac{R}{C_i m}, \]
\[ \langle dW_i(t), dW_j(t) \rangle = \delta_{ij} dt, \]
\[ C_i = 1 + Kn \left[ 1.142 + 0.558e^{-0.999/Kn} \right], \]
\[ Kn = \frac{\lambda}{R}, \]
\[ \lambda = \frac{k_B T}{\sqrt{32\pi R^2} P}. \]

As \( Kn \) increases, influence of friction \( \gamma \) and diffusion \( \sigma \) decrease: particles go more straight.

Cunningham correction is always used later, also for interception and inertial impaction.
Particle Motion including Cunningham correction

\[ d\vec{v} = -\gamma \times (\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) \, dt + \sigma \times d\hat{W}(t), \]
\[ d\vec{x} = \vec{v}(\vec{x}(t)) \, dt, \]
\[ \sigma^2 = \frac{2k_B T \gamma}{m}, \]
\[ \gamma = \frac{\pi \rho \mu}{k_T R}. \]

- \( \vec{u} \): fluid velocity
- \( \vec{v} \): particle velocity
- \( t \): time
- \( T \): temperature
- \( k_B \): Boltzmann constant
- \( m \): particle mass
- \( Kn \): Knudsen number
- \( \kappa_b \): Total pressure

As \( Kn \) increases, influence of friction \( \gamma \) and diffusion \( \sigma \) decrease: particles go more straight.

Cunningham correction is always used later, also for interception and inertial impaction.
Filtration efficiency with and without Cunningham correction

- **Filtration Efficiency [%]**
- **Particle Diameter [μm]**

- **Graph Legend:**
  - Red: No Cunningham correction
  - Yellow: Cunningham Correction
Simulated SEM view of 5 Structures

\[
\begin{align*}
\alpha &= 0.1 & \alpha &= 0.07 & \alpha &= 0.05 & \alpha &= 0.05 & \alpha &= 0.05 \\
 d_F &= 14 \mu m & d_F &= 14 \mu m & d_F &= 14 \mu m & d_F &= 17 \mu m & d_F &= 20 \mu m \\
\end{align*}
\]

\(\alpha\): solid volume fraction of fibers

\(d_F\): fiber diameter
Deposition effects

\[ \alpha = 0.05, \]
\[ d_F = 14, \]
\[ v = 0.1\text{m/s} \]
**Velocity Effects**

\[ \alpha = 0.05, \]
\[ dF = 14, \]

Interception + Impaction + Diffusion

Velocity

\[ v = 0.1 \text{ m/s} \]

Velocity

\[ v = 1 \text{ m/s} \]

Velocity

\[ v = 10 \text{ m/s} \]
Effect of solid volume fraction (SVF)

$dF = 14,$
$v = 1 \text{ m/s},$
Interception + Impaction + Diffusion

SVF $\alpha = 0.05$

SVF $\alpha = 0.07$

SVF $\alpha = 0.1$
Effect of fiber thickness

\( \alpha = 0.05, \)
\( v = 1 \text{ m/s} \)

Interception + Impaction + Diffusion

dF = 14

dF = 17

dF = 20
Effect of slip flow

\[ \alpha = 0.05, \]
\[ dF = 14, \]
\[ v = 1 \text{ m/s} \]

Interception + Impaction + Diffusion

No slip boundary conditions

Fractional slip boundary conditions
Influence of velocity on filter efficiency

- dF = 14 µm
- \(\alpha = 0.05\)
- L = 1.4 mm

Particle diameter [µm]

Filtration efficiency [%]

- 0.1 m/s
- 1.0 m/s
- 10 m/s
Influence of fiber diameter on filter efficiency

\[ U = 1.0 \text{ m/s} \]
\[ \alpha = 0.05 \]
\[ L = 1.4 \text{ mm} \]
Influence of SVF on filter efficiency

Particle diameter [µm]

Filtration efficiency [%]

- Solid volume fraction 0.05
- Solid volume fraction 0.07
- Solid volume fraction 0.10

\( dF = 14 \, \mu m \)
\( U = 1.0 \, m/s \)
\( L = 1.4 \, mm \)
Influence of slip flow on filter efficiency

- Particle diameter [µm]
- Filtration efficiency [%]
- Slippage parameter $\alpha = 0.05$
- Slippage length $L = 1.4$ mm
- Slippage force $dF = 14$ µm
- Velocity $U = 1.0$ m/s

Graph showing the effect of particle diameter on filtration efficiency with and without slip flow.
Influence of individual effects on filter efficiency

- Filtration efficiency
- Brownian diffusion
- Interception
- Inertial impaction

\[ d_F = 14 \text{ m} \]
\[ U = 0.1 \text{ m/s} \]
\[ \alpha = 0.05 \]
\[ L = 1.4 \text{ mm} \]
Comparison with [Balazy & Podgorski Filtech 2007]

Fractional efficiency, $\eta$ [-]

- **filter efficiency**
- **Brownian diffusion**
- **interception**
- **inertial impaction**
- **gravitational settling**

$d_F = 14 \text{ m}$
$U = 0.1 \text{ m/s}$
$\alpha = 0.05$
$L = 1.4 \text{ mm}$

Current work
Effect of mesh refinement on efficiency due to interception

We believe [B &P] results for nano particles. We get their trend for more refined mesh and will investigate what causes the effect for the coarser resolution – the pressure drop is ok, difference hopefully lies in some details of the flow field, particle tracking, or particle collision computations…
Conclusions

Models for nanoscale effects for

- particles
- fibers

added to the model and implemented in the code

Parameters in ‘physicists model’ set to achieve ‘decomposition into classical effects’

- Interception
- Inertial Impaction
- Diffusion

Nano scale results agree qualitatively with literature and measurements, further work is in progress for quantitative agreement
Nonwoven models, computations and figures made with our Software

GEO DICT

www.geodict.com

Thank you for your time and attention