Call for Master thesis:

Modelling for Estimating Aerosol Particle Size from Laser Light-Scattering Measurements

I. INTRODUCTION

The need to measure aerosols has increased dramatically over the last few decades in various fields including public health, atmospheric science, nano-technology, chemical manufacturing, pharmaceuticals, medicine, and specially air pollution.

NILU is developing a Wearable particle detector, LeoPard, allows for high-precision monitoring of aerosols particle exposure of industrial workers.

Leopard is a sensor/alarm device carried by workers in the production industry. It will alert the wearer in cases exceeding limits for both peak and accumulated exposure. Therefore, it is important to control and measure aerosol particle size.

To do such job, the LeoPard device, which is based on Single Particle optical Counting (OPC), is being developed at NILU for measurements of aerosol concentrations and size distributions. OPC-based aerosol particle counters are used to determine the air quality by counting and sizing the number of particles in the air. The instrument principle is utilizing a light source (typically a plasma laser or laser diode) collimated to illuminate a sample volume of aerosol flowing out of a nozzle; a photodetector, off-axis from the light beam, measures the amount of light scattered from single particles by refraction, reflection and diffraction. Both the size and the number of particles are measured simultaneously.

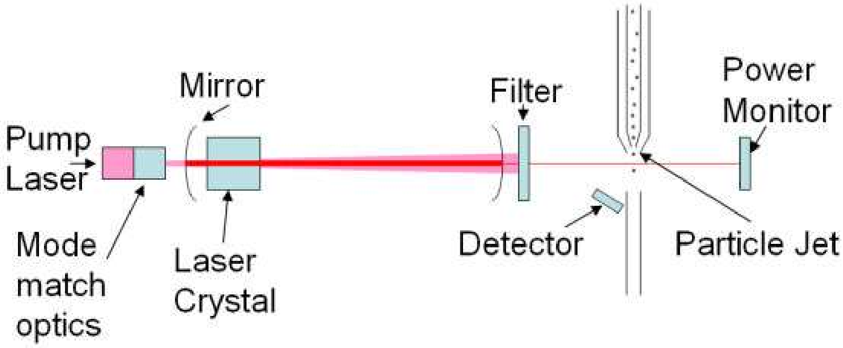
Determination the particle size from the instrument response to single particles is challenging because of the complicated dependence of the response on particle size, particle index of refraction, particle shape, lens geometry of the counter optical system.

Therefore, developing a model to determine particle size from scattered light measurements is important. To estimate correctly with high accuracy, the mathematic model should take account all numerous factors that contribute to scattering intensity, such as the distance to the particle, the scattering angle, the refractive index of the particle, the optical system characteristics…

II. PRINCIPLE

As shown in the below photo, The concept of Laser Light-Scattering Measurements involves the collection of scattered light from a dilute dispersion of particles by detector(s) placed at one or different spatial locations so that they cover a certain span of scattering angles θ.

There is not a simple relationship between particle size and scattered intensity. The angular dependence of the scattered light intensity, originating from a particle, is a function of the size and shape of the particle, as well as the orientation of the particle with respect to the incident laser beam, the particle size and shape can be inferred from the corresponding scattering intensity pattern.



Therefore, the estimation of the Particle Size Distribution (PSD) from the measured scattering intensity pattern involves solving an inverse problem using a suitable scattering model which describes the scattering intensity for particles of a given shape, size and optical properties.

There are many type of shape of the aerosol particles. To determine the size for different shapes of the particles, different approaches must be considered.

1- Spherical particles

For spherical particles of any size, particle size measured from scattered intensity at any given scattering angle is complex and is not fully defined by Mie Theory. Depending on the size of the particle relative to the wavelength of the incident light there are simplifications which may be used to relate particle size to scattered intensity. The size parameter is defined by:

$$\alpha = \frac{\pi D_p}{\lambda}$$

Where α is the size parameter, D_p is the diameter of the scattering particle and λ is the wavelength of the light.

There are three distinct scattering regimes. Most optical particle counters operate with visible or near infrared wavelengths (typically 500-1100nm), putting most of the aerosol size range in the **Mie Scattering regime**. For some instruments measuring larger particles, the **simplified geometric relationship** is applicable and for instruments measuring the smallest aerosol, **Rayleigh scattering** is applicable.

- ***$\alpha \ll \lambda$* (size << wavelength of laser source)**

Rayleigh Scattering theory can be applied, The Rayleigh Scattering Equation calculates the light intensity:

$$I = I_0 \frac{1+\cos^2\theta}{2R^2} \left(\frac{2\pi}{\lambda}\right)^4 \left(\frac{n^2-1}{n^2+2}\right)^2 \left(\frac{d}{2}\right)^6$$

Where I is scattered intensity, I_0 is incident intensity, θ is the scattering angle, R is the distance to the particle, λ is the wavelength of the light, n is the refractive index of the particle and d is the diameter of the particle. For any given detector system and refractive index scattered intensity varies with d^6 in this regime.

- ***α~λ (size ~ wavelength of laser source)***

Mie Scattering theory can be applied. Mie theory requires knowledge of the optical properties (refractive index and imaginary component) of both the sample being measured, along with the refractive index of the dispersant. Usually the optical properties of the dispersant are relatively easy to find from published data, and many modern instruments will have in-built databases that include common dispersants. For samples where the optical properties are not known, the user can either measure them or estimate them using an iterative approach based upon the goodness of fit between the modeled data and the actual data collected for the sample. A full analysis of geometric scattering is also able to closely reproduce the results of Mie Scattering for smaller particles with a significant saving in computation .

- ***α>>λ (size >> wavelength of the laser source)***

Simplified Geometric Scattering theory (Fraunhofer approximation) can be applied:

$$I = I_0 K_{(n,\theta)} d^2$$

where I is scattered intensity, I_0 is incident intensity, K is a function of refractive index (n) and scattering angle (θ), and d is the particle diameter.

Fraunhofer approximation does not require knowledge of the optical properties of the sample. This can provide accurate results for large particles. However it should be used with caution whenever working with samples which might have particles size below 50µm or where the particles are relatively transparent

Considering and Estimating PSD with proper model will help to improve accuracy and quality of the device. Therefore, developing a correct and efficiency model is important.

2- Non- Spherical particles

There are many type of shape of the aerosol particles. A spherical particle can be described using a single number—the diameter— because every dimension is identical. However, non-spherical particles must be described using multiple length and width measures. These descriptions provide better accuracy, but also more complexity. Many techniques make the useful and convenient assumption that every particle is a sphere. In result, final measurement is an equivalent spherical diameter. This approach is simplistic and not perfectly accurate. Therefore, developing a complex model using different theories to estimate the size of non-Spherical particles will help to improve the accuracy of measurements.

III. THE TASKS

- Understanding and interpreting particle size distribution calculations
- Setting particle size specifications
- Investigation on numerous factors that contribute to scattering intensity, such as the distance to the particle, the way to sample the particles, the scattering angle, the refractive index of the particle, the optical properties….
- Investigation into particle shape effects on the light scattering properties
- Developing the models to estimate particles size from Laser Light-Scattering Measurements using some theories:
    + Rayleigh scattering
    + Mie scattering
    + Fraunhofer approximation

- Investigation of the Scattering of Light by Non-spherical Particles and developing the model to calculate the size of Non-spherical Particles using different theories.

- Investigation on Multiple Particle Scattering (optional, for non single-particle-counting).

IV. REQUREMENTS

- Students who are doing Master program on Cybernetics / Sensor technology / Electronics /Physics/ Instrumentation.

- Having some basic knowledges on mathematical modeling techniques for physical systems

- Programing skill on C/C++ or Matlab

V. FUNDING POSSIBILITIES

- Salary for 20% position in 1 year (paid 50% by NILU)

- Fee Office, library, equipment

- Advising from NILU’s employees