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On the Optimality Assessment of Nano-Particle Size Spectrometry and Its Association to the Entropy Concept

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Abstract : Particle size distribution, the most important characteristics of aerosols, is obtained through electrical characterization techniques. The dynamics of charged nano-particles under the influence of electric field in electrical mobility spectrometer (EMS) reveals the size distribution of these particles. The accuracy of this measurement is influenced by flow conditions, geometry, electric field and particle charging process, therefore by the transfer function (transfer matrix) of the instrument. In this work, a wire-cylinder corona charger was designed and the combined field-diffusion charging process of injected poly-disperse aerosol particles was numerically simulated as a prerequisite for the study of a multi-channel EMS. The result, a cloud of particles with non-uniform charge distribution, was introduced to the EMS. The flow pattern and electric field in the EMS were simulated using computational fluid dynamics (CFD) to obtain particle trajectories in the device and therefore to calculate the reported signal by each electrometer. According to the output signals (resulted from bombardment of particles and transferring their charges as currents), we proposed a modification to the size of detecting rings (which are connected to electrometers) in order to evaluate particle size distributions more accurately. Based on the capability of the system to transfer information contents about size distribution of the injected particles, we proposed a benchmark for the assessment of optimality of the design. This method applies the concept of Von Neumann entropy and borrows the definition of entropy from information theory (Shannon entropy) to measure optimality. Entropy, according to the Shannon entropy, is the ''average amount of information contained in an event, sample or character extracted from a data stream''. Evaluating the responses (signals) which were obtained via various configurations of detecting rings, the best configuration which gave the best predictions about the size distributions of injected particles, was the modified configuration. It was also the one that had the maximum amount of entropy. A reasonable consistency was also observed between the accuracy of the predictions and the entropy content of each configuration. In this method, entropy is extracted from the transfer matrix of the instrument for each configuration. Ultimately, various clouds of particles were introduced to the simulations and predicted size distributions were compared to the exact size distributions.

Keywords : aerosol nano-particle, CFD, electrical mobility spectrometer, von neumann entropy
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