Development of a Web-based Electret Filter Performance Modeling and Design Tool

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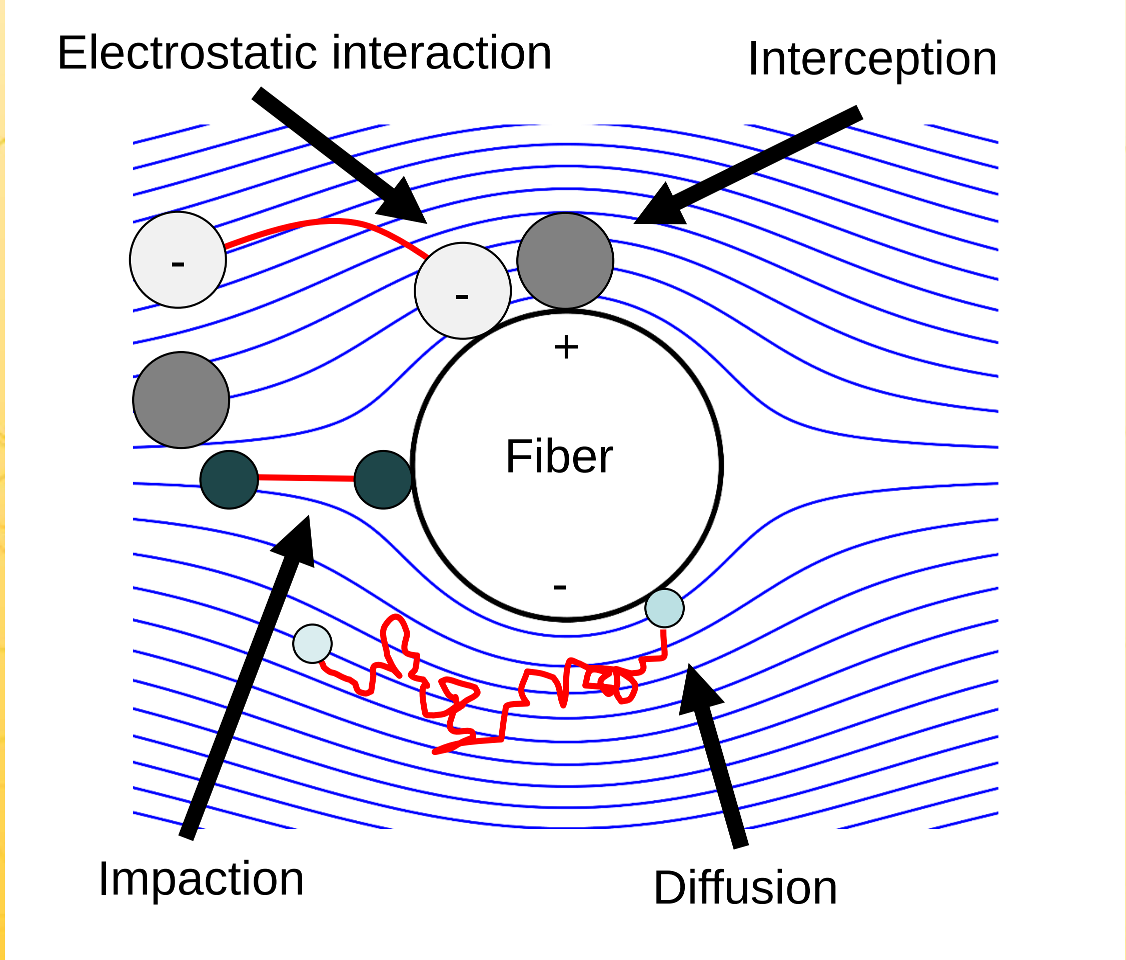
Outline

1. Introduction of electret filter media and theory
2. New model using limiting trajectories
3. Comparison of model with experimental data
4. Development of surrogate models
5. Web-based performance and design tool
6. Future work

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

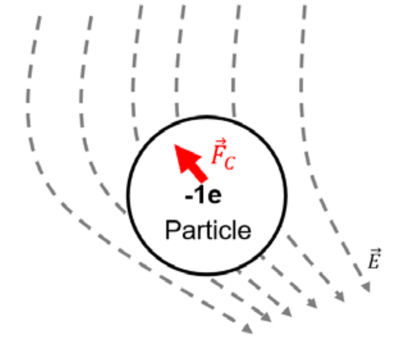


Electrostatic forces

Coulombic force

Charged fiber exerts force on charged particle

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



Polarization force

Charged fiber induces charge on particle

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

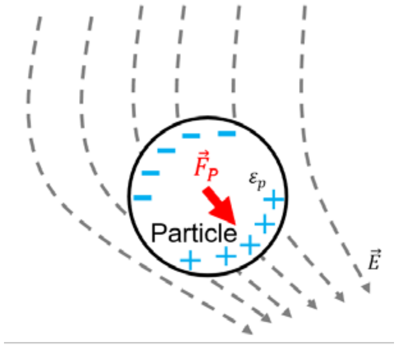
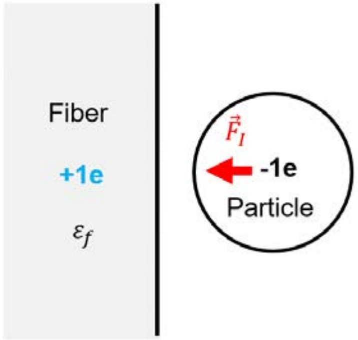


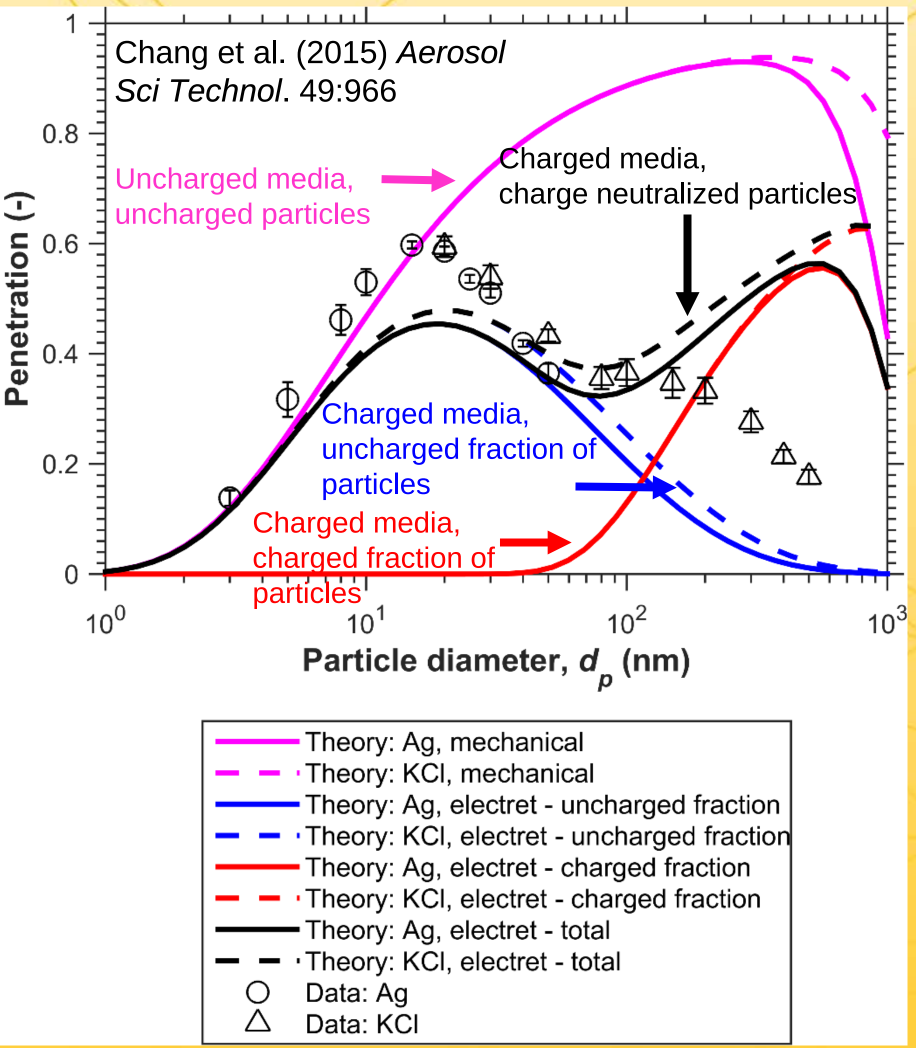
Image force

Charged particle induces charge in fiber

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



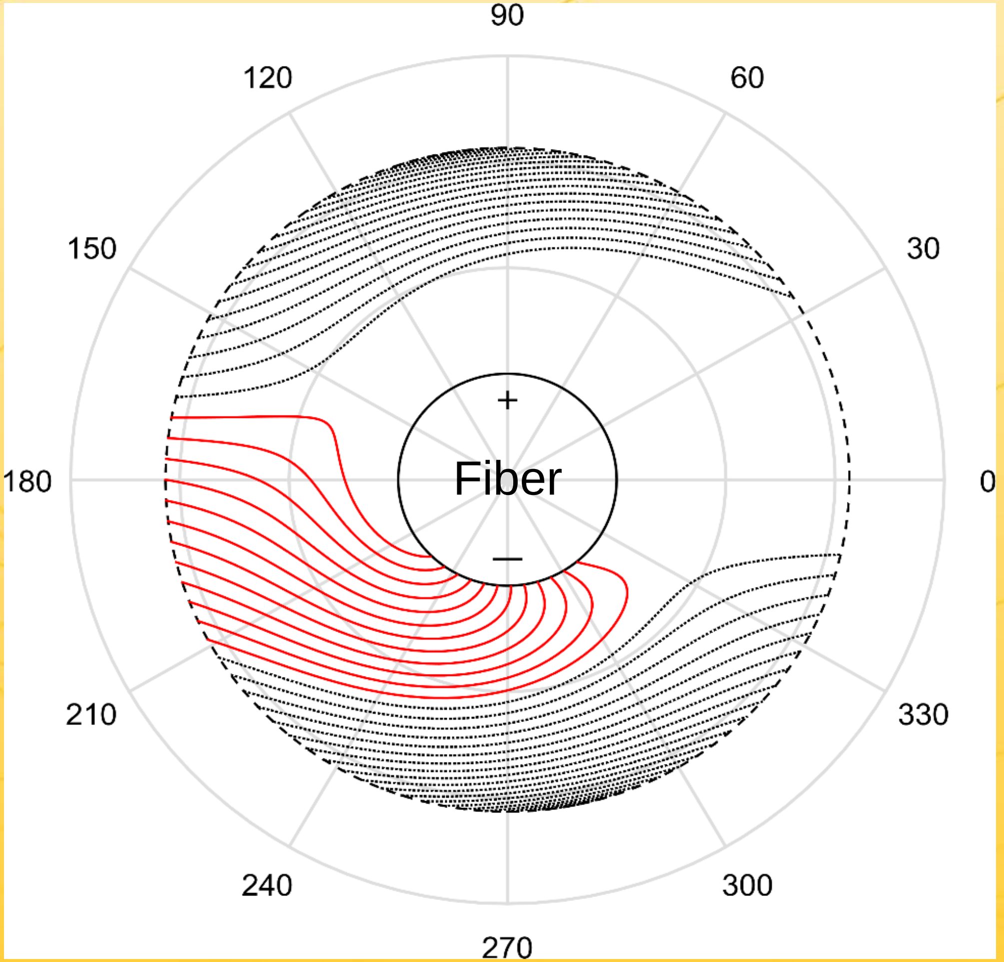
Motivation



- Disagreement between data and model previously used in Chang et al. (2015) for charge neutralized particles because polarization of charged particles was neglected
- Most models are derived considering one electrostatic force at a time and adding their respective efficiencies together
- Lee et al. (2002a,b) found this assumption no longer holds for higher charge densities (1.2 μC/m^2, 20x that studied by Otani et al.,1993) due to negative interaction between polarization and Coulombic forces
- 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 is needed which will account for interaction between electrostatic forces
- A user-friendly filter performance and design tool will utilize this new model

Method of limiting trajectories

- Limiting trajectory is the outermost trajectory a particle can travel and still be captured by the fiber
- Steps for calculating efficiency:
  1) Determine particle's equation of motion
  2) Find limiting trajectories
  3) Integrate particle flux between limiting trajectories



Calculation of particle trajectories

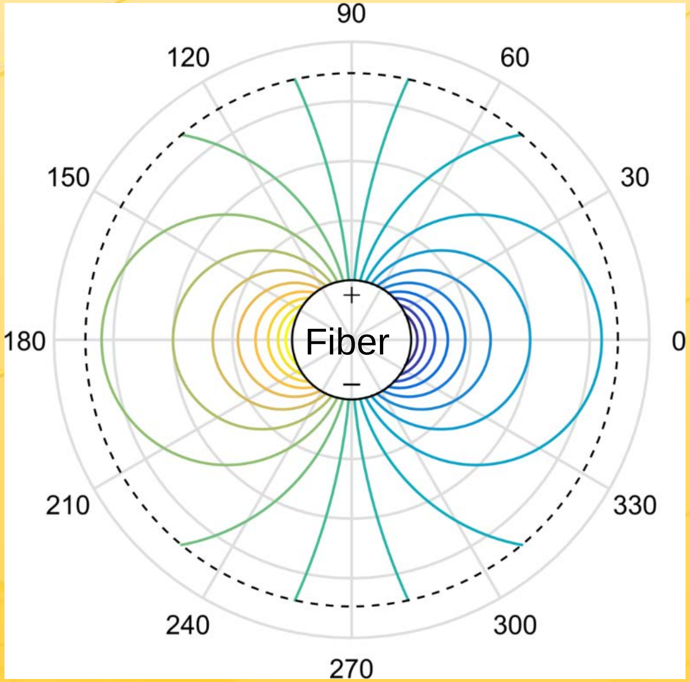
- Particle diffusion and inertia are neglected

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

- 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



Field lines for line-dipole charged fiber

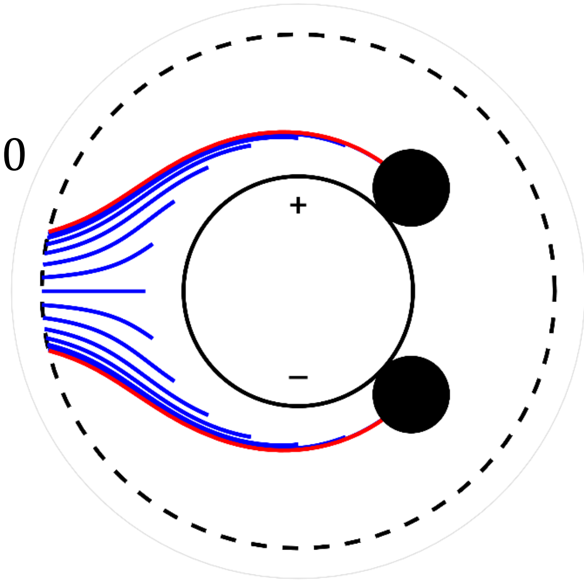
Finding limiting trajectories

- Identify potential limiting trajectories by looking for roots of $v_r\left(\frac{1}{2}d_f + \frac{1}{2}d_p, \theta_c\right)$ and $\vec{v}(r_c, \theta_c)$
- Limit model to cases were roots exist inside flow cell domain (e.g.,$v_r(b, 0) > 0$)
- Solve particle trajectories backwards from location of roots
- If particle reaches cell boundary, search forward trajectories starting on cell boundary until a particle misses the fiber and exits the cell
- Use binary search method between the nearest trajectories which collide and miss the fiber until the single fiber efficiency reaches a convergence criterion

Grazing trajectory

$$v_r\left(\tfrac{1}{2}d_f + \tfrac{1}{2}d_p, \theta_c\right) = 0$$

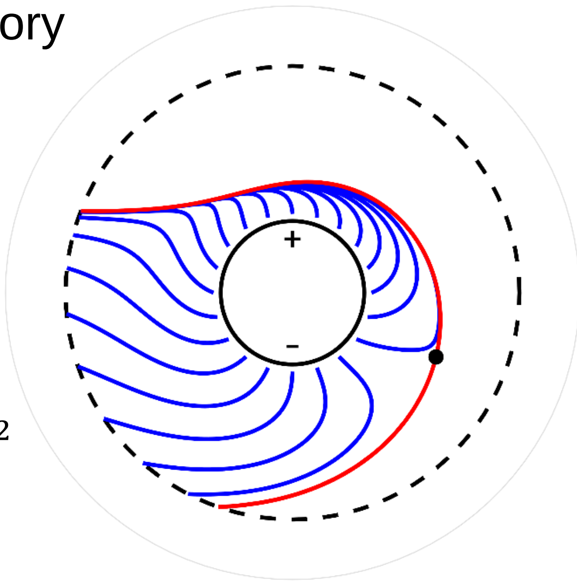
$d_p = 1\ \mu\text{m}$
$q = 0$
$d_f = 3\ \mu\text{m}$
$\sigma_0 = 100\ \mu\text{C/m}^2$
$\alpha = 0.2$
$U_0 = 100\ \text{cm/s}$



Critical trajectory

$$\vec{v}(r_c, \theta_c) = 0$$

$d_p = 0.5\ \mu\text{m}$
$q = 1e$
$d_f = 5\ \mu\text{m}$
$\sigma_0 = 100\ \mu\text{C/m}^2$
$\alpha = 0.1$
$U_0 = 1\ \text{cm/s}$

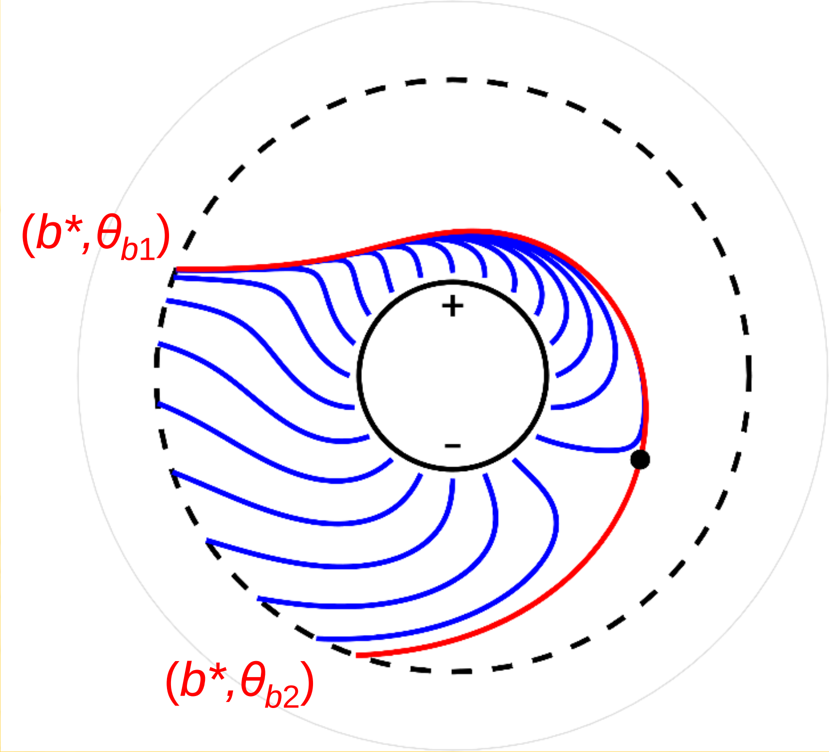


Calculation of single fiber efficiency

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

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

- Particle concentration between limiting streamlines is assumed to be uniform
- If $\theta_{b1} \leq \frac{\pi}{2}$ and $\theta_{b2} \geq \frac{3\pi}{2}$, all particles entering the cell are collected by the fiber. Depth filtration theory is then no longer valid, since all particles would be collected on the surface of the filter.



Forms of single fiber efficiency equation

Coulombic, polarization, and image forces

$\eta_{\sigma q}$ ⇒ 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

$\eta_{\sigma 0}$ ⇒ 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

$$N_R = \frac{d_p}{d_f}$$

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

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

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

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 filtration of nanoparticles

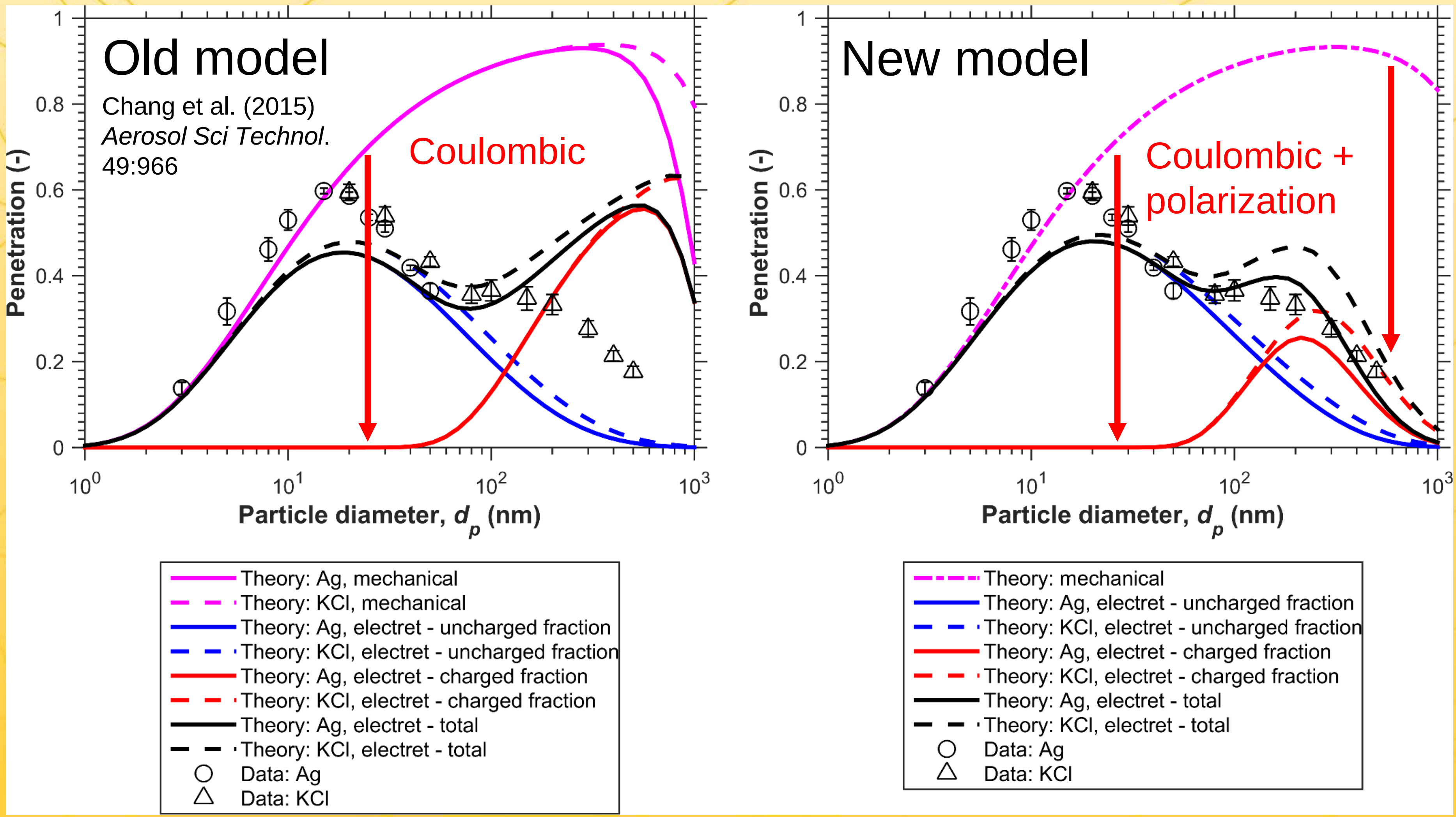
$$\eta_D = 0.84\left(\frac{d_f}{d_{f\Delta p}}\right)^{0.57} [(1-\alpha)Pe]^{-0.43}$$

- 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 Fraction of Particles



Development of a surrogate model from numerical results

- Obtain an surrogate model (or metamodel) for η_{det} from more expensive numerical results
- We will consider two model types: *k*-Nearest Neighbors and Gaussian Processes

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

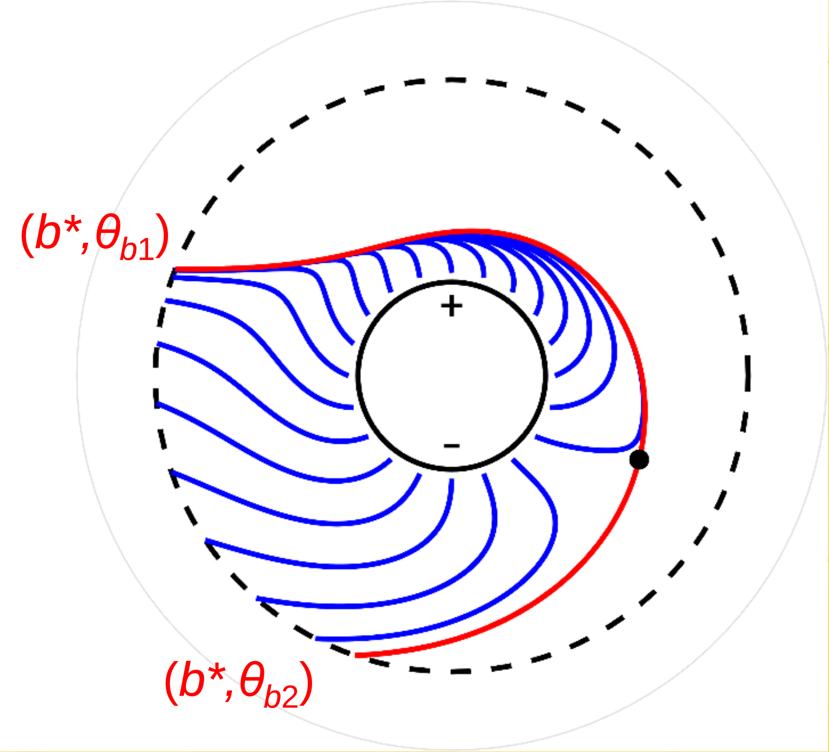
Parameter space

α = 0.01 ~ 0.25
N_R = 10^{-5} ~ 1
N_C = 0, 10^{-6} ~ 10^2
N_P = 10^{-7} ~ 10^5
N_I = 0, 10^{-11} ~ 10

Requirements of surrogate model

- Classification:
  - Determine whether, for the given input parameters, $\theta_{b1} \leq \frac{\pi}{2}$ and $\theta_{b2} \geq \frac{3\pi}{2}$. If so, depth filtration theory is no longer valid, since all particles would be collected on the surface of the filter, and the penetration is zero (effectively $\eta_{det} = \infty$)
- Regression:
  - If depth filtration theory is still valid, estimate η_{det} for the given input parameters

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



Training and testing of surrogate models

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

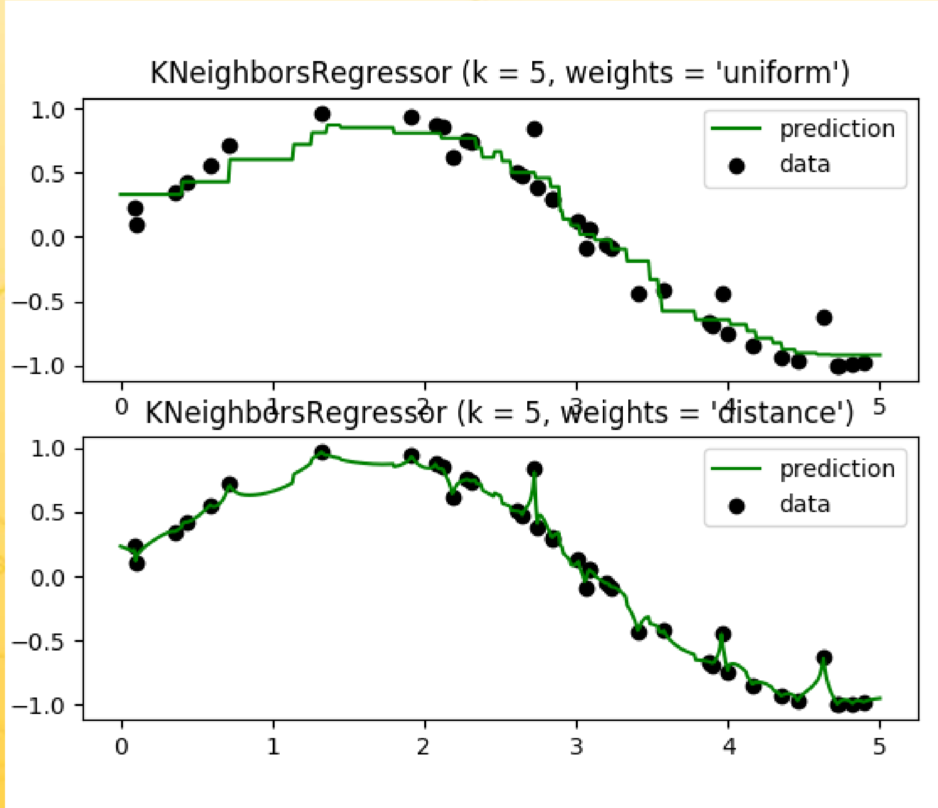
- Training data
  - 20 evenly logarithmically spaced points per decade (710k points total)
- Testing data
  - 73k random logarithmically spaced points

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

- Training data
  - 20 evenly logarithmically spaced points per decade for solidity, 1 point per decade for all other parameters (490k points total)
  - Grid was split into two regions: about 6% where $\eta_{\sigma q}$ was a constant with decreasing parameter values and the other 94%
  - 1.4M random logarithmically spaced points were added in the smaller, more variable region and 378k in the other region
- Testing data
  - 210k random logarithmically spaced points

k-nearest neighbors (*k*-NN)

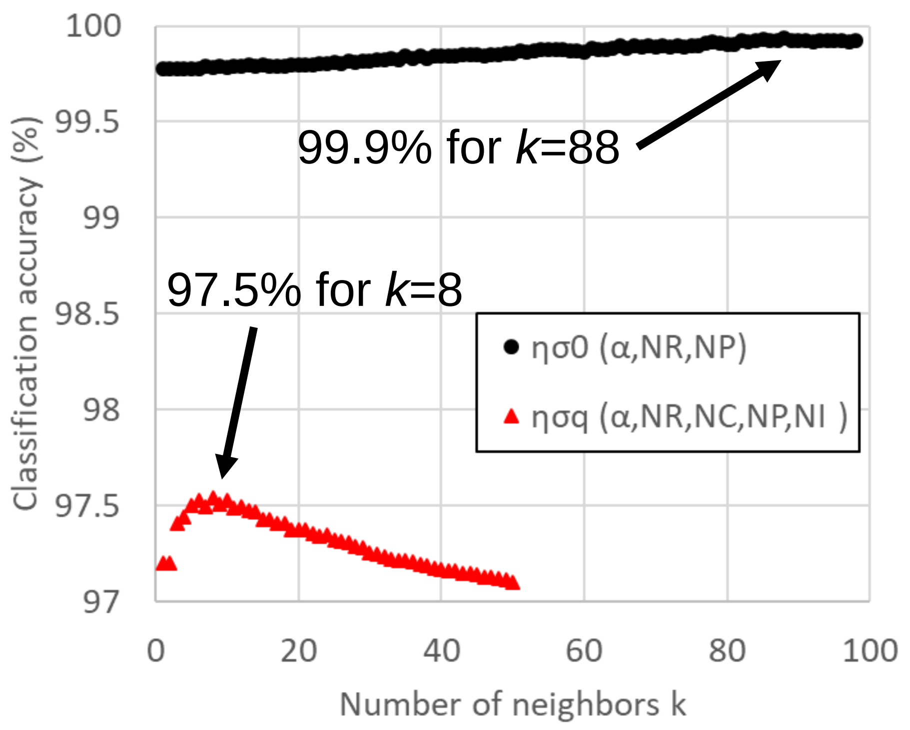
- Takes average value of the *k* number of nearest points
- Points are weighted by the inverse of the distance to the query point
- A *k*-dimensional tree is used to space-partition the data allowing for faster computations
- An optimum value for *k* must be found



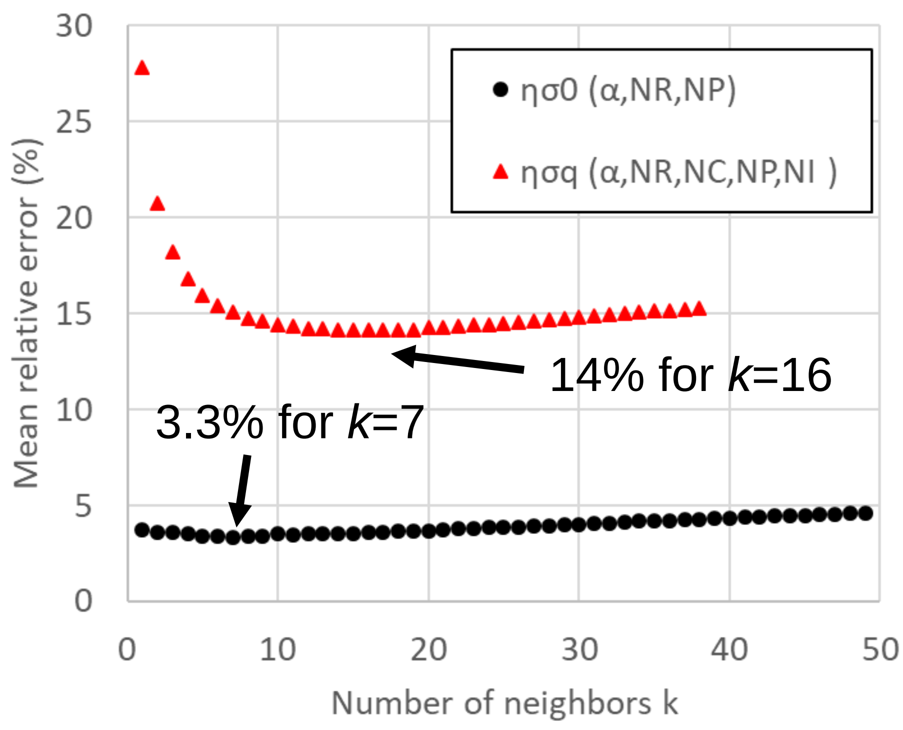
http://scikit-learn.org/stable/modules/neighbors.html

Optimization of the number of neighbors *k*

Classification

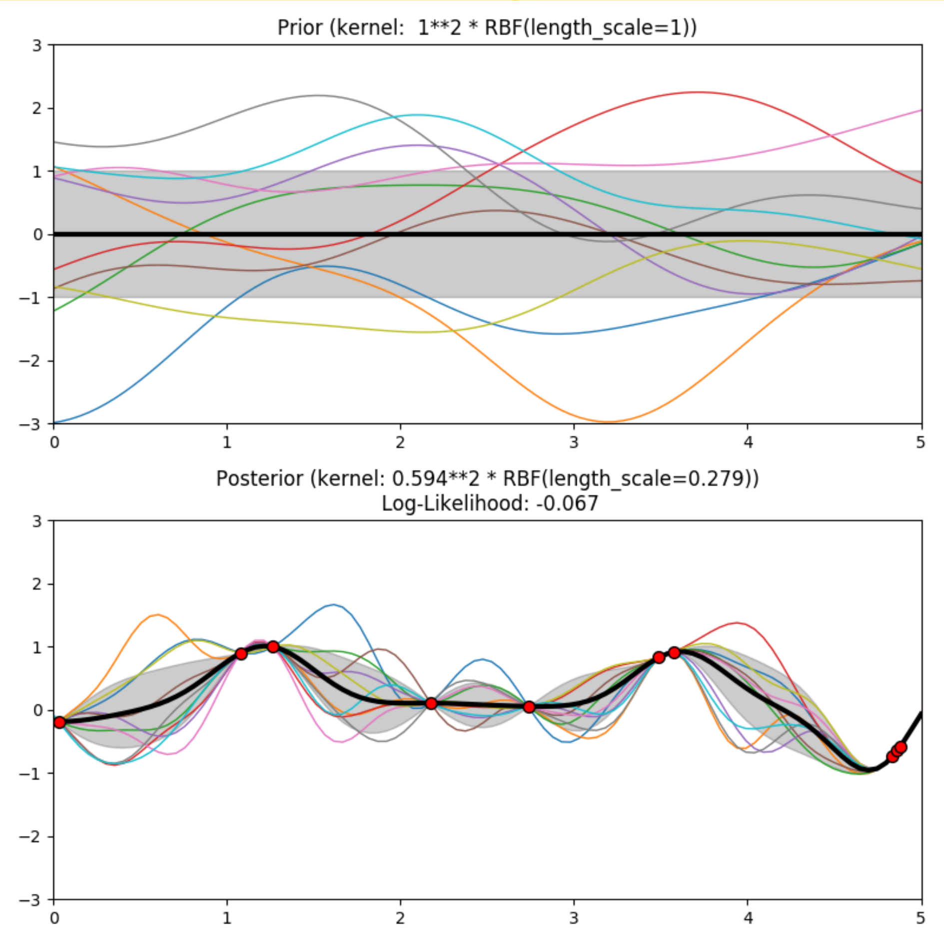


Regression



Gaussian process regression

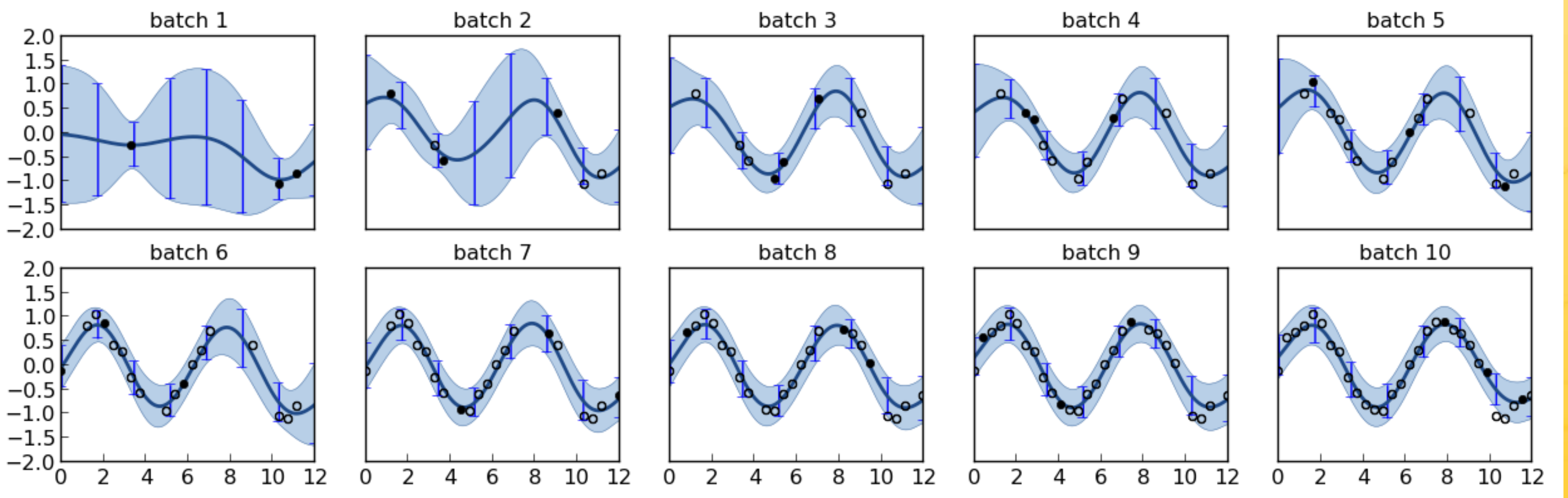
- Gaussian process regression can interpolate observations and compute empirical confidence intervals
- An arbitrary function is viewed as a realization of a random process
- Function is estimated by modeling the covariance of each point with every other point
- To predict the function at a new point, based on the covariance estimated from training data, an optimal weighted linear combination of the training points is taken
- A covariance function, a.k.a. kernel function, must be chosen by user



http://scikit-learn.org/stable/modules/gaussian_process.html

Stochastic variational inference for GPs

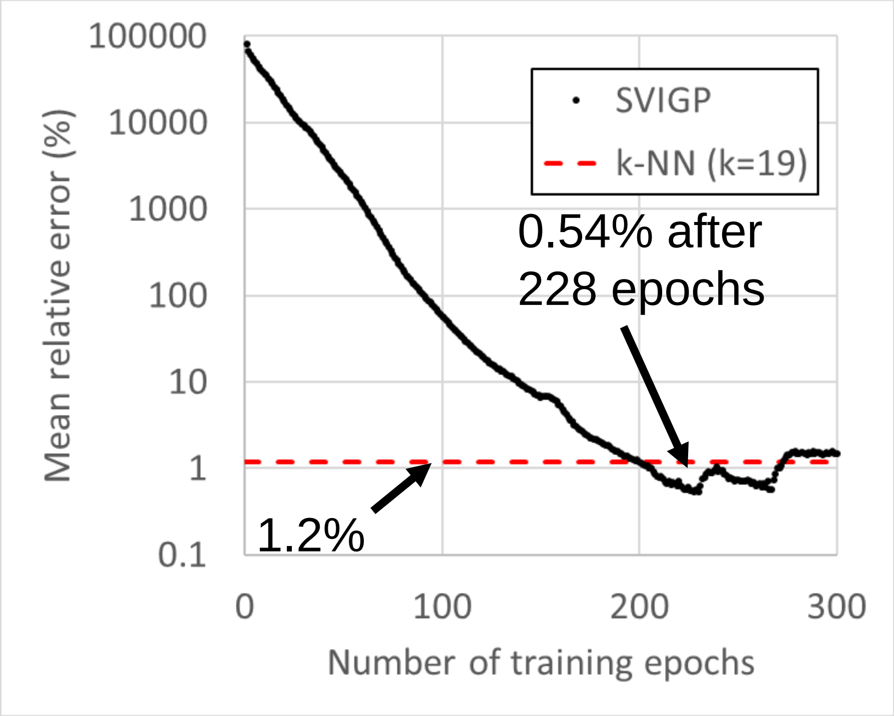
- Traditional Gaussian process regression can typically only handle datasets with fewer than 10k points due to memory limitations
- Hensman et al. (2013) outlined Gaussian processes for Big Data and the results are included in the Stochastic Variational Inference model in GPy (SVIGP) which allows optimization by mini-batch stochastic gradient descent
- This was extended to classification, as well (Hensman et al, 2015)



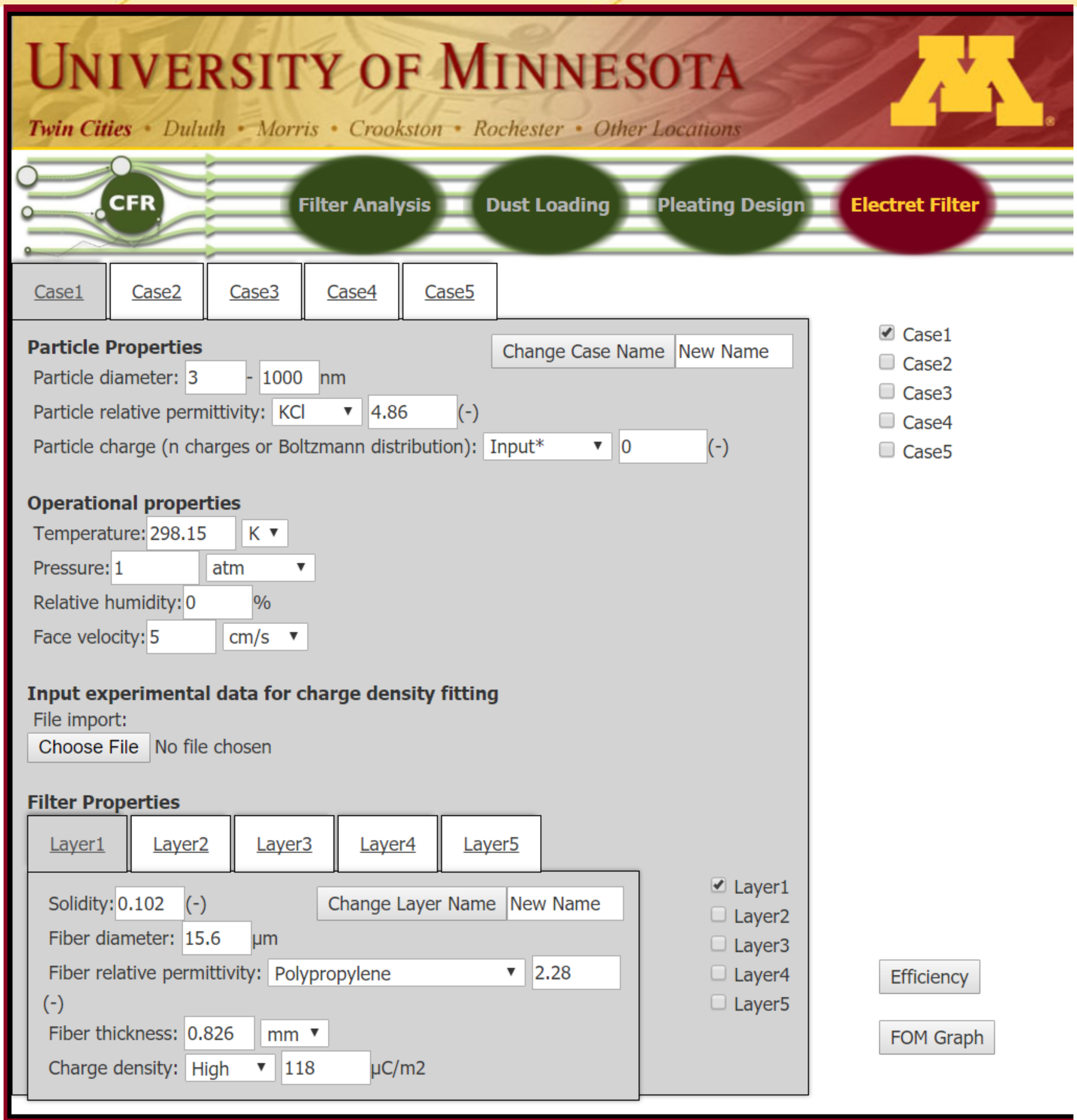
Stochastic variational inference on a trivial GP regression problem. Each pane shows the posterior of the GP after a batch of data, marked as solid points. Previously seen (and discarded) data are marked as empty points, the distribution q(u) is represented by vertical errorbars (Hensman et al., 2013)

SVIGP convergence history for $\eta_P(\alpha, N_P)$

- SVIGP regression outperformed *k*-NN for the simplified case of $\eta_P(\alpha, N_P)$, the collection of uncharged particles where the particle is assumed to be a point mass
- The kernel function was composed of a Radial Basis Function (RBF), with length scale parameters in $\alpha -$ and $N_P -$ directions, a bias function to account for the non-zero mean, and Gaussian white noise
- Work on SVIGP regression for $\eta_{\sigma 0}(\alpha, N_R, N_P)$ and $\eta_{\sigma q}(\alpha, N_R, N_C, N_P, N_I)$ is ongoing



Interface of web-based model



Future work

- Launch current version of website where k-NN is used for surrogate modeling
- Collect additional numerical data for $\eta_{\sigma q}(\alpha, N_R, N_C, N_P, N_I)$ in areas with high estimation error
- Use SVIGP classification and regression to obtain more accurate surrogate models for $\eta_{\sigma 0}(\alpha, N_R, N_P)$ and $\eta_{\sigma q}(\alpha, N_R, N_C, N_P, N_I)$ and update website
- Add functionality to model in order to:
  - Fit a charge density from experimental fractional efficiency data
  - Input relative humidity which will adjust gas properties of dielectric constant, viscosity, and mean free path

Acknowledgements

The authors thank the support of members of the Center for Filtration Research: 3M Co., A.O. Smith, Applied Materials, BASF Corp., Boeing Commercial Airplanes, Corning Incorporated, Cummins Filtration, Donaldson Co., Inc., Entegris Inc., Ford Motor Co., Gore, MSP Corp., Samsung Electronics Co., Ltd., Shengda Filtration Technology Co., Ltd., Shigematsu Works Co., Ltd., TSI Inc., WatYuan Filtration System Co., Ltd., Yancheng Environmental Protection Science and Technology City and affiliate member National Institute for Occupational Safety and Health.

Thank you for your attention

Questions and/or comments:
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