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BAYESIAN INFERENCE APPLIED TO A CFD-GENERATED DATABASE FOR CALIBRATION OF ELECTRICAL MOBILITY SPECTROMETER (EMS) AND SIZE DISTRIBUTION MEASUREMENT OF PARTICLES

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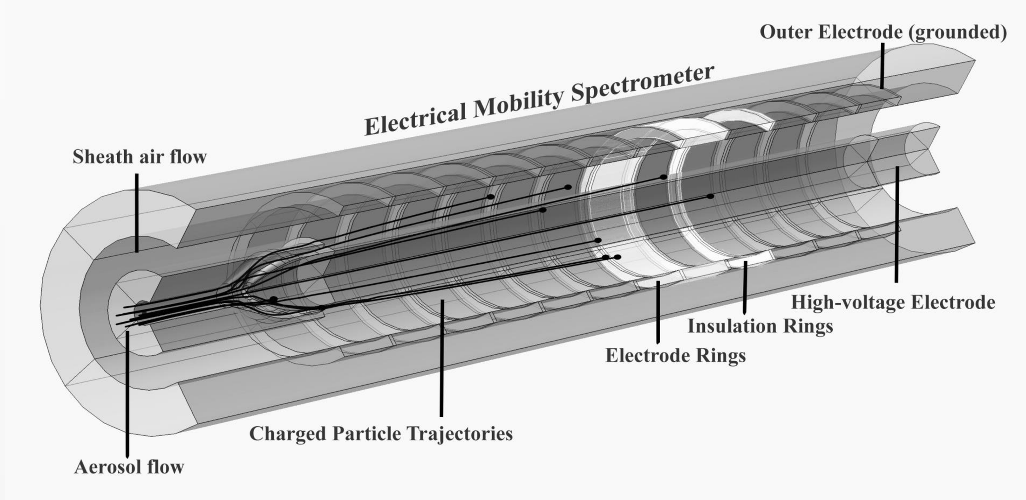
INTRODUCTION

Among the existing methods proposed for size distribution measurements, the most prevalent is on the basis of electrical mobility. Electrical mobility, a function of particle diameter and charge, defines the ability of charged particles to move through a medium in response to an electric field. Knowing induced charge on a particle and its electrical mobility reveals the size of particle. Electrical Mobility Spectrometers (EMSs) are instruments by which aerosol nano particles are classified according to their electrical mobility. Thereupon, size distribution of particles can be determined inversely by inversion of electrical mobility spectra to size spectra.

In this method, aerosol passes through a charger before entering an analyzer (EMS).The EMS has a short column, made of two concentric cylindrical electrodes. The electric field is created by maintaining the central electrode rod at a high voltage while the outer electrode is grounded. A number of electrometer rings are laid along the outer cylinder separated from each other by insulating gaps. Charged particles are routed to the classifier and accelerated to land on detecting rings due to the electric force pushing them away from the central rod. The electric current delivered to the electrometers and recorded as signal ***I*** implies the landing position and particles concentration. The landing position is affected by the geometry, flow characteristics and operating condition of the instrument, as well as charge and diameter of the particle. Knowing the landing position is equivalent of knowing electrical mobility and hence, charge-diameter relation. If the exact induced charge is known, the diameter (hence the size spectrum ***S***(d)) can be easily calculated from signal ***I***. However, because of uncertainties in the instrument and charging process which by itself is random and subjected to probabilities, the induced charge cannot be defined exactly. This makes the signal ***I*** received by each size class fuzzy, and inversion of signal to size spectrum ***S***(d) unstraightforward and ill posed. An schematic EMS is illustrated in Fig. 1.

FIGURE 1. Classification of particles in an EMS



OVERVIEW - OBJECTIVE

In this study, based on Bayesian interpretation, a procedure for inversion of mobility distribution to size distribution is proposed to elevate the accuracy of inversion through a priori knowledge on size distribution of injected particles and instrument responding behavior captured by Computational Fluid Dynamics (CFD) analysis. A database containing size distributions of injected particles and corresponding mobility distributions reported by the classifier is constructed from tracking 10000 particles of poly-disperse size. The instrument responding behavior which is controlled by the transfer function of the instrument, normally acquired through calibration of the device, is captured and obtained by the CFD-generated database. The focus in the present work was on derivation of governing equations for size distribution prediction based on Bayesian statistical framework. Through Bayesian analysis, we predicted size distributions from transferred signals (constructed by injection of particles) and compared our predictions to the exact size distributions. Subsequently, we discussed the sensitivity and accuracy of the predictions with respect to the number of detectors.

INVERSION OF MOBILITY SPECTRUM TO SIZE SPECTRUM

An Inverse problem is the process of obtaining the causal factors called unknown quantities from a set of observations or known quantities which are usually indirect, limited and noisy. The inverse problem (usually ill-posed) is considered the "opposite" of the forward problem (well-posed) by which the model parameters are directly (explicitly) related to the data that we observe. The inverse problem by which the data are transformed to the model parameters is formulated schematically as:

$$\text{Data} \xrightarrow{\text{Transformation}} \text{Model parameters (unknowns)}$$

The transformation from data to model parameters (or vice versa, in the forward problem), is formed through the interaction of a physical system with the object that we want to infer some unknown quantities about. For example, in size distribution measurements of aerosol, the transformation is the process of charge transfer from injected particles to the detectors, the data is the electrometers' signals (electrical mobility spectrum) and the model parameters are parameters of the interest or size spectrum. In this inverse problem, a quantity $\boldsymbol{I} \in \mathbb{R}^K$ is measured (observations) in order to get information about the unknown quantity $\boldsymbol{s} \in \mathbb{R}^n$. An explicit model or data prediction model is required to relate the known ($\boldsymbol{I}$) and unknown ($\boldsymbol{s}$) quantities by:

$$\boldsymbol{I} = \boldsymbol{f}(\boldsymbol{s}, \boldsymbol{\epsilon}) \qquad (1)$$

where $\boldsymbol{f}: \mathbb{R}^n \times \mathbb{R}^{K'} \rightarrow \mathbb{R}^K$ is the model function called transfer function, operator or generative model and $\boldsymbol{\epsilon} \in \mathbb{R}^{K'}$ is a noise vector accounting for the model uncertainties as well as measurement inaccuracies. The inverse problem tries to retrieve the quantity $\boldsymbol{s}$ from the observation $\boldsymbol{I}$ through inversion of the transformation. At the core of this inversion stands the transfer function $\boldsymbol{F}$ of the instrument, by which the size spectrum as a vector is inversely obtained from EMS-reported signal vector $\boldsymbol{I}$ (mobility spectrum). Assuming a continuous size spectrum function $S(d)$, $\boldsymbol{s}$ is defined as the discrete size spectrum function or the spectrum vector and each member s_i represents a discrete number concentration corresponding to a discrete diameter. Therefore the total number concentration from diameter d_1 to d_n can be obtained by the integral $\int_{d_1}^{d_n} S(d)\mathrm{d}d$.

MATHEMATICAL REPRESENTATION IN BAYESIAN FRAMEWORK

Given the transfer function of the instrument and K detectors' response, the size spectrum vector or size distribution of injected aerosol with n discretized classes (of diameter) can be obtained by inversion of the following general relation:

$$\boldsymbol{I} = \boldsymbol{f}(\boldsymbol{s}, \boldsymbol{\epsilon}) \xrightarrow{\text{linear discrete form}} \begin{bmatrix} i_1 \\ \vdots \\ i_K \end{bmatrix} = \begin{bmatrix} F_{11} & \cdots & F_{1n} \\ \vdots & \ddots & \vdots \\ F_{K1} & \cdots & F_{Kn} \end{bmatrix} \begin{bmatrix} s_1 \\ \vdots \\ s_n \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_K \end{bmatrix} \qquad (2)$$

where a general rule $\boldsymbol{f}$ as the transfer function of the instrument acts on $\boldsymbol{s}$, the size spectrum vector to generate detectors' current vector $\boldsymbol{I}$ (i.e. the mobility spectrum) within the error term or instrument noise $\boldsymbol{\epsilon} = \mathcal{N}(\boldsymbol{\mu}_e, \boldsymbol{\Sigma}_e)$.

Bayes' theorem predicts the parameters $\boldsymbol{w}$ (called weights) given the set of data $\boldsymbol{D}$, by maximizing the posterior probability of parameters $P(\boldsymbol{w} \mid \boldsymbol{D})$ through the following relation:

$$P(\boldsymbol{w} \mid \boldsymbol{D}) = \frac{P(\boldsymbol{w})\, P(\boldsymbol{D} \mid \boldsymbol{w})}{P(\boldsymbol{D})} \qquad (3)$$

where $\boldsymbol{w}$ are unknown parameters of size distribution function, and $\boldsymbol{D}$ are measured vectors $\boldsymbol{I}$. The Bayes theorem predicts the parameters based on the likelihood $P(\boldsymbol{D} \mid \boldsymbol{w})$ (the probability of the measured currents given a set of parameters) and the priori information about the parameters $P(\boldsymbol{w})$. The posterior probability distribution is the solution of the inverse problem (Bayesian inverse model).

GOVERNED EQUATIONS FOR SIZE MEASUREMENTS AND SENSITIVITY ANALYSIS

The posterior probability of parameters assuming multimodal Gaussian size distribution $\boldsymbol{s}_{\mathcal{N}}$

$$P(\boldsymbol{w} \mid \boldsymbol{D}) = P(\boldsymbol{I}' \mid \boldsymbol{I}, \boldsymbol{\epsilon}) \propto \exp\left(\frac{-1}{2}(\boldsymbol{w} - \bar{\boldsymbol{w}})^T \boldsymbol{\Sigma_p}^{-1} (\boldsymbol{w} - \bar{\boldsymbol{w}}) + \frac{-1}{2}(\boldsymbol{I} - \boldsymbol{F}\boldsymbol{s}_{\mathcal{N}})^T \boldsymbol{\Sigma_e}^{-1} (\boldsymbol{I} - \boldsymbol{F}\boldsymbol{s}_{\mathcal{N}})\right) \qquad (4)$$

The posterior probability of parameters without any assumptions on distribution $\boldsymbol{s}$

$$\boldsymbol{P}(\boldsymbol{I}' \mid \boldsymbol{I}, \boldsymbol{\epsilon}) \propto \mathcal{N}(\boldsymbol{s} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{N}\left(\boldsymbol{s} \,\middle|\, \left(\boldsymbol{F^T}\boldsymbol{\Sigma_e}^{-1}\boldsymbol{F} + \boldsymbol{\Sigma_p}^{-1}\right)^{-1} \left(\boldsymbol{F^T}\boldsymbol{\Sigma_e}^{-1}\boldsymbol{I} + \boldsymbol{\Sigma_p}^{-1}\bar{\boldsymbol{s}}\right), \left(\boldsymbol{F^T}\boldsymbol{\Sigma_e}^{-1}\boldsymbol{F} + \boldsymbol{\Sigma_p}^{-1}\right)^{-1}\right) \qquad (5)$$

$$= \exp\left(\frac{-1}{2}(\boldsymbol{s} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{s} - \boldsymbol{\mu})\right)$$

$$\boldsymbol{\mu} = \bar{\boldsymbol{s}} + \boldsymbol{\Sigma_p}\boldsymbol{F^T}\left(\boldsymbol{F}\boldsymbol{\Sigma_p}\boldsymbol{F^T} + \boldsymbol{\Sigma_e}\right)^{-1}(\boldsymbol{I} - \boldsymbol{F}\bar{\boldsymbol{s}})$$

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma_p} - \boldsymbol{\Sigma_p}\boldsymbol{F^T}\left(\boldsymbol{F}\boldsymbol{\Sigma_p}\boldsymbol{F^T} + \boldsymbol{\Sigma_e}\right)^{-1}\boldsymbol{F}\boldsymbol{\Sigma_p}$$

COLIBRATION EQUATIONS

Each surface f can be approximated by a superposition of a number of bivariate Gaussian functions g_m within error ϵ_f as:

$$f_j\left(\begin{bmatrix} V \\ d \end{bmatrix}\right) = g_m\left(\begin{bmatrix} V \\ d \end{bmatrix}\right) + \epsilon_f\left(\begin{bmatrix} V \\ d \end{bmatrix}\right) \qquad (6)$$

$$P(parameters|signal) \propto \left(\prod_{i=1}^{m} P\left(\phi_0, \phi_i, \mu_{V_i}\, \mu_{d_i}, \Sigma_{V,d_i}\right)\right) . \exp\left(\sum_{v=1}^{T} \frac{-1}{2\sigma_{i_{j_v}}^{\ 2}} \left\|\epsilon_{i_j}\right\|^2\right) \qquad (7)$$

The total posterior from C calibrating aerosols for an electrometer is:

$$\prod_{c=1}^{C} P_c(parameters|signal) \qquad (8)$$

CALIBRATION

In order to interpret size spectrum from mobility spectrum, the transfer function $\boldsymbol{F}$ of the device (in the form of a matrix) should be obtained through calibration. Through CFD simulation and releasing the narrow-sized classes of unit concentration particles, we change the operating voltage of the EMS and record the signals received from all electrometers in all voltages. This gives a 3D surface of signal intensity $f\left(\begin{bmatrix} V \\ d \end{bmatrix}\right)$ for each electrometer, representing one dimension for the diameter classes of discretized spectrum, another dimension for the voltage classes, and the third, the signal intensity reported by each electrometer as a function of independent variables voltage and diameter, for injection of unit concentration particles in each diameter class. Fig.2 depicts the heat-maps of such surfaces for the EMS with 12 channels simulated in this study. Through Bayesian interpretation, the prior information and the model structure captured based on CFD simulation, $\boldsymbol{F}$ is obtained.

To obtain the total signal received from all diameter classes, one should integrate f multiplied by unit concentration on the diameter spectrum. For instance, this has been done for channels one, seven, and twelve shown on the second row in Fig. 3. On the third row, the total signal for all 12 electrometers are shown when particles injected with unit concentration in each diameter class.

FIGURE 2. Heat-maps of surface f showing signal intensity received by each electrometer with changing the operating voltage and injecting unit concentration particles in each diameter class

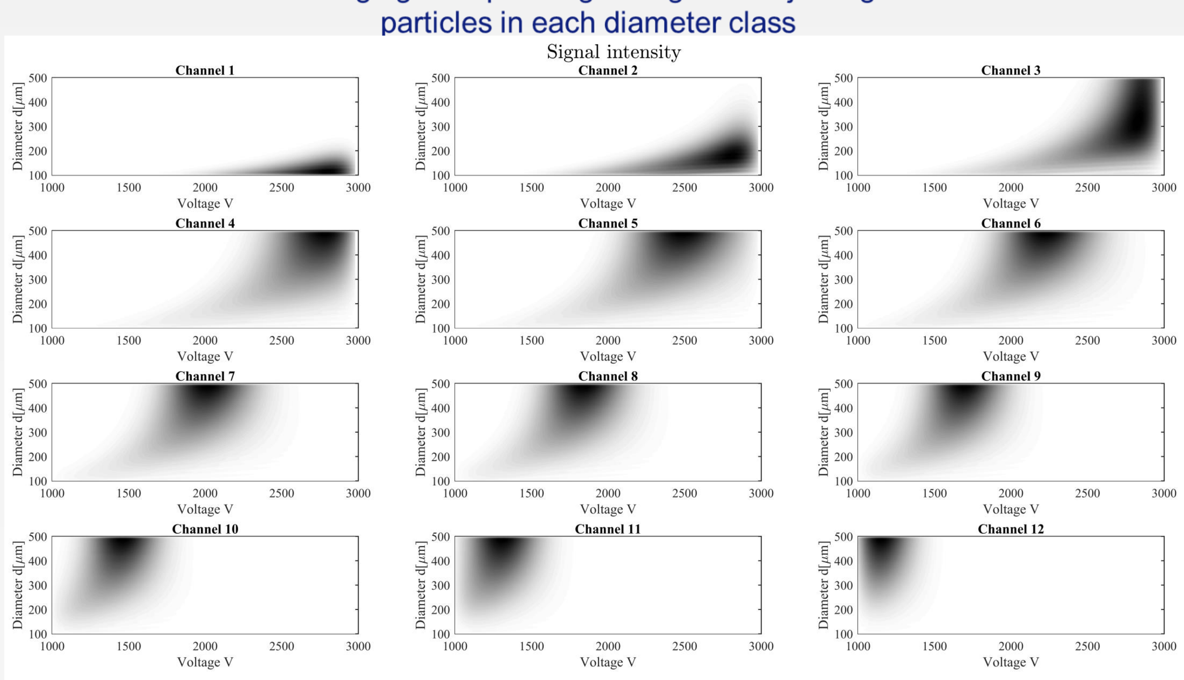
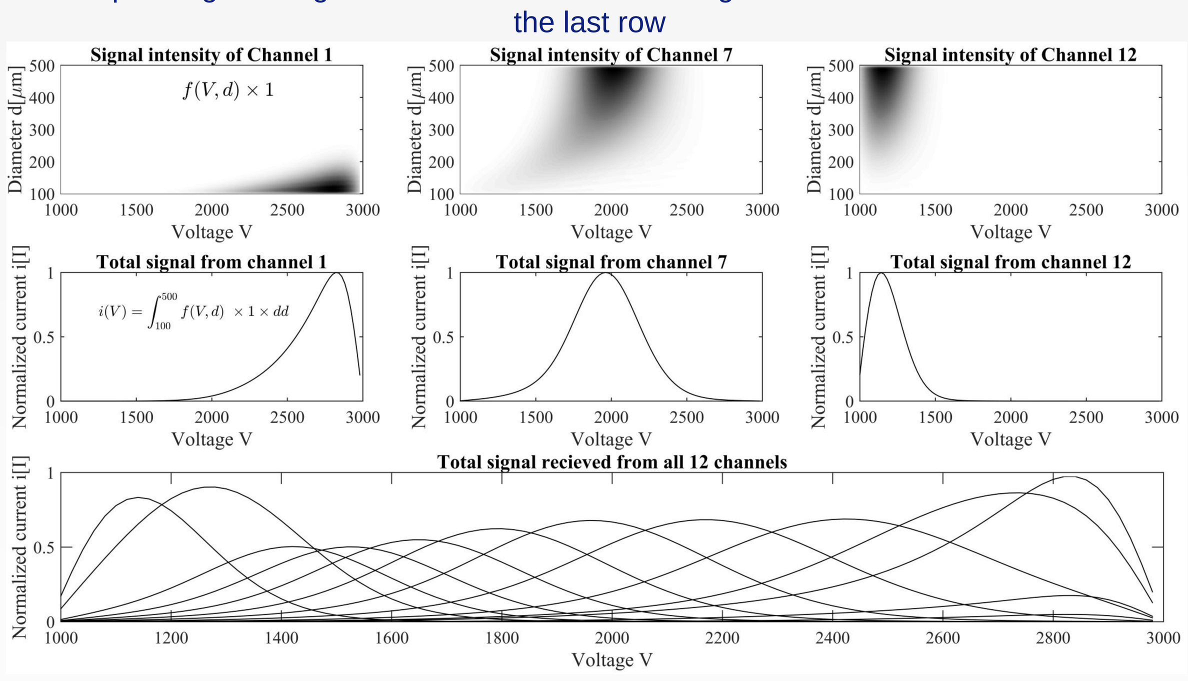


FIGURE 3. Heat-maps of surface f showing signal intensity and their corresponding total signal in the second row. Total signal for all 12 channels shown in the last row



RESULTS

Three electrode configurations 12, 9 and 6-channel EMS were examined in this study to analyze sensitivity of size measurements to the added noise (without size function assumption). Measurements of unimodal and bimodal aerosols with 1% standard deviation for noise are shown in Fig. 4. Fig. 5 compares noisy predictions of 12 and 6 channel EMS assuming 1%, 2% and 3% standard deviations for noise. Four configurations 12, 9, 6 and 3 channels EMS were examined to analyze sensitivity of size measurements to the added noise (with unimodal size function assumption). Measurements of unimodal aerosol with 10% standard deviation for noise are shown in Fig. 6.

FIGURE 4. Measurements of unimodal and bimodal aerosols with 1% standard deviation for noise

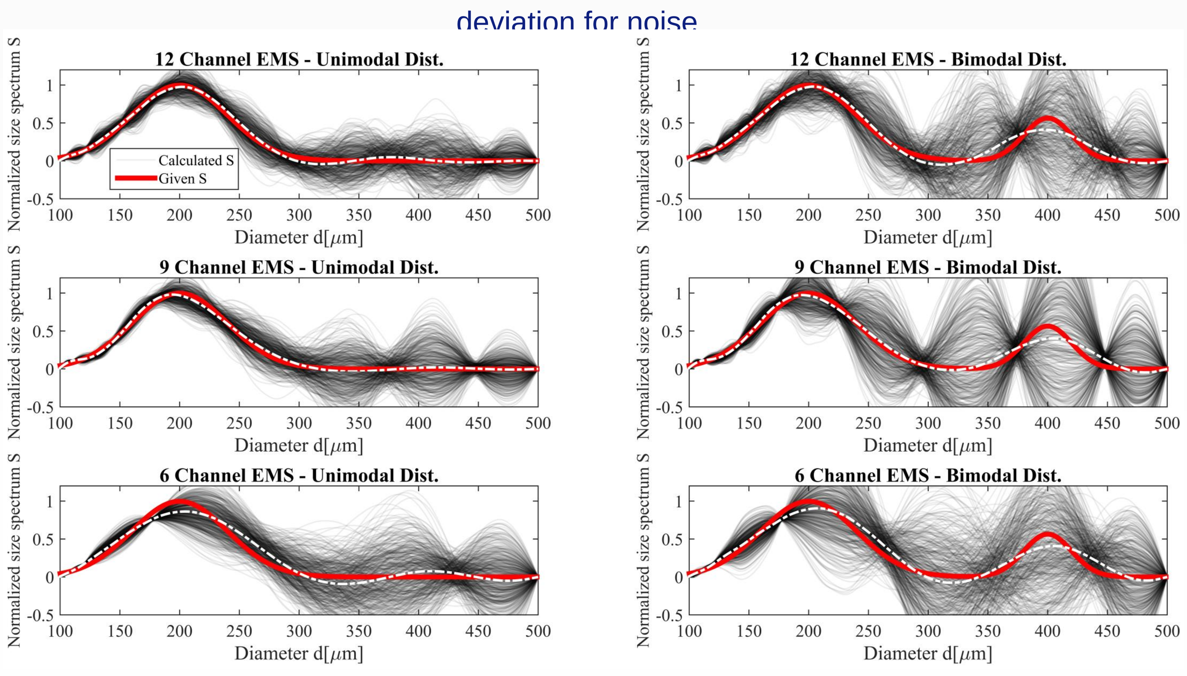


FIGURE 5. Measurements of unimodal aerosol with 1%, 2% and 3% standard deviations for noise

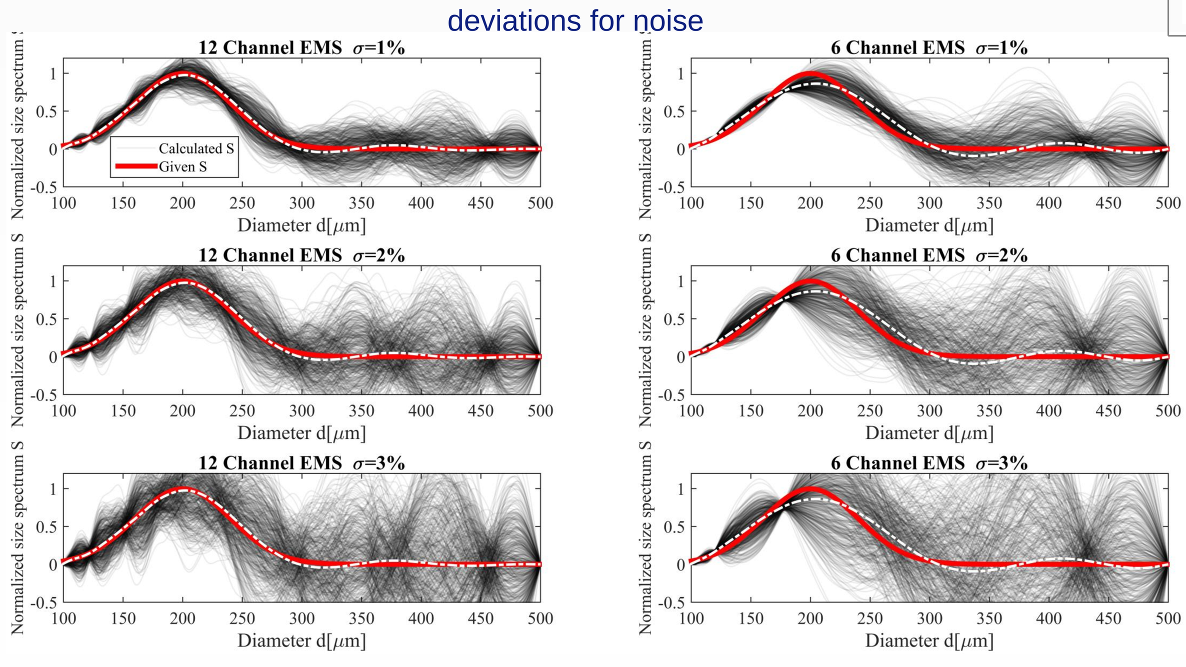
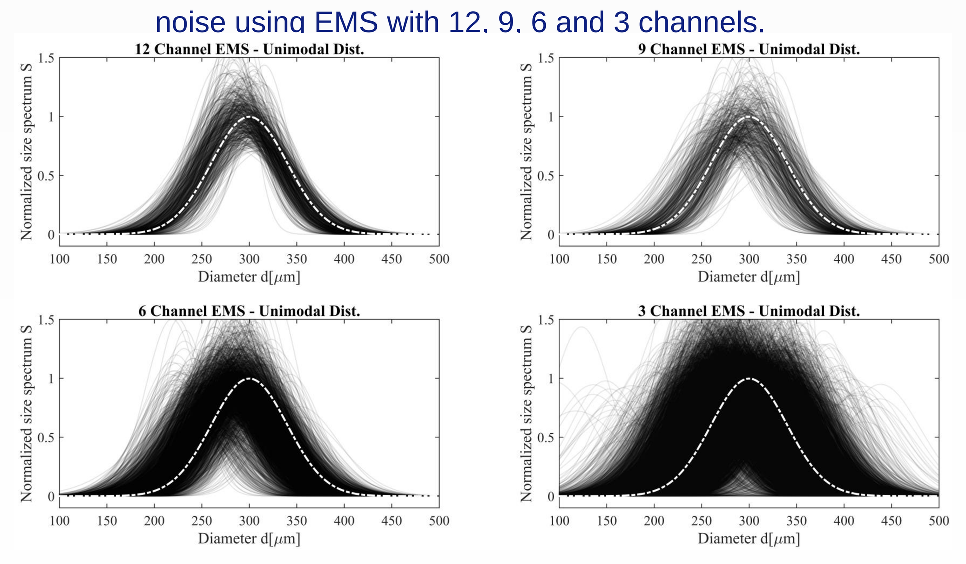


FIGURE 6. Measurements of unimodal aerosol with 10%, standard deviation for noise using EMS with 12, 9, 6 and 3 channels.



CONCLUSIONS

It was found that the size distribution predictions were strongly sensitive to the number of detectors and noisy response when size distribution assumed to be of unimodal distribution. Without any assumption on size distribution function, predictions were moderately sensitive to noisy response in comparison. As the number of detectors grows, measurement accuracy also increases and this effect was more evident for measuring unimodal aerosols than for bimodal. The improvement of accuracy from 9 to 12-chanel EMS is less obvious than improvement from 6 to 9-channel EMS. This suggests that for unimodal and bimodal aerosols optimum number of detectors would be between 6 and 12.