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DESIGN AND OPTIMIZATION OF A COMPACT LOW-COST OPTICAL PARTICLE SIZER

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Abstract

Direct measurements of time- and size-resolved particulate matter (PM) concentrations are of major importance in air quality studies and pollution monitoring. Low-cost, compact optical particle counters (OPCs), which provide accurate PM measurements independent of the particle complex index of refraction (CRI), can be useful in personal exposure monitoring and distributed sensor network studies applications. A methodology is presented for the optimization of the sensor design and operation parameter space aimed at reducing the effect of the CRI on particle sizing errors. The Monte Carlo numerical simulation, which utilizes Mie scattering calculations, is used to determine the optimal detector angle for the specific set of constraints described by the weighting coefficients. The optimized detector position ($\theta = 48^\circ$) has the lowest dependency on CRI over the entire particle size range of 0.5–10 microns. The near-forward, optimized, and perpendicular detector angles are compared experimentally using monodisperse 2 μm and 4 μm particles of silica, PSL, and alumina; the light collection cone angle is set at $\alpha = 20^\circ$ in all experiments. The data agree well with the numerical results for all tested scenarios. Overall, the perpendicular detector location has the best precision and worst accuracy related to the CRI variations. The optimized detector position has the best accuracy for both silica and alumina particles. The use of low-cost components, such as laser diodes, photodiodes, miniaturized integrated electronics, and simple component layouts allows for the development of compact OPCs capable of accurately sizing PM. The number of sizing bins, sizing accuracy and precision, and other parameters of interest can be used as an input to an optimization algorithm.

Graphical Abstract

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2 INTRODUCTION

Direct measurements of time- and size-resolved particle concentrations are of major importance in applications of aerosol research (e.g., personal exposure assessments, air quality studies, and pollution monitoring). Human exposure to particulate matter (PM) is associated with multiple adverse health effects, including cardiovascular disease, cardiopulmonary disease, and lung cancer [1–7]. Estimates show that approximately 3% of cardiopulmonary and 5% of lung cancer deaths are attributed to PM exposure globally. The health and environmental research communities have standardized three categories of PM as its primary interest: particles smaller than 1 μm (PM_{10} , submicron particles), particles smaller than 2.5 μm ($\text{PM}_{2.5}$, fine particles), and particles smaller than 10 μm (PM_{10}) [8]. Studies have evidenced how particle deposition in the human respiratory tract and the resultant adverse health effects depend on the size distribution of the particles [9, 10]. Additionally, PM concentrations and distributions are known to vary significantly in both space and time [11, 12]. Hence, time- and size-resolved PM measurements are more informative than traditional total PM weight measurements when assessing these negative effects on human health. The U.S. Environmental Protection Agency (EPA) and the EU have adopted the PM_{10} and $\text{PM}_{2.5}$ criteria for monitoring ambient air quality [8, 13]. However, the density of monitoring sites varies widely across the globe, making annual exposure estimations a challenge [14]. A variety of methods are currently used to measure particle concentrations, including traditional gravimetric filters, aerodynamic particle sizers, beta attenuation monitors, and scanning electrical mobility sizers. These methods are highly accurate and precise, but their large size and high price make them impractical for use as personal monitors. Often, applications demand more practical instruments that are compact, automatic, and low-cost, without forgoing sizing accuracy and reliability. Such applications include mass deployments of ambient air monitoring instruments and wearable exposure monitors.

Instruments that rely on the elastic scattering of light to measure time- and size-resolved PM concentrations have already proven their worth in aerosol research, particularly when measuring particles in the 0.1 to 10 μm range. They enable the automatic measurements of size- and time-resolved PM concentrations and are simpler, less expensive, and generally smaller than the alternatives. Aerosol photometers measure the bulk light scatter of multiple particles simultaneously, while devices that measure the light scatter of individual particles are called optical particle counters (OPCs). The development of OPCs over the last half

century has provided them with more accurate particle sizing capabilities, rendering the “counter” terminology unfitting. Optical particle sizers (OPSs) are available on the market, but their cost and complexity limit their use as personal exposure monitors. Particle sensors gauge the average optical properties of PM in the air and can be calibrated to provide indications of PM concentrations with some success, e.g., [15]. They are compact, low-cost, can be integrated into small devices, and have been used in large-scale PM exposure studies [16, 17]. In contrast, with proper calibration, OPSs count the individual particles and provide more accurate size-resolved profiles of PM number concentrations.

Light scattering devices, by definition, utilize the same physical principle—the elastic scattering of light. OPSs measure light scattered by the particles and determine the size of each particle based on the measured intensity of the scattered light. Single-detector sensors suffer from the same weaknesses: (i) the scattered light intensity is sensitive to small variations in the complex refractive index (CRI) of particles, and (ii) the scattered light intensity displays non-monotonic size dependence as a function of particle sizes and their CRI. These issues create ambiguity in sizing particles with unknown CRI; which is typical in environmental PM monitoring and personal exposure assessments. Since current PM regulations are based on mass measurements, better estimations of particle size are important for any light scattering device. For example, an underestimation of the particle diameter by 10% leads to an error in the particle volume (mass) calculation of 33%, while a 50% sizing error leads to about a 340% error in PM mass estimates. CRI sensitivity is particularly apparent in compact, low-cost devices; a recent study found that low-cost (< \$100) particle sensors consistently provide erroneous number concentrations when exposed to particles that differed from the calibration particles [18]. Another study evaluated three commercially available low-cost particle sensors; the results show that all three sensors depend highly on the particle composition and size, providing measurements with errors of up to 1000% [19]. Measurements obtained using low-cost sensors suffer from sensor-to-sensor variability due to the lack of quality control and differences in the individual components [15, 18].

Researchers have addressed CRI sensitivity by designing OPSs that measure scattered light at multiple different angles simultaneously [20] or by employing dual wavelength techniques [21]. However, these solutions involve complex and expensive components not suitable for compact, low-cost devices. A common workaround for less expensive solutions is to collect PM on a filter after or parallel to the OPS measurements. The filters are analyzed to determine their average particle CRI; these data are then used to correct the optical measurements after the fact. Retrieving average CRI values is a labor-intensive task which presents difficulties for collecting measurements in large studies or in scenarios where the PM composition may change during the collection period. Low-cost, compact, easy to use OPSs providing accurate real-time and size-resolved PM measurements, independent of CRI, can be useful for a variety of applications. Traditionally, such sensors are used in real-time personal exposure assessment scenarios, monitoring HVAC systems, and managing general air quality.

This manuscript describes the process of the design optimization and experimental validation of a low-cost OPS capable of aerosol size measurements in the 0.5–10 micron size

range. The optimization of the sensor geometry is guided by the Monte Carlo optimizations of the parameter space. The sensor design goals are to (i) have a low sensitivity to variations in the CRI of the particles, (ii) provide accurate particle sizing, (iii) have a small form factor, and (iv) be low-cost. The manuscript is organized as follows: (a) a description of the optimization methodology to minimize sensitivity to the CRI related to the particle sizing accuracy, (b) a comparison of the optimized geometry with two alternatives (i.e., perpendicular and near-forward scattering models), and (c) an experimental validation of the numerical findings and a comparison with the two commonly used alternative geometries.

3 BACKGROUND, OPTIMIZATION, AND DESIGN

3.1 THEORETICAL BACKGROUND

The operating principle of an OPS is based on collecting and measuring the intensity of light scattered from the individual particle as it traverses a focused light beam. A portion of the scattered light is collected by a photodetector, which converts the scattered light into a voltage signal. Thereby, each particle generates a pulse, whose amplitude depends on the particle diameter, CRI, shape, and surface roughness. Ideally, the sensor has a unique relationship between the particle diameter and the measured electrical signal, independent of the particle's CRI, shape, and surface roughness, providing distinctive particle sizing. The spatial distribution of light scattered by a spherical particle can be calculated using the Mie theory [22, 23]. The spatial distribution is described with polar scattering in the scattering plane, containing the particle and the incident light beam and the azimuthal scattering around the axis of the incident light beam. For a linearly polarized light beam irradiating a particle from one direction, the OPS response, R , is given by Equation 2,

$$R = \frac{\lambda^2}{4\pi^2} \int_{\phi_1}^{\phi_2} \int_{\theta_1}^{\theta_2} G(x, m, \theta, \phi) (I_{\text{hor}}(x, m, \theta, \phi) + I_{\text{ver}}(x, m, \theta, \phi)) d\theta d\phi \quad (2)$$

where G represents the characteristics specific to each device (i.e., amplification, signal processing, stray light), I_{hor} and I_{ver} are the scattered light intensities polarized horizontal and vertical to the plane of the incoming plane wave, $m = n - ik$ is the CRI of the particle, $x = \pi d/\lambda$ is the dimensionless particle size parameter, d is the particle's diameter, and λ is the wavelength of the incoming light. For spherical and homogeneous particles, the two intensities I_{hor} and I_{ver} can be calculated with the Mie theory. Angles θ and ϕ correspond to the central axis of the photodetector; the solid angle is α (detector light collection cone) is defined by detector dimensions and distance from the optical interrogation volume. Figure 1 shows the spatial coordinate system used in the Mie scattering calculations.

The in-house Mie scattering code is used to perform the scattering calculations in a Monte Carlo simulation for the optimization of the sensor parameters. The code allows computation of particle light scattering intensities for a range of detector positions, light collecting cone angles, and particle sizes and their CRIs. Figure 2 shows a typical result from the Mie calculation – the scattering light intensity of the particles as a function of their size, CRI, and

the light scattering angle. Most discrete angles display oscillatory behavior with respect to particle size, although the intensity can be smoothed by integrating over specific angular ranges. One often-used strategy is to employ large collecting optics to improve the sensitivity and introduce the spatial integration of the scattering light. However, this solution increases the size and complexity of the optical cell. Non-monotonic size dependence is apparent in Figure 2 (Left) for CRI=1.5-0i, illumination wavelength $\lambda=450\text{nm}$, and scattering angles $\theta \sim 20^\circ$ and $110^\circ > \theta > 160^\circ$ (i.e., smaller particles scatter more light than larger particles, leading to multivaluedness in the sensor response). Figure 2 (Right) shows the scattering intensity for a $1\text{ }\mu\text{m}$ particle as a function of the angle and CRI. The scattered intensity varies substantially for the fixed particle size, and for the fixed values of the scattering angle, the scattering intensity can vary by two orders of magnitude; the backscattering angles show the greatest variations. The non-monotonic size dependence and the multivaluedness in the sensor response make unique particle sizing very difficult.

The sensor response is proportional to the scattered light intensity. More strictly, it is a function of the parameters in Equation 2, including the integrated angular range (which represents the collection area of the photodetector), the wavelength and polarization of the incident light beam, and the optical properties, shapes, and surface roughnesses of the measured particles. Previous studies have suggested that near-forward scattering (for our case, $\theta = 15^\circ$) is less sensitive to the CRI [20]; this angular range is often referred to as the Mie lobe and contains the mostly diffracted light that is less affected by variations in the CRI. The perpendicular positioning of the photodetector ($\theta = 90^\circ$) limits the effects of stray light inside the device; it is simple to manufacture, offers the smallest optical volume, and has traditionally been the most commonly used angular range in OPCs [24]. In this optimization study, we consider all possible angle ranges to minimize the effect of the CRI on the particle sizing accuracy. The optimized geometry is compared with the near forward and perpendicular scattering scenarios.

In addition to the sizing accuracy considerations, the other performance characteristics of interest are the minimum detectable particle size and the sensor dynamic range. Figure 2 shows that the scattered light intensity increases as the scattering angle approaches $\theta = 0^\circ$, thereby improving the device's capabilities of measuring smaller particles, i.e., the limit of detection (LOD). The LOD is defined as the smallest measured particle size that provides an S/N ratio in 3 to 5 range, where S is the sensor response to a particle scattering event and N is the sensor background noise. Lower threshold values result in detection of smaller particles. The dynamic range of the sensor is defined as the ratio of the highest measured intensity over the lowest; a ratio that varies substantially for different positions and the collecting angle of the photodetector. A greater range of the scattering intensities, as received by the detector, requires the use of more complex electronics and may limit the range of the measurable particle sizes.

3.2 OPTIMIZATION PROCEDURE

Instead of heuristically examining multiple angular ranges for system response, our approach is to build an optimization scheme for finding the optimal geometry of the optical components within the design parameters and limitation of the size and performance of any

given components. In particular, the angular detector position is optimized to minimize the following four characteristics: (i) the sensitivity towards the CRI, (ii) the non-monotonic nature of the scattering intensity with respect to the particle size, (iii) the dynamic range of the detector response, and (iv) the LOD. Together, they form the cost functions for the optimization of the sensor design. The optimization algorithm uses the Mie theory to calculate the response characteristics of each scattering angle range. The collected light cone angle (α) is determined by the size and proximity of the photodetector to the optical volume located at the intersection of the particle stream and the laser beam. The algorithm considers a multi-objective optimization with multiple equally possible solutions. To find a single solution, each optimization criterion is normalized and weighted in the range from zero to unity. Thereby, the scheme can find the optimal angular range using the weighted criteria defined by the user. The quantitative outcome for variation in each input parameter must be independent of the other parameters; the approach taken here is to quantify each input parameter mathematically. Table 1 shows the input parameters and their weighting in the optimization algorithm used in this study; these input parameters can be varied by the user, depending on the design goals. In this example, the set of parameters and the constraints are chosen to design the low-cost, compact OPC for sizing PM_{2.5} and PM₁₀ particles. CRI sensitivity is essential for the accurate sizing of the PM and is assigned a weight of unity; the response to the CRI is quantified as the Coefficient of Variation (CV), the ratio of the standard deviation to the mean for varying CRI and a given particle size. The monotonicity as a function of the particle diameter is assigned a weight of unity; it is quantified as the number of multivalued instances for all particles in the size range. The dynamic range is assigned a lower weight because the response can be compensated by the design of the electronic amplification circuit. The LOD criterion is assigned a weight of one-half.

The constraints listed in Table 1 are chosen based on the targeted application of the monitoring of size-resolved concentrations of PM_{2.5} and PM₁₀ for typical rural and urban environments. Studies show that the properties of PM found in these environments range from non- to weakly-absorbing particles; specifically, the real part of the refractive index ranges from 1.3 to 2.0 for individual particles, with 1.5 to 1.6 being the average. The imaginary part ranges from almost zero in rural areas to 0.1 in urban areas [25–27]. The range of particles chosen for the optimization are non- and weakly-absorbing spherical particles with diameters from 0.1 to 10 μm and CRIs ($m = n - ik$) in the range of $n = 1.3$ to 2.0 and $k = 0$ to 0.1. Several other factors constrain the optimization, mainly stemming from the physical design of the device: its small form factor and low cost. The angle between the illumination beam and the center line of the detector ranges from 15 – 165° due to the restrictions imposed by the laser source and laser dump. The maximum collection cone angle is 20° due to the sensor assembly and photodiode size constraints. The presented optimization does not include the use of collection optics (i.e., mirror, lenses). The polarization of the incident light source is assumed to be linear (i.e., horizontal or vertical) as the laser diodes considered in the design are linearly polarized. The selected optimization criteria, constraints, and their relative weight are chosen for the specific use case; other inputs, constraints, and weighting selections can be utilized in the algorithm and will likely result in a different sensor geometry.

Monte Carlo simulations are performed using a custom Matlab subroutine to optimize for the best detector angle for the given constraints. The angle $\theta = 48^\circ$ to the detector centerline was found to be the best scenario. The variability of the response, R , as a function of CRI over the particle size range from 0.1 to 10 μm is shown in Figure 3. The optimized sensor geometry is compared to two alternatives geometries, commonly used in commercially available sensors: the perpendicular ($\theta = 90^\circ$) and near-forward ($\theta = 15^\circ$) range. For each scenario, the collecting cone angle is $\alpha = 20^\circ$. The scattering intensity for these sensor positions is calculated using the Mie code. The amplitude of the response increases as the angular range gets closer to the forward scattering (Mie lobe); the near-forward range has the highest intensity out of the three detector positions considered. The variance of the optimized detector placement is the smallest, especially for particles larger than 1 μm . The perpendicular sensor position displays the highest sensitivity to variations in the CRI for all particle sizes, while the near-forward range is the most sensitive when smaller particles are considered.

Figure 4 shows the CV as a function of particle diameter for the three angular detector positions; the optimized position has the least sensitivity to CRI variations, especially for particles larger than 1 μm . The perpendicular arrangement has the highest CV overall; near-forward scattering shows only a slightly higher coefficient of variation, except for the particles in the smaller size range, which may not be very important for a low-cost device with relatively high particle size detection cutoff (0.5–0.8 micron) due to power and size limitations.

The geometry optimization performed by the Monte Carlo simulation using Mie scattering calculations shows the feasibility of constructing a simple particle sizer with significant improvements in particle sizing over the traditional designs. The results of the numerical study are tested experimentally in the following section.

4 EXPERIMENTAL SETUP

4.1 Optical Cell Design

To evaluate the modeling results, we experimentally tested the sensor response as a function of the detector placement using the experimental setup shown in Figure 5. The optical cell is placed within the 300 mm $\times$ 300 mm $\times$ 250 mm hermetically sealed enclosure; the interior is painted with non-reflective matte black paint. The entire enclosure is placed on an optical table to allow for the precise alignment of optical components and aerosol stream. The test particles are aerosolized from an aqueous solution using a Lovelace nebulizer (In-Tox, Moriarty, NM), mixed with filtered dry air in a heated mixing chamber before traveling through a Nafion membrane dryer that reduces the moisture content of the aerosol stream. The prepared aerosol mixture is injected into a particle chamber where the pressure is close to atmospheric conditions. The aerosol mixture is then aspirated into the optical cell; the TSI Aerodynamic Particle Sizer (TSI APS, Model 3310) provides the necessary vacuum. The flow rate of the APS is 1 slpm, confirmed by the Gillibrator (Sensidyne, St. Petersburg, FL) measurements. The APS is used as a reference for the particle count and to monitor that the aerosol mixture contains only the particles of the correct size. The following monodisperse spherical particles are used in the experiments: 2 μm and 4 μm PSL spheres with CRI of

1.61-0i (Thermo-Fisher, Waltham, MA), 2 μm and 4 μm silica particles with CRI of 1.53-0i (Cospheric, Santa Barbara, CA), and 2 μm and 4 μm alumina particles with a CRI of 1.78-0i (Corpuscular, Cold Spring, NY). Figure 5 shows a diagram of the optical cell used for testing. Though the experimental setup used in these experiments is constructed on an optical table and has several large auxiliary components, the optical components tested in these experiments are suitable for the construction of a compact, low-cost device. The experimental setup provides precise component placement and enough flexibility to perform size control aerosol injections. The incident light source is a 120 mW laser diode (Osram PL450B) that emits blue light (450 nm); the diode is operated at 70 mW (running below maximum power for increased durability and stability). The laser beam is linearly polarized and focused using a 6 mm diameter lens into an elliptical volume at the location of the particle stream intersection. The laser beam passes through two rectangular apertures to minimize stray light and to shape the final beam before it traverses the collimated particle stream. At the intersection point, the elliptically shaped laser beam measures approximately 0.5 $\times$ 2 mm, with the longer axis angled perpendicular to the particle flow. The laser beam is trapped in a custom laser beam dump that uses an absorptive neutral density filter (OD = 3.0) followed by a geometrical beam trap. The particle stream inlet is a 1.8 mm (ID) stainless steel tube, and the outlet uses a 3 mm (ID) tube; the distance between the inlet and outlet is 5 mm. Sheath flow is not used in the design to minimize the size and the complexity of the sensor. The intersection of the particle stream and the laser beam creates a cylindrical optical volume with a diameter of 1.8 mm and length of 1 mm. The detector is a photodiode with a 3.2 mm square active area positioned on a manual rotary optical mount allowing to adjust detector angle. The size and the proximity of the photodiode to the optical volume determine the solid angle. In the experimental setup the light collection shape is not strictly a cone, but a square base pyramid. The reported solid angle $\alpha = 20^\circ$ is calculated based on the cone shape in the computational model using the equal cone base area. The corners of the square base detector are visible to the optical interrogation region. In order to compare the experimental results to the calculated scattering intensities, we consider a cone with the base area equal to the area of the square detector. Based on the square pyramid assumptions, the solid angle is in the range of 17.8 $^\circ$ –24.8 $^\circ$. Some uncertainty related to the use of the square detector is apparent, it is unlikely to result in the significant changes in the mean values of the particle size distribution. The goal of the experimental study is to compare different scattering angles; the detector solid angle is the same for all tested detection angles. The main advantages of this optical cell design are simplicity, adjustability, and flexibility, which allows for the testing of multiple geometrical arrangements and optical components. The experimental setup is also used to study the effect that the number of sizing bins has on the sizing accuracy (to test data acquisition strategies) and the electronic components (to test the sizing algorithms) with a short turnaround in the design cycles. In this work, we test a relatively simple geometry that can be manufactured easily with minimum requirements for alignment and recalibration. The total cost of the optical components including the laser driver is under \$100; the signal processing hardware is not included in the estimation.

4.2 SIGNAL PROCESSING & PERFORMANCE ESTIMATES

When a particle traverses the laser beam with Gaussian intensity, it scatters light in all directions; a portion of the light in the collection cone is detected by the photodiode and is

converted to a voltage signal. The photodiode output is a near Gaussian shaped pulse, which is then amplified by a two-stage trans-impedance amplifier with active filtering. The signal is processed by an Atmel AVR microcontroller with a built-in analog to digital converter, a sampling rate of 52 kHz, and a 10-bit analog to digital resolution in the 0–1 V range. An adaptive peak detection algorithm determines the amplitude of the voltage pulse and subsequently sorts the amplitude into bins corresponding to the size of the particle. Figure 6 shows a representative time-resolved signal from a 2 μm spherical PSL particle measured at a flow rate of 1 slpm.

The optical cell has particle inlet ID=1.8 mm and outlet ID=3 mm. The flow rate is 1 slpm, which translates to an average air velocity at an optical volume of 3.7 m/s. A particle traveling at that velocity crosses the 1 mm long optical volume and has a residence time of about 270 μs , which agrees well with the pulse width recorded by the detector as observed in Figure 6. The microcontroller samples at 52 kHz corresponding to an average of 12 samples for each particle that traverses the optical volume. Based on the particle residence in focal volume and sampling rate of the device, the theoretical maximum particle count is 3670 particles per second ($\sim 2.2\text{e}+5$ per min) at 1 lpm flow rate it translates a concentration of 220 particles per cubic centimeter. Several strategies can be readily used to improve the sample saturation issue, including increasing the data acquisition rate, reducing the optical volume, and reducing the particle residence time in the volume. Though strategies are not discussed in this manuscript in detail, the practical sensor device would address the optimization between the sensor sensitivity, propensity to the coincidence events, and the saturation limit.

5 MODEL VALIDATION

In the experimental study, we test the system's response for three detector positions, the optimized range ($\theta = 48^\circ$), the perpendicular range ($\theta = 90^\circ$), and the near-forward range ($\theta = 15^\circ$). The photodiode dimension and the proximity to the optical volume determine the collected light cone angle ($\alpha = 20^\circ$). All experiments use the experimental setup shown in Figure 5. For each angular range, the system is first calibrated using monodisperse PSL spheres of 2 μm and 4 μm . After the calibration, the setup is used to count and size monodisperse particles of the same two sizes, with different CRIs, namely silica and alumina microspheres. For illumination wavelength of 450nm, the PSL particles have a CRI of 1.61-0i, the silica particles – 1.53-0i, and the alumina particles – 1.78-0i. This approach represents a range of the CRIs, where the particles with unknown optical properties are measured by a sensor calibrated for a specific CRI value. For particles with CRI below 1.53-0i, the experimental comparison is not performed though some of the atmospheric aerosols may have lower values. Based on the modeling (see Figure 3) the response of the optimized sensor is better than other geometries considered in the study in both monotonicity and sensitivity to CRI. The experiments are performed for each combination of detector angle, particle size, and particle CRI; a total of 18 unique combinations are considered. In each experiment, at least one thousand particles had been counted and sized; resulting in 18 datasets with one thousand data points each.

Figure 7 shows the comparison of the response as predicted by the UW Mie scattering code and data from the optical cell. The experimental response is displayed as a marker (the

mean) with error bars extending to one standard deviation from the mean. The experimental response is well within the predicted curves for all tested scenarios. However, there is a small systematic tendency of the experimental values being lower than the theoretical curves. This is likely due to the “glancing effect” related to the Gaussian intensity profile of the laser beam. Particles that do not intersect the laser beam at the center of the beam experience lower incident light intensity compared to particles that do cross the laser beam in the middle [20]. Some of the strategies for minimizing this effect are to focus the laser beam into a uniform line using a focusing lens or focusing the particle toward the center of the laser beam by introducing sheath air or particle focusing inlet. These options are not considered for this sensor due to cost considerations. The under-sizing is more pronounced for smaller particles as they have a smaller Stokes number and are more susceptible to aerosol stream expansion and flow instabilities than larger particles. Figure 7 also shows that the near forward scattering has the highest intensity while the perpendicular detector orientation has the lowest intensities; this is observed in the numerical simulation and confirmed by the experimental measurements. The CRI dependence on the computed and measured scattering intensities is lowest for the optimized geometry; this is discussed in more detail below.

To assess the sizing performance (i.e., precision and accuracy) of each angular range, we compare the system measured signal for each particle of the known size and the CRI of that particle. The relative sizing error (RSE) is computed for each experimental data point (individual particle). Figure 8 and Figure 9 show the RSE distributions for all tested angular ranges. The width of each distribution indicates precision while its location (relative to the middle) represents the sizing accuracy. The 2 μm and 4 μm PSL particles used for calibration are colored in green and light blue respectively; as expected, they are located in the middle of each distribution. Figure 8 shows the experimental results for 2 μm particles, where the device is calibrated to PSL and is then used to size silica and alumina particles. The near-forward angular range has an RSE distribution with three distinct peaks, corresponding to the three types of particles tested; both the silica and alumina particles are undersized. The optimized angular range has three overlapping RSE distributions, showing virtually no dependence on the CRI. The perpendicular angular range has three distinct peaks in the RSE distribution; the data shows the undersizing of the silica particles and the oversizing of the alumina particles. The individual RSE distributions are the tightest for the perpendicular detector position. As expected, the perpendicular detector placement has the smallest optical volume and the lowest influence of stray light, allowing for increased precision. Another important observation is that all data shows longer “tails” for the negative RSE values, suggesting that more particles get undersized due to the glancing effects associated with poor particle focusing in the Gaussian beam profile.

Figure 9 shows the RSE distribution for 4 μm monodisperse particles. The near-forward detector position oversizes both silica and alumina particles. The optimized angular range slightly undersizes alumina particles and slightly oversizes silica particles. The perpendicular arrangement undersizes both silica and alumina particles. In comparison to the 2 μm RSE distributions, all three angular ranges show tighter distributions for 4 μm particles. This is likely due to the better particle stream collimation associated with the greater Stokes number of the larger particles.

6 CONCLUSIONS AND DISCUSSIONS

In this manuscript, a new methodology for the OPS geometry optimization is described, and the sensor performance is validated. The procedure is guided by a Monte Carlo optimization of the parameter space based on the design goals of having a low sensitivity to variations in the CRI of the particles, accurate sizing, a small form factor, and a low cost.

Previous research has shown that variations of the intensity with scattering angles are strongly dependent on the refractive index of the particles, e.g., [28] and [29]. Several researchers proposed simultaneous measurements at two different angles to elucidate the particle nature [30], [31] or using a ring of detectors covering the entire scattering angle range [32]. Near forward angles are dominated by light diffraction, and this region is reported to be less sensitive to the refractive index; the scattered light intensity is mainly dependent on the size of the particles, allowing for a better determination of the corresponding size distribution, e.g., [33]. On the other hand, the measurements at 60° are found to be very sensitive to the refractive index, e.g., [34]. These results are consistent with the modeling presented here as the near forward scattering geometry shows less dependence on the particle index of refraction (see Figure 4). However, our experimental data show only minimal improvements for near-forward scattering measurements, possibly due to the difficulties with stray-light contamination; the real-time signal correction of this signal offset due to the stray light has been previously proposed [35]. Another possible explanation for only modest improvement at the angles closest to near-forward scattering is the fact that the forward scattering lobe becomes narrower with the increasing particle size and particle refractive index as shown in Figure 2 and reported by other investigators, e.g., [36], [37]. A detector positioned at a scattering angle of 15° , and the solid angle of 20° is capturing the first minimum in the scattered light intensity adjacent to the forward lobe.

The undersizing of the particles with lower CRI in the 90° optical cell has been previously reported, e.g., [38]; the data is consistent with modeling and experimental data presented here. The apparent diameter of the silica particles (the lowest CRI tested) is always smaller than the PSL or alumina particles at the 90-degree scattering angle. This undersizing trend is predicted by the model and observed experimentally (Figures 7–9). We find that in the forward scattering scenario this trend is not present, as the error in the particle sizing changes sign: *2 micron* silica particles are oversized by $\sim 40\%$, and *4 micron* silica particles are oversized by $\sim 45\%$. In the comparison of the results, the authors recognize that in the presented experimental setup the scattered light solid angle is greater than in the high-cost instruments and the wavelength of the illumination source may be different. The modeling results for the $\lambda=450\text{nm}$ illumination wavelength (Figure 2) have a similar trend to the results shown in the literature [39] for particles with a CRI of $m=1.5-0.0i$ and a wavelength of $\lambda=633\text{nm}$. The modeling analysis of the forward scattering angles shows the region with a lower variation of scattered light intensity at angles of $\sim 30^\circ$ and $\sim 45^\circ$.

6.1 Conclusions

The following conclusions related to the design and performance of the sensor can be made:

- Numerical Monte Carlo simulation utilizing Mie scattering code can be used for the optimization of the sensor geometry. The detector angle is optimized for a range of operational parameters and particle sizes to minimize sensitivity to the CRI. Other criteria and weighting coefficients can be used as the optimization cost function. The geometry optimization performed by the Monte Carlo simulation using Mie scattering calculations shows the feasibility of constructing a simple particle sizer with significant improvements in particle sizing over traditional designs.
- Numerical comparisons of the optimized geometry with the perpendicular and near-forward scattering models show that all angles display oscillatory sensor response vs. particle size. The optimized detector position ($\theta = 48^\circ$) shows the best results for the entire particle size range considered in this study (0.5–10 microns). The angle corresponds to the region where the scattering intensity has the weakest dependency on the CRI for the considered detector solid angle. The near-forward scattering angle had a slightly worse dependency on the CRI and had the highest scattering intensity signals. The perpendicular detector placement has the highest dependency on the CRI.
- The near-forward, optimized, and perpendicular angular detector placements are compared experimentally using monodisperse 2 μm and 4 μm particles of silica, PSL, and alumina. The data agree well with the predicted curves for all tested scenarios. Overall, the perpendicular angular range has the best precision and the worst accuracy related to the CRI variations. The optimized detector position ($\theta = 48^\circ$) has the best accuracy for both silica and alumina particles.

6.2 Limitations and Future work

Based on the geometry and operating conditions of the current experimental setup, the maximum particle concentration is about 220 particles per cubic centimeter. This can be improved by the modifications of the design and operation of the sensor, such as reducing the optical volume, increasing the particle velocity, and faster signal processing. A practical sensor design should address optimization in the sensor sensitivity, coincidence events, and the saturation limit.

Although the experiments show good agreement with the model, the data has a systematic tendency of undersizing the particles, which is likely due to the “glancing effect” related to the Gaussian intensity profile of the laser beam. Better aerodynamic particle focusing toward the middle optical volume may be needed. Sheath-air inlets and conical inlets have been shown to improve the resolution and sampling efficiency of the counters [40]; particle focusing by a forward facing step flow geometry can be used [41], the approach is similar to the studies related to aerosol stream conditioning in aerodynamic lenses [42–44].

For atmospheric science and security applications where the concentration of aerosols can be relatively low, an increase in particle concentration may be required. The overall aerosol sampling rate can be increased if the aerosol concentrator is used upstream of the detector. Virtual impactors [45] and aerodynamic lens concentrators can increase the concentration an order of magnitude. Aerodynamic lenses have low pressure drops and can reduce the size of

the particle beam; these have been recently used as inlets for atmospheric sampling applications [46] and in air-to-microfluidic interfaces [47].

6.3 Generalization comments

Flexible optimization methodologies can be tuned to a specific application during the design stage. Although this manuscript deals with optimizing the parameters to increase sizing accuracy in a low-cost optical device, the method can be used for other aerosol science applications and fields.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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NOMENCLATURE AND DEFINITIONS

CRI	Complex index of refraction
CV	Coefficient of variation, the ratio of the standard deviation to the mean
LOD	Limit of Detection
OPC	Optical particle counter
OPS	Optical particle sizer
PM	Particulate matter
R	Sensor response
RSE	Relative sizing error
I_{hor}, I_{ver}	Scattered light intensities horizontal and vertical to the plane, calculated with the Mie theory
d	Particle diameter
m = n – ik	complex index of refraction components
x = $\pi d/\lambda$	the dimensionless particle size parameter
α	detector light collection cone

λ	wavelength of light
θ	light scattering angle in x-y plane related to the position of the detector
ϕ	light scattering angle in x-z plane related to the position of the detector, also referred as the azimuthal angle

Research Highlights

- Numerical Monte Carlo simulation utilizing Mie scattering code can be used for the optimization of the sensor geometry; the method shows the feasibility of constructing a simple particle sizer with significant improvements in particle sizing over traditional designs.
- The optimized detector position ($\theta = 48^\circ$) has the lowest dependency on the particle index of refraction over the particle size range of interest (0.8–10 micron).
- The near-forward, optimized, and perpendicular angular detector placements are compared experimentally; the data agree well with the predicted curves for all tested scenarios. The optimized detector position has the best accuracy for both silica and alumina particles.
- Flexible optimization methodology can be tuned to a specific application during the design stage.

Figure 1. Schematic diagram of the miniature OPS design and the spatial coordinates for particle scattering used in the Mie scattering calculation: projection on the horizontal plane.

Figure 2.

Scattered light intensity as a function of the scattering angle for a linearly (vertically) polarized light source. Left – constant CRI, particle size range 0.5–2.0 μm . Right – $d_p = 1$ micron, CRI varied range 1.3-0i to 1.6-0i. $\theta = 0^\circ$ is forward scattering, and $\theta = 180^\circ$ is backscatter.

Figure 3.

Sensitivity of each configuration toward variations in the CRI of the particles. The flat profile with respect to the RI axis indicates better sensor response. Monotonicity can be assessed by the features in the top-panel contour plots; the less distinct the features, the more monotonic the sensor response to the particle size and CRI.

Figure 4. Coefficient of Variation (CV) for the near-forward, optimized, and perpendicular angular ranges. The particle diameter ranges from 0.1 to 10 μm and the refractive index ranges from 1.3-0i to 2.0-0i.

Figure 5.

Diagram of the experimental setup: the dry aerosolized particle enters the particle chamber, which is used as a particle source in the experiments; the geometry of the optical and flow arrangement are varied. The TSI APS 3310 provides suction and a reference for the optical cell measurements. The top view of the optical cell (blue outline) is shown in Figure 1.

Figure 6. Time-resolved signal for a 2 μm PSL particle traversing the focal volume. The abscissa is the time; the minor gradation is 19.23 μs . The ordinate shows the amplified voltage from the photodiode.

Figure 7.

Comparison of the theoretical and measured scattered light intensity for the three angular ranges. Each experimental range is shown as a marker (mean) with error bars extending to one standard deviation from the mean. The experiments include 2 μm and 4 μm monodisperse particles of silica, PSL, and alumina.

Figure 8. Experimental RSE distribution for near-forward, optimized, and perpendicular angular range using monodisperse 2 μm particles of silica, PSL, and alumina. Each dataset (color) is normalized so that the sum of the bars equals unity.

Figure 9. Experimental RSE distribution for near-forward, optimized, and perpendicular angular range using monodisperse 4 μm particles of silica, PSL, and alumina. Each dataset (color) is normalized so that the sum of the bars equals unity.

Table 1

Optimization criteria and constraints

Criterion	Description	Pseudocode	Weight	Constraint	Value
CRI Sensitivity	Coefficient of Variation	$\sigma(R) = f(d_i, CRI \text{ varied})$ $\mu(R) = f(d_i, CRI \text{ varied})$	1	Particle diameter RI – Real Part	0.1 to 10 μm 1.3 to 2.0
Monotonicity	Instances of multivaluedness	for $i = 1$ to end: $R(d_i) < \text{any}(R(d_{i-1}, i, 2, \dots))$	1	RI – Imag. Part Max Scattering Cone Angle	0 to 0.1 20°
Dynamic Range	Response range	$\frac{\max(R)}{\min(R)}$	0.3	Angular Range	15 to 165°
LOD	Scattering intensity of 0.1 μm particle	$R(d_{\text{smallest}})$	0.5	Particle shape Polarization	Spherical Linear