Parametric Model for Estimation of Mass Concentration based on Particle Count Distribution for Ambient Air Monitoring

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Abstract. The application of optical based instrument in particulate matter monitoring has gained interest among researchers in recent years due to their high degree of automation in providing real time reading of particulate matter concentrations. Such instrument usually comes in compact form making it compatible for in-situ monitoring especially for dense monitoring network. Theoretically, optical based instrument is unable to measure the mass concentration of particulate matter which is the key parameter in air quality monitoring. Instead, the mass concentration is calculated based on particle size distribution under assumptions that all particles is spherical using a known density. This being said, the accuracy of the reported mass concentration by optical instrument can be easily deteriorated if one of these assumptions is violated. Therefore, there is a need for a thorough evaluation on the particle to mass conversion factor in order to improve the accuracy of the reported mass concentrations by an optical instrument. In this study, the reported mass concentration from an optical based instrument as a function of particle distribution through random air sampling was investigated. The obtained data was then used to develop a parametric model for calculation of particulate mass concentration based on particle count distribution. The model developed was evaluated at several site and reported a good accuracy with high correlation ($R^2 > 0.97$) in estimation of mass concentration.

1. Introduction
The application of optical based instrument in particulate matter monitoring has gained interest among researchers in recent years due to their high degree of automation in providing real time reading of particulate matter concentrations. Besides that, such instrument also comes in lower price in comparison with the conventional Federal Reference Method (FRM) and Federal Equivalent (FEM) instrument making it highly compatible for dense network monitoring deployment. Its compact form also makes it feasible for real time in situ monitoring [1-3].
Despite being highly advantageous, the performance of optical based instrument for particulate matter monitoring still remains a stigma especially among researchers who needs highly accurate data [4-5]. Theoretically, optical based instrument does not directly measure the mass concentration of particulate matter which is the key factor in air quality monitoring. Instead the mass concentration is calculated based on particle size distribution under assumptions that all particles is spherical and density is known [6-7]. This being said, the accuracy of the reported mass concentration by optical instrument can be easily deteriorated if one of these assumptions is violated [8].

Several previous study had evaluated the performance of these optical based instrument for particulate matter monitoring by exposing the instrument to a simulated aerosol in order to investigate the effect of particle composition and size distribution to their performance [8-11]. Based on the studies, both particle composition and particle count have significant impact on the performance of these optical instruments. Exposure to different type of particle composition (Sodium Chloride, Sucrose and Ammonium Nitrate) of the same concentration tend to report different mass concentrations, where organic compound tends to overestimate the mass concentration reading [9].

The fact that the reported particulate mass concentration from an optical based instrument may vary depending on particle size variation, there is a need for continuous evaluation. The application of an accurate density factor is crucial in the calculation of particle count to mass conversion. The aim of this study was to investigate the relationship between particle count and particle mass from an optical based instrument. Based on the correlation, a Parametric Model for Estimation of Mass Concentration based on Particle Count Distribution for Ambient Air Monitoring was developed and evaluated at several site.

2. Research Approach

2.1 Reference Instrument

The instrument used in this study was the PurpleAir-II (PA-II) which is an optical based instrument capable of reporting both particle mass and particle count simultaneously. This instrument detects particle count in six sizes ranges from 0.3µm to 10µm as well as particle mass for PM 1.0, PM 2.5 and PM 10.0 using two sets of algorithms namely the AT and CF. The selection of the PA-II was due to its excellent correlation when evaluated alongside the Federal Equivalent Method (FEM) [12] as shown in Table 1.

| Instrument | Evaluation Period | R²   |   |   |
|------------|-------------------|------|---|---|
|            |                   | PM 1.0 | PM 2.5 | PM 10.0 |
| BAM        | 1 Hour            | N/A   | 0.9208 | 0.640   |
|            | 24 Hour           |       | 0.9721 | 0.7475  |
| GRIMM      | 1 Minute          | 0.9849 | 0.9785 | 0.7037  |
|            | 1 Hour            | 0.9891 | 0.9831 | 0.7235  |
|            | 24 Hour           | 0.9928 | 0.9873 | 0.7833  |

Table 1. Evaluation Summary between PA-II and FEM instrument.
2.2 Observed Parameters

In this study, the particle count from the PA-II was categorized into 5 smaller range based on their aerodynamic diameter as follow:

- **A**: 0.3 – 0.5 µm
- **B**: > 0.5 – 1.0 µm
- **C**: > 1.0 - 2.5 µm
- **D**: > 2.5 – 5.0 µm
- **E**: > 5.0 – 10.0 µm

The smallest particle diameters that is detectable by the PA-II is 0.3 µm whereas for the maximum particle diameter size, the range is only up to 10 µm as particle bigger than this diameter would not be able to enter the detection cavity [10].

For particle mass, the AT algorithm was selected in this study since the experiment was carried out in an indoor environment. The AT algorithm represents the pollutants commonly found in an indoor environment [8] and is compatible with the study site.

The instrument was set to continuously sample the ambient air in an indoor environment from an elevation of 1.5 m from the ground for a period of seven days from 10th March 2018 until 17th March 2018. To avoid bias, no simulated aerosol was introduced to the instrument throughout the sampling period. Figure 1 shows the sensor setup side by side with reference instrument.

![Figure 1. Sensor Setup Side by Side with Reference Instrument.](image)

3. Results and Discussion

3.1 Particle Count to Particle Mass conversion

Particulate mass concentration has always been used as an indicator in air quality monitoring [13]. Conventionally, the mass concentration is measured using the gravimetric method by weighing the mass of filter paper before and after suspension of airborne dust over a certain period, usually 24 hours [14-15]. The mass concentration from optical based instrument is calculated based on particle size distribution equation 1 [6-7]:

\[
\text{mass concentration, } \frac{kg}{m^3} = \rho \int \frac{\pi d_p^3}{6} N(d_p) \]

(1)
where \( \rho \) is the density factor, \( \frac{nd^3}{6} \) is the particle size volume in respect to the mean diameter, \( d \) and \( N(d) \) is the total number of particles in their respective range. Since the density factor used by the PA-II for conversion of particle count to particle mass was not published elsewhere, the contributing particle count range was specifically identified to respective the particle mass as follow:

- **PM 1.0**: 0.3 – 1.0 \( \mu m \) (A to B)
- **PM 2.5**: 0.3 – 2.5 \( \mu m \) (A to C)
- **PM 10.0**: 0.3 – 10.0 \( \mu m \) (A to E)

In this study only PM 1.0, PM 2.5 and PM 10.0 are correlated with the particle count as these are the most common parameters observed in air quality monitoring. The correlation between the particle mass with their respective contributing particle count is as shown in Figure 2.

![Figure 2](attachment:image.png)

**Figure 2.** correlation between the particle mass with their respective contributing particle count.
3.2 Determination of Density Function

Based on the identified contributing particle count, the density function for each of the respective particle mass were then derived using inverse of equation 1 which is given by

\[
\text{Density Function, } \rho = \frac{1}{\text{mass concentration, kg/m}^3} \times \int \frac{n d p^3}{6} N(d_p) \tag{2}
\]

where \( N \) is the total number of particle count and \( d_p \) is the average particle diameter in the contributing particle count range which was calculated as the arithmetic mean of the stated interval for range A to E as shown in Table 2.

| Range | Particle Size, µm | Sum | N | Mean Diameter, µm |
|-------|-------------------|-----|---|-------------------|
| A     | 0.4, 0.5          | 1.2 | 3 | 0.45              |
| B     | 0.6, 0.7, 0.8, 0.9, 1.0 | 4   | 5 | 0.80              |
| C     | 1.1, 1.2, 1.3, 1.4, 1.5, ... , 2.5 | 27  | 15 | 1.80              |
| D     | 2.6, 2.7, 2.8, 2.9, 3.0, ... , 5.0 | 95  | 25 | 3.80              |
| E     | 5.1, 5.2, 5.3, 5.4, 5.5, ... , 10.0 | 377.5 | 50 | 7.55              |

Using equation 2, the density function for conversion of each particle mass was determined and plotted against time as shown in Figure 3.

![Figure 3 (a). Density factor distribution for PM 1.0.](image)
As illustrated in Figure 3(a),(b) and (c) the density factor for each particle mass conversion is constantly changing over time thus violating the condition of equation 1 where the density must be a known value [16]. Therefore, in order to ensure the validation of the applied density function, correlation between total contributing particle count and density function for each of the particle mass was plotted as shown in Figure 4.
Figure 4. Regression plot between particle count and density function.

Based on the correlation, it was observed that the total contributing particle count and the density function is excellently correlated by logarithmic relation with $R^2$ is more than 0.8 for PM 1.0 and PM 2.5. However, there is no clear correlation between the density factor and contributing particle count for PM 10.0 with $R^2$ less than 0.3 hence the density function for PM 10 is neglected for further calculation. Therefore, the parametric model for estimation of density function was constructed for PM 1.0 and PM 2.5 which is given by

$$\text{Density Function PM 1.0} = 1 \times 10^{12} \times \ln \sum_b \text{particle count} - 2 \times 10^{13}$$  \hspace{1cm} (3) \\
$$\text{Density Function PM 2.5} = 6 \times 10^{11} \times \ln \sum_b \text{particle count} - 6 \times 10^{12}$$  \hspace{1cm} (4)

By using equation (3) and (4), the density function for conversion of particle count to particle mass as a function of total contributing particle count can then be determined thus fulfilling the requirement of equation (1).

3.3 Validation of Developed Model

In this study, accuracy of the developed model as shown in Equation (3) and (4) was validated by comparing the particle mass obtained using the density function from the developed model against the actual reported Particle mass from the PA-II. The comparison was made by replicating the experiment in a new site which is located in Kg Babah Bunduon, a rural area Located in Penampang, Sabah for the same 7 days period.

The particle count of 1.0 µm and 2.5µm obtained from the replicated experiment was then applied to equation (3) and (4) to obtain the density function. Using the density function, the estimated particle mass was then calculated using equation (1). A correlation analysis was then conducted to compare the actual particle mass reported by the PA-II against the estimated particle mass as shown in Figure 5.
Based on the regression plot between the estimated mass concentration against the actual mass concentration from PA-II, it was observed that there is a strong positive correlation of $R^2 > 0.9$. Therefore, the functionality of the model was proven thus making the model applicable in both indoor and outdoor environment. In this study, the correlation for PM 2.5 is slightly higher in comparison to PM 10.0. This is due to the mechanical configuration of the sensor used in this study. Since the sensor relies on small exhaust fan for its air intake mechanism, therefore, bigger particles may not be effectively drawn in to the detection chamber.

4. Conclusion
While having cost advantages over the FEM and FRM instrument, the accuracy of the reported particle mass from an optical based instrument can easily get deteriorated if the applied density factor is unknown. This study had successfully correlated the particle count and particle mass from an optical based instrument and identified the contributing particle count range to respective particle mass for PM 1.0, PM 2.5 and PM 10.0. Based on the correlation, a model for estimation of density function as a function of particle count was developed. Next, in order to evaluate the validity of this model, the experiment was replicated in a new set of outdoor environment and data from the new site was applied to the model. Based on the evaluation, the estimated particulate mass derived from the model showed positively strong correlation with the actual mass concentration with $R^2 > 0.9$. Therefore, the model is applicable for application in both indoor and outdoor environment. This model is crucial to ensure the correct density factor is being applied for derivation of particulate mass concentration by an optical instrument thus ensuring reliability and accuracy.

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