Web-based Modeling of Electret Filter and Nanofiber Composite: Performance and Design

Drew Thompson, Min Tang, Sheng-Chieh Chen, Seong Chan Kim, and David Y.H. Pui

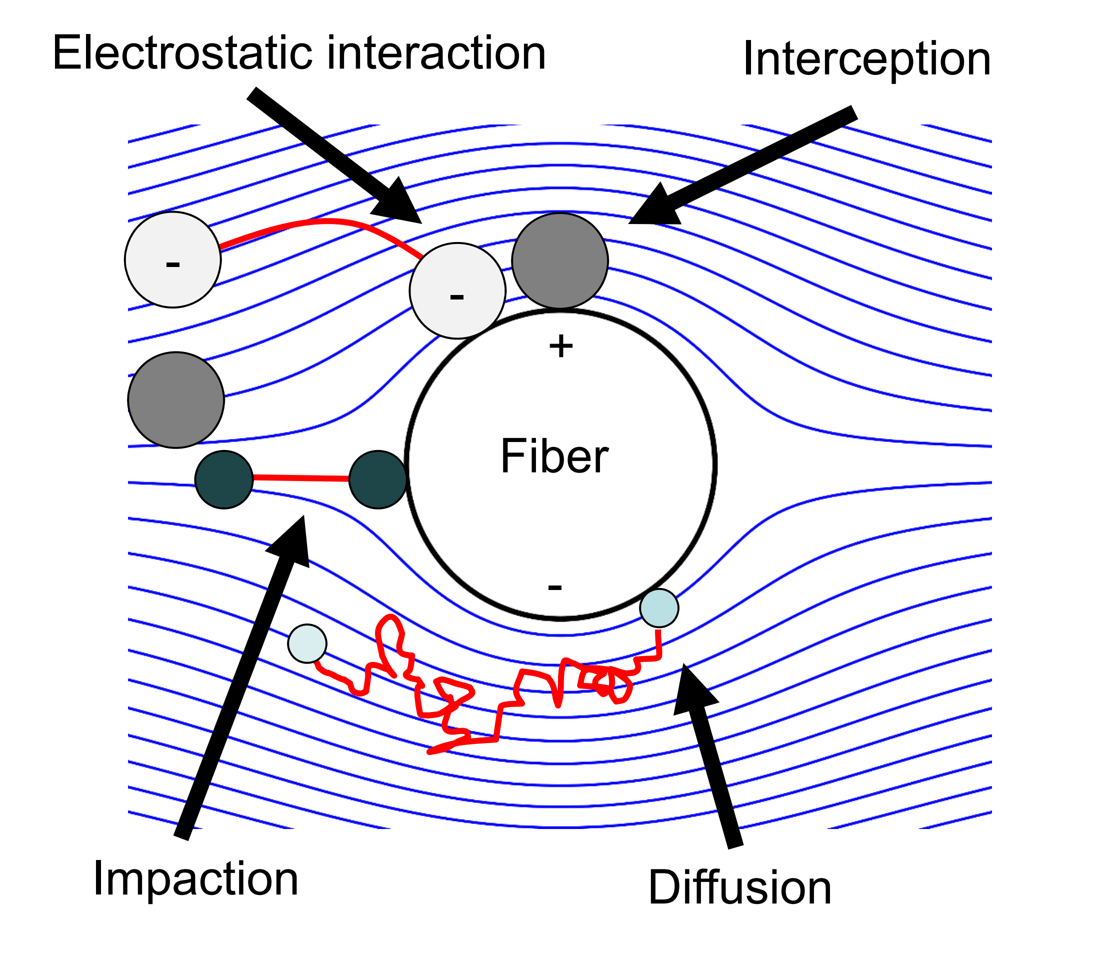
Particle Technology Laboratory, University of Minnesota

Center for Filtration Research

University of Minnesota

Electret filtration

- Mechanical filter media capture particles by:
  - Interception
  - Impaction
  - Diffusion
- Electret filter media have semi-permanently charged fibers
- Electrostatic interactions between particles and fibers increase filtration efficiency without increasing pressure drop

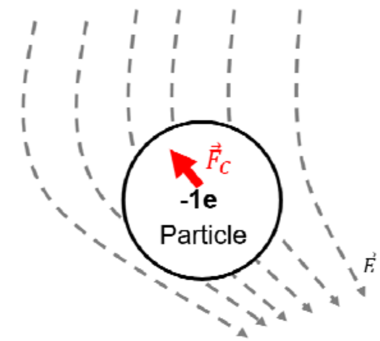


Electrostatic forces

Coulombic force

Charged fiber exerts force on charged particle

$$\vec{F}_C = q\vec{E}$$



Polarization force

Charged fiber induces charge on particle

$$\vec{F}_P = \frac{\pi {d_p}^3 \varepsilon_0 \varepsilon_g}{4}\left(\frac{\varepsilon_p - \varepsilon_g}{\varepsilon_p + 2\varepsilon_g}\right)\nabla\left(\vec{E}^2\right)$$

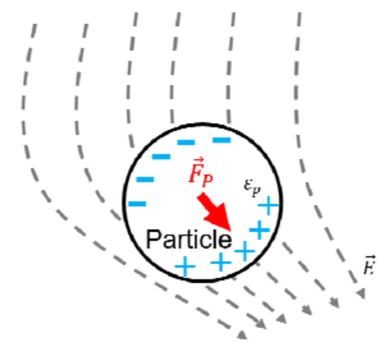
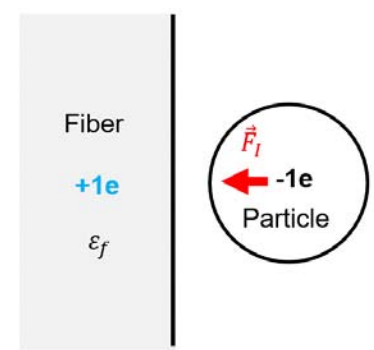


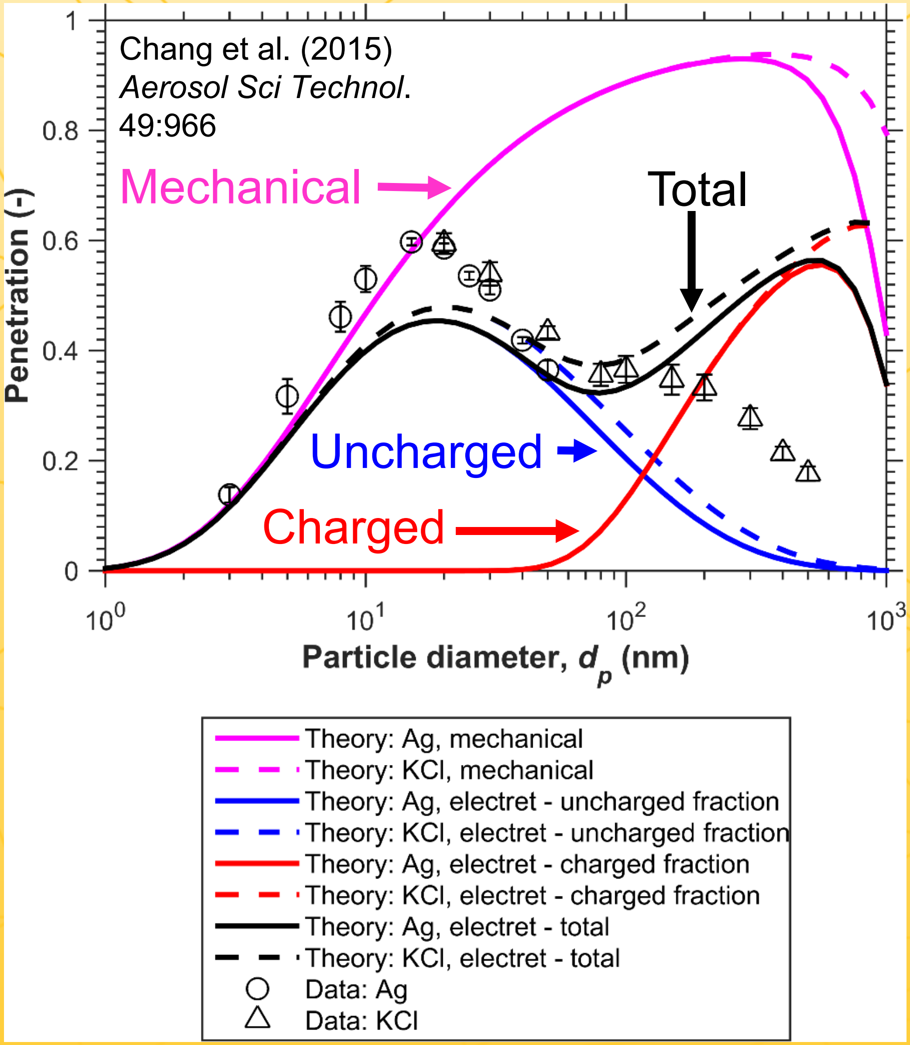
Image force

Charged particle induces charge in fiber

$$\vec{F}_I = -\left(\frac{\varepsilon_f - \varepsilon_g}{\varepsilon_f + \varepsilon_g}\right)\frac{q^2}{16\pi\varepsilon_0\varepsilon_g\left(r - \frac{d_f}{2}\right)^2}\hat{\boldsymbol{r}}$$



Motivation



- Disagreement between data and model previously used in Chang et al. (2015) because polarization of charged particles was neglected
- Most models are derived considering one electrostatic force at a time and adding their respective efficiencies together
- Assumption no longer holds for higher charge densities due to negative interaction between polarization and Coulombic forces (Lee et al. 2002a,b)
- Semi-empirical expression in Emi et al. (1987) which accounts for interaction of forces does not give functional relationships for charge density dependent constants
- New model which accounts for interaction between electrostatic forces and charge density dependencies is needed
- A user-friendly filter performance and design tool will utilize this new model

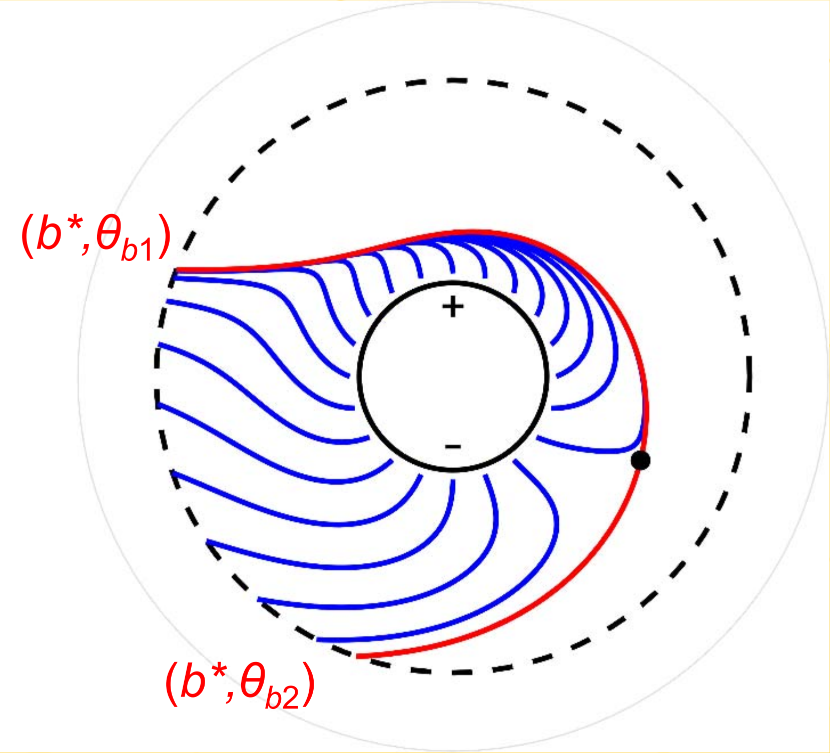
Calculation of single fiber efficiency

- Particle trajectories are found solving the equations of motion using numerical methods for ordinary differential equations

$$\vec{v} = \vec{u} + B\left(\vec{F}_C + \vec{F}_P + \vec{F}_I\right)$$

- Deterministic single fiber efficiency is calculated from the particle flux between limiting trajectories

$$\eta_{det} = -\frac{1}{2\sqrt{\alpha}} \int_{\theta_{b1}}^{\theta_{b2}} v_r^* d\theta \Bigg|_{r^*=b^*}$$

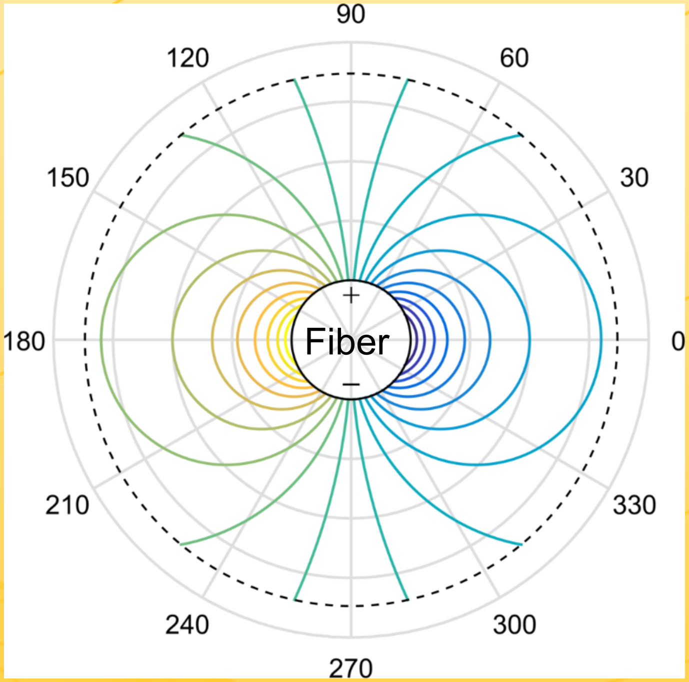


Assumptions in numerical model

- Particle diffusion and inertia are neglected
- Kuwabara flow cell model (1959)
- Fibers have sinusoidally distributed surface charge density (Brown, 1981)

$$\sigma(\theta) = \sigma_0 \cos(\theta - \theta_0)$$

- The electric field from neighboring fibers is neglected
- Particle concentration between limiting streamlines is uniform



Field lines for line-dipole charged fiber

Forms of single fiber efficiency equation

Coulombic, polarization, and image forces

$\eta_{\sigma q} \Rightarrow$ charged fiber (σ) and charged particle (q)

$$\eta_{\sigma q}(\alpha, N_R, N_C, N_P, N_I) = \frac{1}{\pi}\int_0^{\pi}\left[-\frac{1}{2\sqrt{\alpha}}\sin\theta - \frac{\sqrt{\alpha}N_C}{2}\sin(\theta-\theta_0) + \left(\frac{\alpha^2 N_P}{2} + \frac{\sqrt{\alpha}N_I}{2\left(1-\sqrt{\alpha}\right)^2}\right)\theta\right]_{\theta_{b1}(\theta_0)}^{\theta_{b2}(\theta_0)} d\theta_0$$

Polarization force only

$\eta_{\sigma 0} \Rightarrow$ charged fiber (σ) and uncharged particle ($q = 0$)

$$\eta_{\sigma 0}(\alpha, N_R, N_P) = \frac{1}{\sqrt{\alpha}}\sin\theta_b + \alpha^2 N_P(\pi - \theta_b)$$

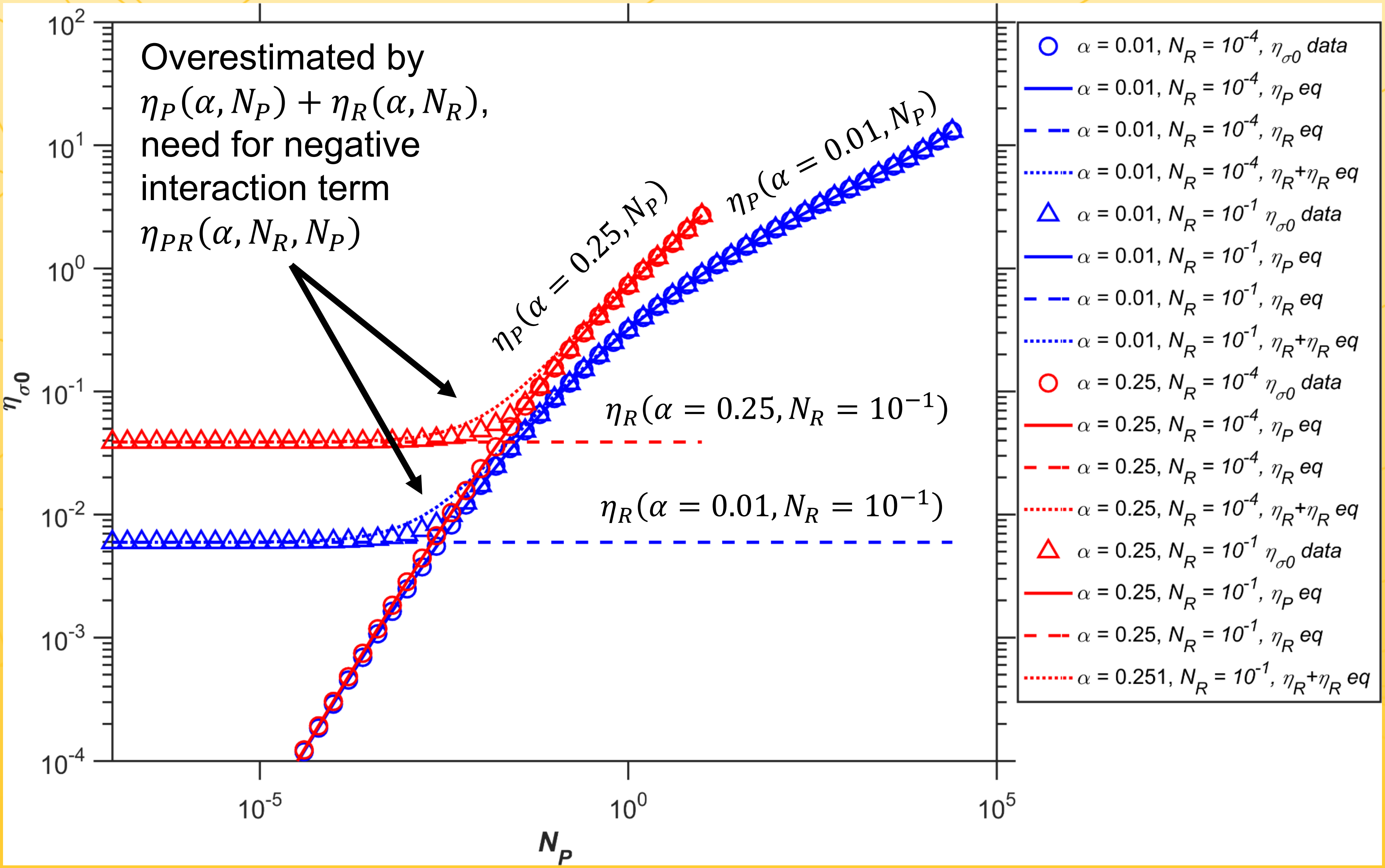
Non-dimensional numbers

$$N_R = \frac{d_p}{d_f} \qquad N_C = \frac{\sigma_0 q C(d_p)}{3\pi\varepsilon_0(\varepsilon_f + \varepsilon_g)\mu U d_p}$$

$$N_P = \frac{2}{3}\left(\frac{\varepsilon_p - \varepsilon_g}{\varepsilon_p + 2\varepsilon_g}\right)\frac{\varepsilon_g {\sigma_0}^2 {d_p}^2 C(d_p)}{\varepsilon_0\left(\varepsilon_f + \varepsilon_g\right)^2 \mu U d_f} \qquad N_I = \left(\frac{\varepsilon_f - \varepsilon_g}{\varepsilon_f + \varepsilon_g}\right)\frac{q^2 C(d_p)}{12\pi^2 \varepsilon_0 \varepsilon_g \mu U d_p {d_f}^2}$$

Regression equation for $\eta_{\sigma 0}(\alpha, N_R, N_P)$

$$\eta_{\sigma 0}(\alpha, N_R, N_P) = \eta_P(\alpha, N_P) + \eta_R(\alpha, N_R) + \eta_{PR}(\alpha, N_R, N_P)$$



Surrogate model for $\eta_{\sigma q}(\alpha, N_R, N_C, N_P, N_I)$

Filter, particle, and flow properties

α = 0.01 – 0.25
d_F = 1 – 100 μm
σ_0 = 0 – 10^{-3} C/m^2
ε_F ~ 1
U_0 = 0.01 – 1 m/s
d_p = 1 – 1,000 nm
ε_p ~ 1
q = 0 – 10e

⇒

Parameter space

α = 0.01 ~ 0.25
N_R = 10^{-5} ~ 1
N_C = 10^{-6} ~ 10^2
N_P = 10^{-7} ~ 10^5
N_I = 10^{-11} ~ 10

- Too many dependent variables to develop regression equations
- A surrogate model will simulate the behavior of the numerical model
- Gradient-Enhanced Kriging will predict the output of the numerical model based on a small number of computationally expensive numerical data points

Additional considerations for performance model

- Single fiber efficiency assumed to be sum of deterministic mechanisms (e.g., drag and electrostatic forces) and stochastic mechanisms (i.e., diffusion) (Bałazy and Podgórski, 2007)

$$\eta = \eta_D + \eta_{det}$$

- Diffusional single fiber efficiency given by empirical model of Wang et al. (2007) for nanoparticles and theory of Stechkina and Fuchs (1966) for larger particles

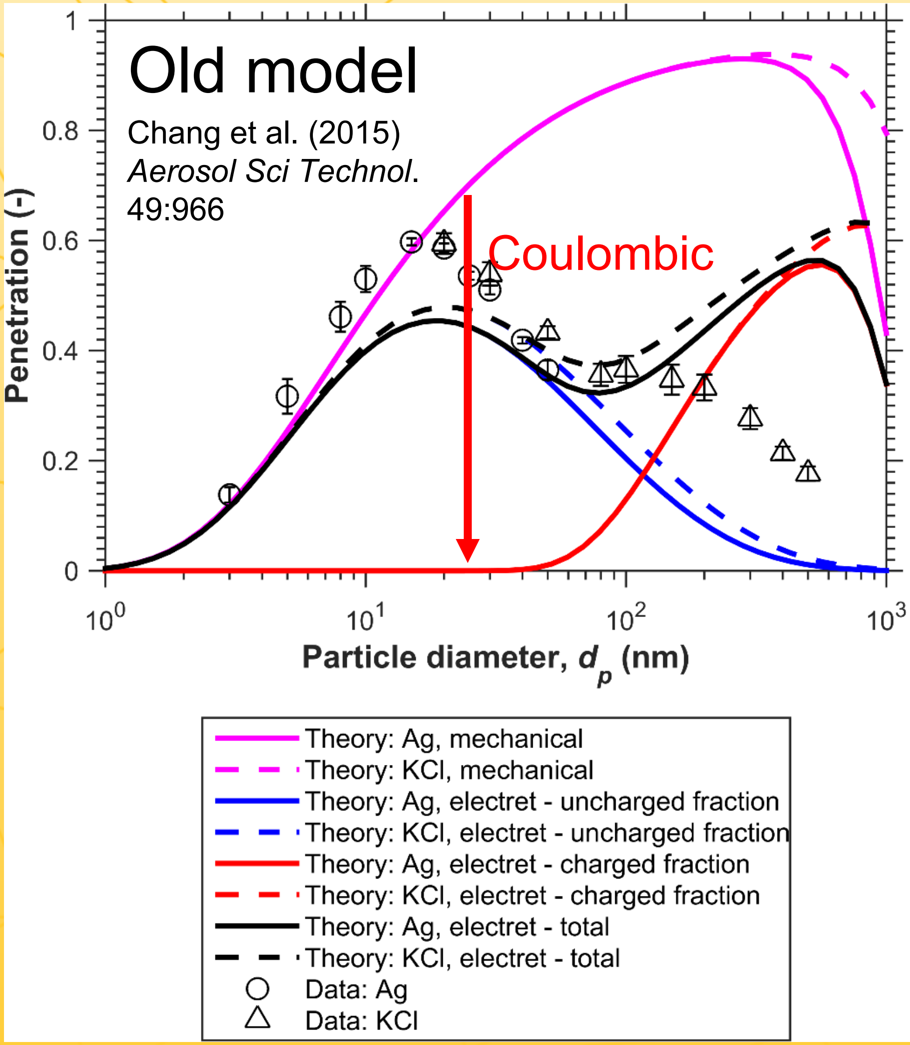
$$\eta_D = \min\left\{0.84\left(\frac{d_f}{d_{f\,\Delta p}}\right)^{0.57}[(1-\alpha)Pe]^{-0.43}, \qquad 2.9Ku^{-\frac{1}{3}}Pe^{-\frac{2}{3}} + 0.524Pe^{-1}\right\}$$

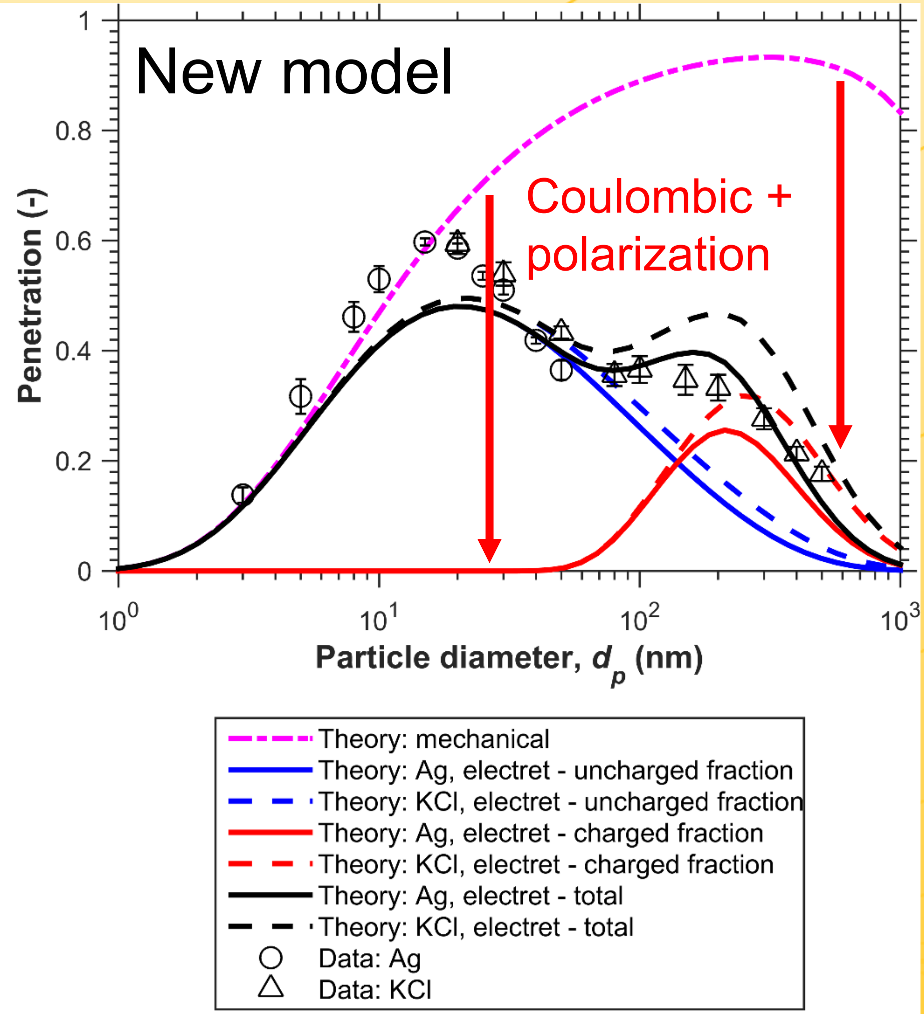
- For particles in charge equilibrium the charge distribution $f(n)$ (Wiedensohler, 1988) was considered

$$P = \sum_{n=-10}^{10} f(n)\exp\left\{-\frac{4\alpha h}{\pi(1-\alpha)d_f}[\eta_D + \eta_{det}(n)]\right\}$$

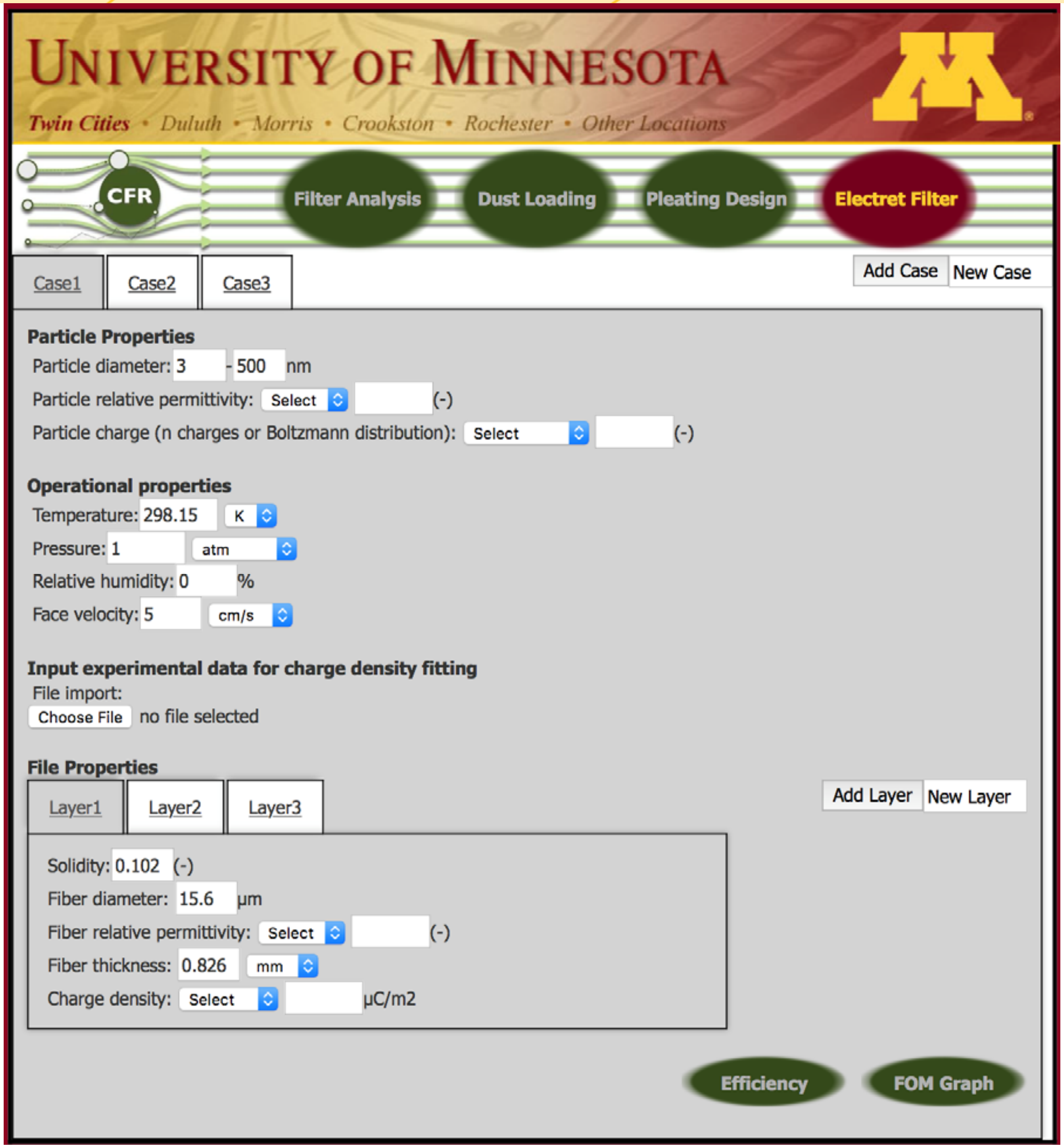
- Pressure drop calculated using theory of Pich (1966) for Kuwabara flow field with aerodynamic slip

Enhancement of Collection of Charged and Uncharged Fractions of Particles





Interface of web-based model



Future work

- Electret filter model
  - Obtain regression equation for interaction of interception and polarization
  - Refine surrogate model
  - Add functionality to input relative humidity which will adjust gas properties of dielectric constant, viscosity, and mean free path
- CFR web-based model website
  - Upload electret filter model
  - Update other modules with new user interface and Python backend
  - Add liquid filtration module

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Thank you for your attention

Questions and/or comments:
thom3527@umn.edu

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