Electrode Interface Design for High-accuracy Size Distribution Measurement of Aerosol Nanoparticles using Electrical Mobility Spectrometer Integrated with Triplet Charger

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Introduction

- Application of nanoparticles classification and measurement is ubiquitous in scientific and industrial fields. Accurate size distribution measurement of a wide spectrum of polydisperse nanoparticles is quite challenging. On the left side of the size spectrum, Brownian motions of ions and ultrafine particles, and on the right side, multiple charging phenomena or non-uniformity of charge distributions account for this difficulty.

- The present study employs Computational Fluid Dynamics (CFD) simulations of Electrical Mobility Spectrometer (EMS) integrated with a corona charger, and particle tracking method, to map regions in the classifying section of the instrument targeted by particles with the highest probabilities. This gives the signals (charges) which can be potentially transferred to electrometers by particles, through landing on the detectors connected to the electrometers. In a traditional EMS, detectors are identical electrode rings placed sequentially in the classifying section. Fig. 1. Schematically illustrates the typical of EMS.

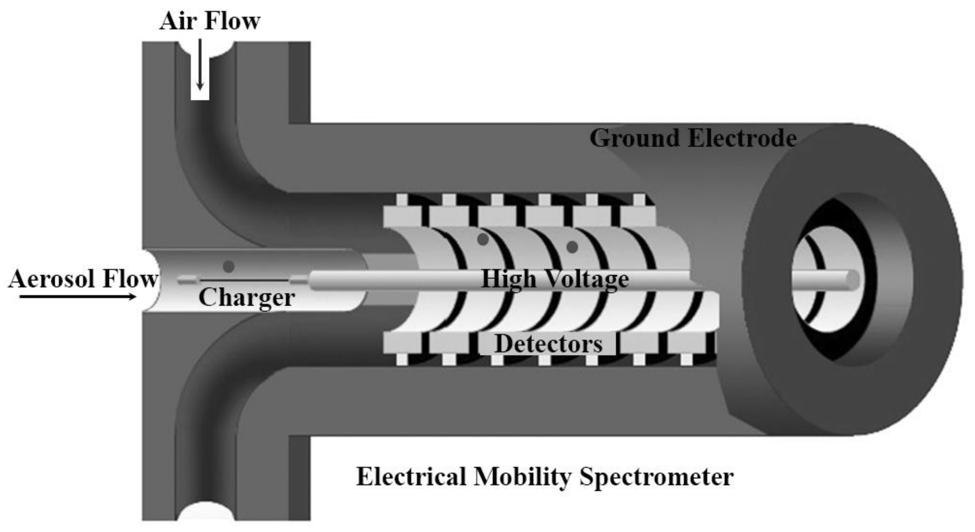

Figure 1. Schematic view of an Electrical Mobility Spectrometer (EMS). Corona charger is installed upstream and the flow is provided with clean sheath air before entering the measurement zone.

- Configuration of the detectors has direct impact on the transfer matrix of the instrument and therefore accuracy of the measurements. This work bridges the gap between data interpretation and uncertainties dictated by underlying physics; Feeding CFD results into Genetic Algorithm (GA), optimal configuration of electrodes (called interface) is found, corresponding to the transfer matrix with the highest rank and entropy. This matrix transfers maximum information possible, about size distributions of injected particles.

Transfer Matrix and Data Interpretation

Transfer matrix contains a vector signal for every monodisperse diameter in the spectrum, given by the set of electrodes. Any size distribution can be reconstructed by a linear combination of these vectors. Consider a polydisperse (in size) calibrating aerosol with concentration N^c (a continuous concentration function of diameter). Assume we divide the size distribution into J mono-disperse classes of diameter d_j and treat each class independently. Therefore we can easily find concentration in each size class, N_j^c (scalar). For an EMS with K channels (electrometers):

1- If particles of a mono-disperse aerosol of size d_j are introduced into the device, a signal vector of K elements ($\boldsymbol{I}_j$) is produced where,

$$\boldsymbol{I}_j = [i_{1j} \dots i_{kj} \dots i_{Kj}]^T \qquad (1)$$

2- If a poly-disperse aerosol is introduced, a signal vector ($\boldsymbol{I}$) of the same length (K) is produced which is the sum of the signal vectors produced by each size class ($\boldsymbol{I}=\sum_j \boldsymbol{I}_j$).

3- The signal strength is proportional to the concentration with factor a_j. Therefore the signal produced by any other concentration is linearly related to the signal produced by calibrating aerosol.

$$N_j = a_j . N_j^c \quad => \quad \boldsymbol{I}_j = a_j . \boldsymbol{I}_j^c \qquad (2)$$

Mathematical representation of the three above statements in the matrix form reads:

$$\begin{bmatrix} i_{11}^c & \cdots & i_{1J}^c \\ \vdots & \ddots & \vdots \\ i_{K1}^c & \cdots & i_{KJ}^c \end{bmatrix} . \begin{bmatrix} a_1 \\ \vdots \\ a_J \end{bmatrix} = \begin{bmatrix} i_1 \\ \vdots \\ i_K \end{bmatrix} \rightarrow \boldsymbol{F}.\boldsymbol{N} = \boldsymbol{I} \qquad (3)$$

where $\boldsymbol{F}$ is called transfer matrix of the EMS, $\boldsymbol{N}$ contains size distribution of injected particles and $\boldsymbol{I}$ is the signal read by electrometers as a vector.

Now, estimated size distribution of injected particles is given by inversion of data ($\boldsymbol{N}_{est}=\boldsymbol{F}^{-1}.\boldsymbol{I}$) or for an underdetermined system is given by:

$$\boldsymbol{N}_{est} = (\boldsymbol{F}^T\boldsymbol{F} + \lambda \boldsymbol{D}^T\boldsymbol{D})^{-1}\boldsymbol{F}^T\boldsymbol{I} \qquad (4)$$

Here, λ is a positive real number as regularization factor and smoothing matrix $\boldsymbol{D}$ is a sparse matrix defined as:

$$\boldsymbol{D} = \begin{bmatrix} 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix}_{J-2\times J} \qquad (5)$$

With this definition, a transfer matrix with higher rank gives more accurate size distributions.

Steps and Methods

1- Numerical simulation of Corona discharge in the charger to estimate space charge density in the charging chamber. This includes Maxwell's equations, charge transport equation, Navier-Stokes and continuity equations.

2- Numerical simulation of aerosol charging due to Diffusion and Brownian motions using birth-and-death theory and estimation of charge distributions on each mono-disperse class d_j.

3- CFD simulation of EMS and particle tracking in the classifier to map landing positions of particles holding different number of charges and to obtain the map of charges (or currents) transferred to the electrometers for each class d_j.

4- Configuration of electrodes means physical location of electrodes under the map of currents. Different configuration means different vector, transferred and reported by electrometers. Transfer matrix is obtained by releasing calibrating aerosol spanning the entire size spectrum, and recording the signals given in each size d_j.

5- Using GA, random electrode configurations are produced to obtain corresponding transfer matrices. The objective is to find a matrix with highest possible rank and maximum entropy.

CFD Simulation and Particle Trajectories

Following diagrams (Fig. 2) depict particle trajectories in the classifying section (cylinder) for three size samples d_j equal to 100, 300 and 500 nm. The monochromatic images (left column) show the map of concentrations or probabilities in each class. Darker means higher concentration. Fig. 3. gives the map of landing positions and particle diameters, colored by the fraction per nanometer. For example, roughly 27 % of all 300 nm particles (d_j) land at distance of approximately 20 cm from inlet marked as the red dot. Velocity field and sample trajectories in 3D are shown in Fig. 4 and Fig. 5.

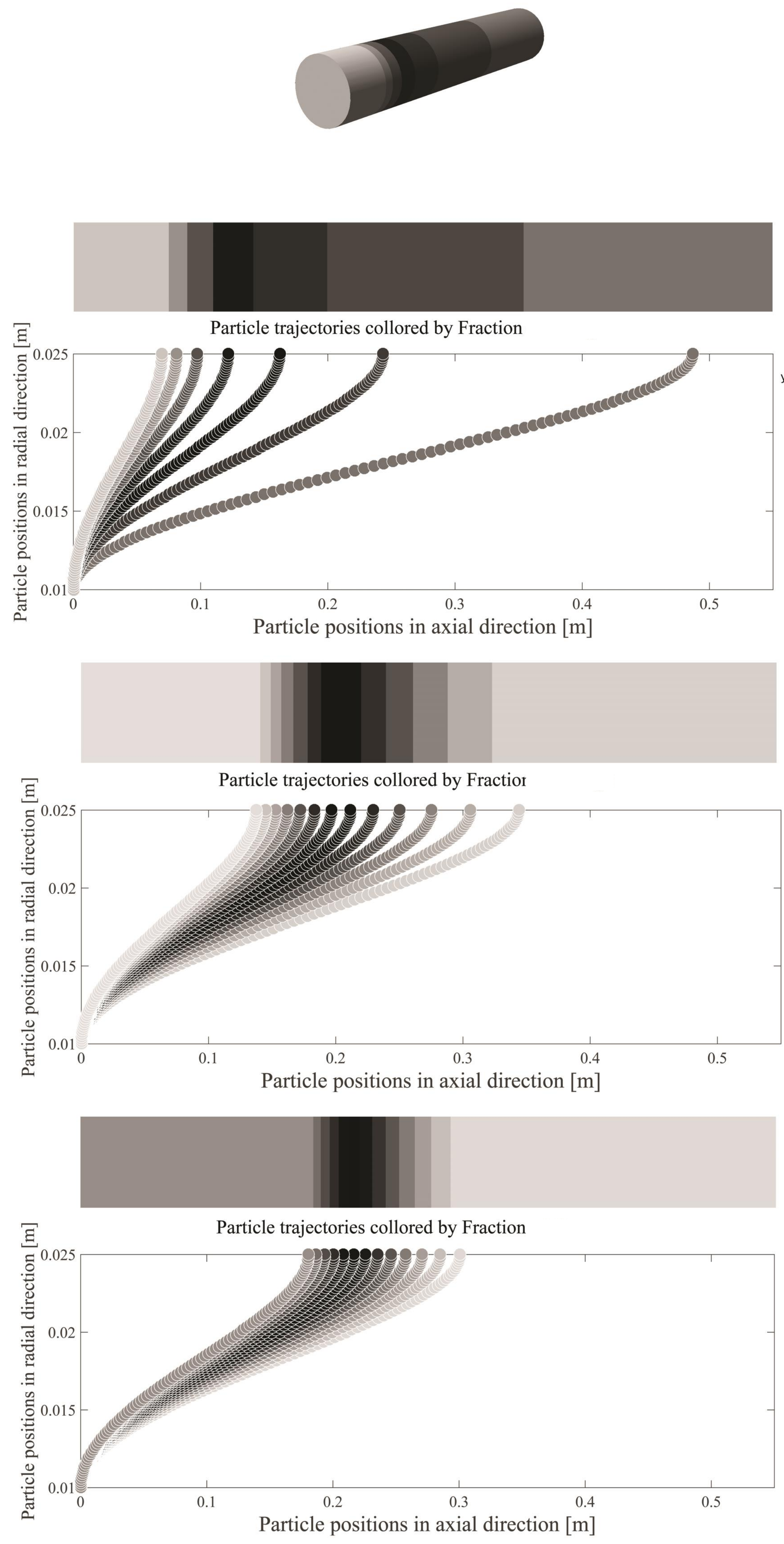

Figure 2. 2D axisymmetric view of particle trajectories for 100nm (first), 300nm (second), and 500nm (third), with different charge distributions

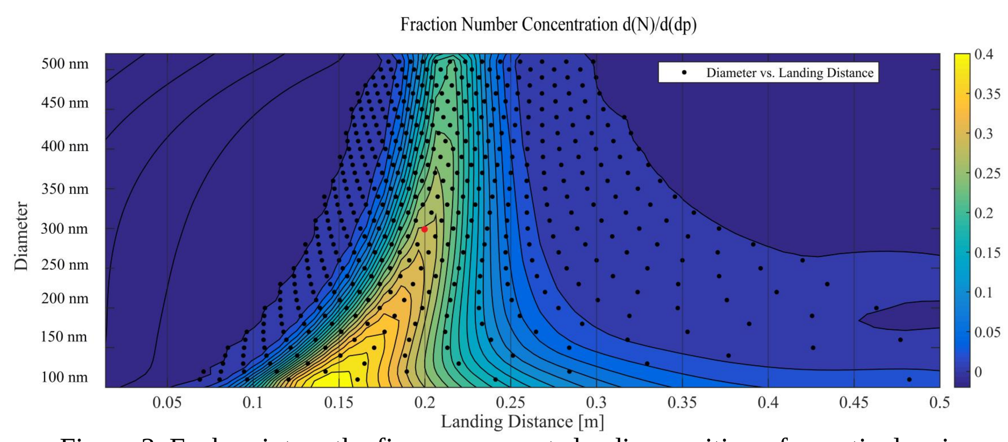

Figure 3. Each point on the figure represents landing position of a particular size particle and the color at that point indicates the fraction of the particles of that size landing at that particular distance

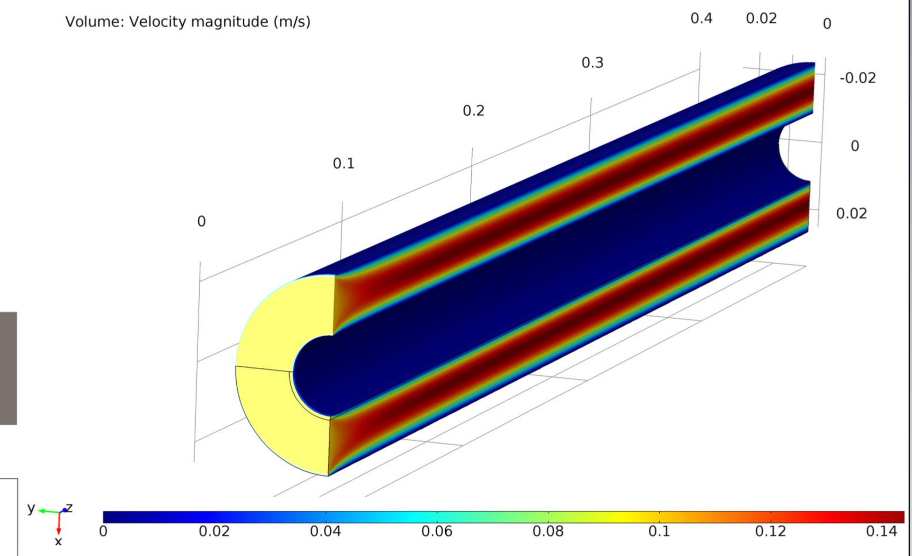

Figure 4. Velocity field in the classifying section

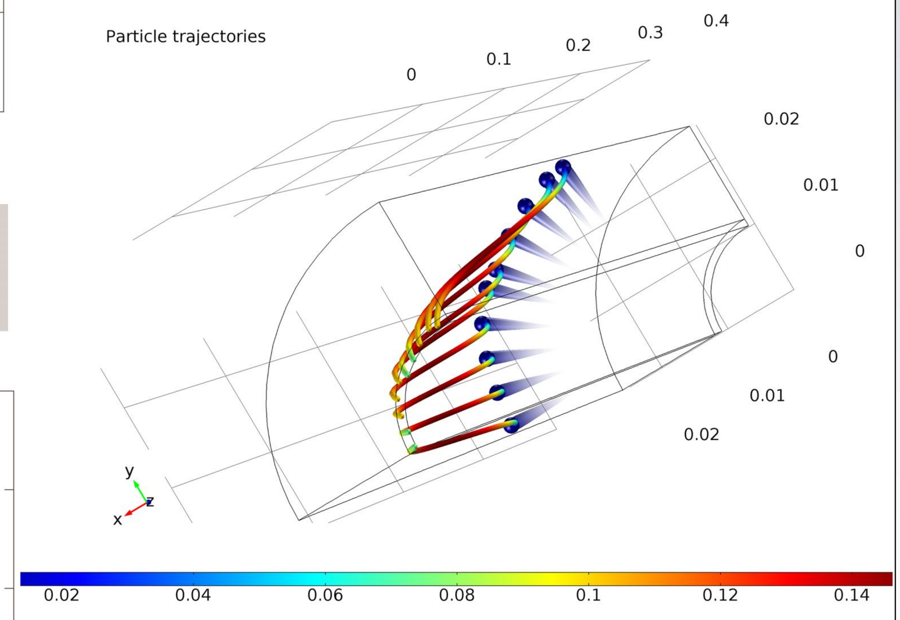

Figure 5. Particle trajectories in ¼ of the Geometry

Entropy of the Transfer matrix or GA's Objective

The singular value decomposition (SVD) of the matrix F is in the form:

$$\boldsymbol{F} = \boldsymbol{USV}^T \qquad (6)$$

where the columns of $\boldsymbol{U}$ are left singular vectors of $\boldsymbol{F}$ or orthonormal eigenvectors of $\boldsymbol{FF}^T$, the columns of $\boldsymbol{V}$ are right singular vectors of $\boldsymbol{F}$ or orthonormal eigenvectors of $\boldsymbol{F}^T\boldsymbol{F}$ and $\boldsymbol{S}$ is a diagonal matrix containing n singular values of $\boldsymbol{F}$ or square roots of eigenvalues (λi) of $\boldsymbol{F}^T\boldsymbol{F}$ in descending order.

Objective function of GA is the entropy of transfer matrix $\boldsymbol{F}$ defined by:

$$H_F = -\sum_{j=1}^{n} \frac{\sqrt{\lambda_j}}{\sum \sqrt{\lambda_i}} \ln \frac{\sqrt{\lambda_j}}{\sum \sqrt{\lambda_i}} \qquad (7)$$

Why more than one charger?!

As it is evident according to depictions, probability of landing increases as particles travel along the cylinder and then decreases until a very small fraction escape from the instrument. Concentrating the electrodes in the regions with high probability of landing results in producing a transfer matrix with higher entropy and therefore more accurate size distribution estimation. Since width of the aerosol inlet decreases the resolution of the instrument and imposes limits on the size of electrodes, instead of decreasing beyond the resolution limit, increasing the number of electrodes peripherally in angular direction (as apposed to axial direction), and dividing the aerosol inlet into the number of chargers (with different charging conditions) compensate the limitations in axial direction and increases the accuracy of size distribution measurements. Fig. 6 shows three corona chargers, division of aerosol inlet and optimum configuration of electrodes called interface.

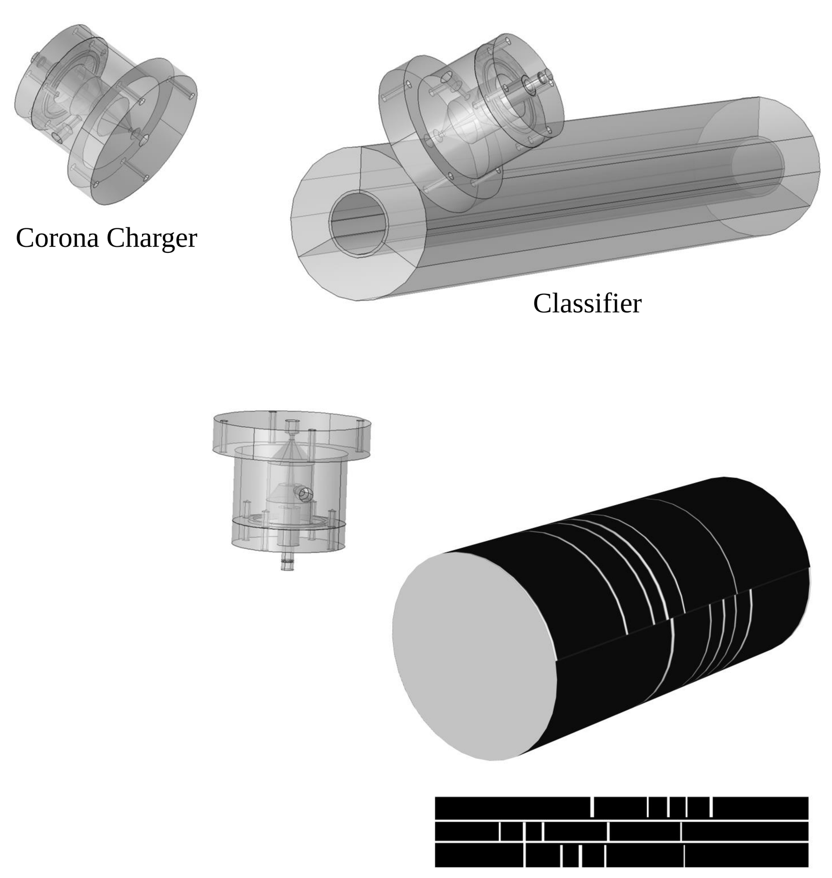

Figure 6. Schematic of three chargers and optimized electrode configuration

Conclusions

According to Shannon's information theory, This transfer matrix of optimized electrode configuration transfers maximum information possible, about size distributions of injected particles. Utilizing a triplet charger (with three different charging conditions) can add more information to the system, and lead to more accurate measurements if well-chosen electrode interface is embodied. Incorporating the electrode interface, not only helps for gaining more accurate measurements, but reduces computational costs of data interpretations, as well.

ETHzürich 20th ETH-Conference on Combustion Generated Nanoparticles June 13th – 16st 2016