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Inversion of electrical mobility measurements using bipolar or unipolar chargers for the arbitrary distribution of channels

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ABSTRACT

The inversion of the particle size distribution from electrical mobility measurements is analyzed. Three different methods are adapted for a dot-matrix approach to the problem, especially for non-square or singular matrices, and applied to electrical mobility measurements from fixed or scanning voltages. Multiply charged particles, diffusion losses, arbitrary voltage steps and noise were considered, which results in non-adjoining and overlapping transfer functions. The individual contribution of the transfer functions in each size interval was geometrically estimated, which requires only its characteristic mobilities. The methodology is applied to mobility measurements from particles charged with unipolar and bipolar chargers. However, the method can be extrapolated to any charging method with a defined charge distribution, and retrieval of the singly charged particle distribution and mean charge from a tandem differential mobility analysis configuration was successfully demonstrated.

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Introduction

Knowledge of the particle size distribution (PSD) is a fundamental requisite to characterize an aerosol population. Differential mobility analysis (DMA) is the most common principle to measure submicron PSDs, because it is able to characterize a wide range of sizes with high resolution in almost real time independently of the composition of the particles.

However, the PSD cannot be directly measured and must be inferred from related mobility measurements using inversion techniques. The first attempt at inversion was by Knutson and Whitby (1975a, 1975b) based on integration of the particle trajectory equation inside the DMA. The particle size was represented by the size of a sphere with the same mobility Z_p as the particle, which is called the *mobility diameter* (D_{Z_p}):

$$Z_p = \frac{qeC_c(D_{Z_p})}{3\pi\mu D_{Z_p}}, \tag{1}$$

where q is the number of elementary charges e on the particle, μ is the dynamic viscosity of the gas flow, and $C_c(D_{Z_p})$ is the Cunningham slip correction factor.

The particle size distribution $N(D_p)$ and particle mobility distribution $M(D_{Z_p})$ are related through the non-negative Kernel function $\mathcal{K}_q(D_p, D_{Z_p})$ by a Fredholm-type integral equation that also considers the uncertainty in the measurements $\varepsilon(D_{Z_p})$:

$$M(D_{Z_p}) = \int_{D_{p\,min}}^{D_{p\,max}} K_q(D_p, D_{Z_p})N(D_p)dD_p + \varepsilon(D_{Z_p}). \tag{2}$$

When the Kernel is linear with respect to the size distribution, Eq. (2) can be expressed in matrix form as

$$M_m \approx K^q_{mn}N_n + \varepsilon_m. \tag{3}$$

The equation is approximate because of the error $\varepsilon_m \in \mathbb{R}^m$ not only in the data, but also in the approach of the integral (Eq. (2)) to a set of discrete linear equations. The indices m and n are the number of discrete measurements and output channels, respectively.

Abbreviations: CN, condition number; CPC, condensation particle counter; DMA, differential mobility analyzer; DMPS, differential mobility particle sizer; FWHM, full width at half maximum; GSD, geometric standard deviation; GCV, generalized cross-validation; LC, L-Curve; LS, least squares; NNLS, non-negative least squares; NRMSE, normalized root mean square error; PSD, particle size distribution; SMPS, scanning mobility particle sizer; SVD, singular value decomposition; TDMA, tandem differential mobility analysis; TF, transfer function.

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Nomenclature

A_Ω	area of the transfer function
C_c	Cunningham slip correction factor
d	ratio between diameters
D_{gap}	vertical distance from needle tip to output of ionizing region in corona
D_p	particle diameter
D_{pg}	geometric mean diameter
D_{Z_p}	mobility diameter
e	elementary unit of charge (1.602×10^{-19}) C
f_c	fraction of charged particles
H	height of the fitting TF triangle
k_B	Boltzmann's constant (1.380×10^{-23}) J/K
K	kernel matrix
L	length of DMA
m	number of measurement intervals
M	particle mobility distribution
n	number of output intervals
N	particle size distribution
P	pressure
P_n	penetration efficiency
Pe	Peclet number
q	number of elementary charges on a particle
Q_i	ion dilution flow
Q_a	aerosol flow
Q_{ex}	excess flow
Q_m	aerosol monodisperse flow
Q_{sh}	sheath flow
R_i, R_0	inner and outer radius of the DMA electrodes
t	residence time
V_0	voltage applied to the DMA central rod
Z_c	centroid mobility of transfer function
Z_l, Z_u	lower and upper boundaries from the mobility TF intervals
Z_l^*, Z_u^*	lower and upper boundaries from the size intervals
Z_p	electrical particle mobility

Greek letters

β_0	relative width of the TF
ε	error
λ	regularization parameter
μ	dynamic viscosity of gases
σ_g	geometric standard deviation
τ	scan time
Ω	transfer function (math.)

One of the main drawbacks of this technique is that large particles with multiple charges can have the same mobility as small singly charged particles. It is an *ill-posed problem* in the sense that a stable solution may not exist or may not be unique.

In general, the rank of the control matrix $\mathcal{K}^q_{mn}$ determines the reliability of finding a solution. For determined systems ($m = n$), there may be a unique solution. If the system is under-determined ($m < n$), it has many possible solutions, whereas if $m > n$ it is an overdetermined system and there is no exact solution (Voutilainen, 2001; Talukdar & Swihart, 2003).

Data inversion technique

The ill-posedness of the problem can be rectified by replacing it with an approximate well-posed problem whose solution is assumed to be close to the actual PSD. The main methodology to solve Eq. (3) is based on methods derived from the least squares (LS):

$$N_{LS} = arg \quad \min \left\| \mathcal{K}\, N_{inv} - M \right\|. \tag{4}$$

In this work, only deterministic techniques were applied, such as iterative (Alofs & Balakumar, 1982; Bazan & Francisco, 2009; Collins, Flagan, & Seinfeld, 2002; Crump & Seinfeld, 1981; Fiebig, Stein, Schröder, Feldpausch, & Petzold, 2005; Hagen & Alofs, 1983; Pfeifer et al., 2013; Rojas & Steihaug, 2002; Talukdar & Swihart, 2003; Twomey, 1975), regularization (Hansen & O'Leary, 1993; Talukdar & Swihart, 2003), or linear inversion methods (Hagen & Alofs, 1983), although recently the statistical techniques have been improved (Dubey & Dhaniyala, 2013; Voutilainen, 2001).

When the control matrix is strongly ill-conditioned, small errors in the data can be greatly magnified in the solution, even allowing negative values for the PSD. One way to avoid negative values is to use the non-negative least squares (NNLS) algorithm (Lawson & Hanson, 1974), which is a reformulation of the LS solution in which a dual vector $w = \mathcal{K}^T(M - \mathcal{K}N)$ forces the solution to be positive:

$$N_N = arg \quad \min \left\| \mathcal{K}\, N_{inv} - M \right\|; \quad N_N \geq 0. \tag{5}$$

The biggest drawback of this method is the convergence: there is no single factorization and the results can converge to a different local minimum. Moreover, it is only valid for systems where $m \geq n$, excluding under-determined problems.

The Tikhonov regularization (Willoughby, 1979) is widely used to solve problems of signal processing such as noise reduction, image restoration, and data inversion. The method replaces Eq. (4) by a minimization problem:

$$N_\lambda = N \in \mathbb{R}^n arg \quad \min \left\{ \left\| \mathcal{K}\, N - M \right\|^2 + \lambda \left\| N \right\|^2 \right\}, \tag{6}$$

where λ is the *regularization parameter*, which is a positive constant that balances the fit and smoothness of the distribution and is chosen such that N_λ becomes as close as possible to the noise-free solution.

The main advantage of the Tikhonov regularization is that diagnosis of the problem can be made through the singular value decomposition (SVD). It achieves a pseudo-inverse of the kernel matrix, $\mathcal{K}^+$, by disaggregating it into two orthogonal matrices, $U \in \mathbb{R}^{m \times m}$ and $W \in \mathbb{R}^{n \times n}$, and a diagonal matrix formed by non-negative elements, the *singular values*, $\Sigma \in \mathbb{R}^{m \times n}$:

$$\mathcal{K}^+ = W \Sigma^+ U^T = \sum_k \frac{w_k u_k^T}{\sigma_k}. \tag{7}$$

Expressing Eq. (6) in vectorized form, the inverted PSD is

$$N_\lambda = (\mathcal{K}^+ \mathcal{K} + \lambda \mathbb{III})^{-1} \mathcal{K}^+ M = \sum_{k=1}^{r} \zeta_k \frac{u_k^T M}{\sigma_k} w_k, \tag{8}$$

where ζ_k are the filter factors or Wiener weights:

$$\zeta_k = \frac{\sigma_k^2}{\sigma_k^2 + \lambda}. \tag{9}$$

The L-Curve (Hagen & Alofs, 1983; Hansen & O'Leary, 1993; Lloyd, Taylor, Lawson, & Shields, 1997) is a powerful tool for estimating the optimal regularization parameter. In brief, it consists of minimizing Eq. (8) for each value of λ until the point of maximum curvature is found (Johnston & Gulrajani, 2000). Another regularization method is based on generalized cross-validation (GCV). It

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