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Development of an Analytical Line Source Dispersion Model to Predict Ground Level Concentrations for Particulate Matter (PM) of Different Particle Size Ranges †

Saisantosh Vamshi Harsha Madiraju [1] and Ashok Kumar [1,]*

[1] The College of Engineering, The University of Toledo, Toledo, OH 43606, USA; smadira@rockets.utoledo.edu
[2] Affiliation 2; e-mail@e-mail.com
* Correspondence: ashok.kumar@utoledo.edu; Tel.: +1-419-530-8136
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Abstract: Particulate matter (PM) is released in varying quantity from mobile sources depending on the type of fossil fuel used in combustion. According to the USEPA, PM exposure could cause a variety of problems like premature deaths, nonfatal heart attacks, irregular heartbeat, asthma, reduced lung function, and respiratory issues. Therefore, it is necessary to predict the downwind concentrations near highways from mobile sources for protecting public from adverse health effects. The current study concentrates on developing an analytical line source dispersion model to account for different particle size ranges for particulate matter released from mobile sources. Available line source models do not consider explicitly different ranges of particle size present in the exhaust. The present study discusses the development of a dispersion model to predict downwind concentrations of PM by incorporating a range of particle sizes for an infinite and a finite length mobile source. The dry deposition of particles is also considered during development. Emission rate, wind speed, wind direction, atmospheric turbulence, and dry deposition velocity of the particles are the model inputs. The sensitivity of the model is determined by simultaneously varying the independent input variables using Monte Carlo simulation.

Keywords: Line Source Model; Dispersion; Particulate Matter; Particle size; Dry deposition; Sensitivity Analysis; Crystal Ball software.

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1. Introduction

In the US, cars and other motorized vehicles have been the source of about half of the air pollution [1]. This pollution originates in both direct tailpipe emissions and the mechanical wear of different parts of the vehicle. The major emissions from automobiles include carbon monoxide, hydrocarbons, nitrogen oxides, lead, and particulate matter [2]. The concentration of these emissions should be estimated for the implementation of federal and local regulations [3].

Particulate matter (PM) is made up of tiny particles of solids/liquids that are in the air. These particles may include dust, dirt, soot, smoke, and drops of liquid. They could affect human health irrespective of their size [4]. Breathing in particle pollution can be harmful to your health. Dust from roads, farms, dry riverbeds, construction sites, and mines are particulate matter less than 10 um (PM_{10}) [5].

Many models are available in the literature to predict the concentrations of contaminants at downwind distances from different sources. Most of these models are aerosol dynamics models considering particle size method. Each model has their own criteria for the particle size that it is used for. UHMA (University of Helsinki Multicomponent Aerosol Model) is a dispersion model developed at the University of

Helsinki with a focus on growth and development of new particles. The model is evaluated in the studies conducted by Pitjola et al and Korhonen et al [6], [7]. MONO32 is a model containing 4 size modes and follow monodisperse approach especially for the particle size between 7- 450 nm. This model was examined and evaluated by Pohjola et al within 25 seconds after the emission [8]. AERO is a dispersion model developed for the particle sizes between 0.01-10μm with 8 size distribution sections and composition was assumed to be uniform [9]. GATOR (Gas Aerosol Transport Radiation Model) is a Eulerian dispersion model used for the moving size or the stationary size particles in urban and meso-scale environments [10]. MADRID (Model of Aerosol Dynamics, Reaction, ionization and Dissolution) is developed for multiple size particles [11]. AEROFOR2 is a sectional box model considering 200 evenly distributed sections for the particle size method and externally or internally mixed varying within each size group distributed logarithmically. URM is a Eulerian dispersion model containing four groups under 10μm size. RPM model is considered for the particle sizes between 0.01-0.07μm. CIT model developed by California Institute of Technology is for the particle sizes between 0.5-10μm. All the discussed models consider the effect of condensation/evaporation. The phenomenon of coagulation is considered by all the above-mentioned models except URM and CIT in simulating predictions. The effect of dry deposition is incorporated in all the discussed models. However, the effect of wet deposition is considered only by AEROFOR, URM, and RPM [12].

The literature shows that the reported models for the estimation of concentrations are not designed for releases from mobile sources. This study develops SLINE PM 1.0 that could be used to calculate the ground level concentrations of the PM considering different particle size ranges. The model is developed for an infinite and a finite-length source.

2. Model Development

The basic approach to developing the SLINE PM 1.0 model is based on the analytical solution of the convective–diffusion equation for a velocity field represented by a power law. This allows us to incorporate the variation of the wind velocity magnitude near the ground during the dispersion of PM released from mobile sources. The concentration Equation (1) given by Ermak [13]; and used by Nimmatoori and Kumar [14] for a point at (x, y, z) from an elevated source is used for developing SLINE PM 1.0.

$$C_{(x,y,z)} = \frac{q}{2\pi\sigma_y\sigma_z u}\exp\left\{\frac{-y^2}{2\sigma_y^2}\right\}\exp\left\{\frac{-V_g(z-h)}{2K}-\frac{V_g^2\sigma_z^2}{8K^2}\right\}\left[\exp\left\{\frac{-(z-h)^2}{2\sigma_z^2}\right\}+\exp\left\{\frac{-(z+h)^2}{2\sigma_z^2}\right\}-\sqrt{2\pi}\frac{V_1\sigma_z}{K}\exp\left\{\frac{V_1(z+h)}{K}+\frac{V_1^2\sigma_z^2}{2K^2}\right\}erfc\left\{\frac{V_1\sigma_z}{\sqrt{2}K}+\frac{z+h}{\sqrt{2}\sigma_z}\right\}\right] \quad (1)$$

where,

$C_{(x,y,z)}$ = concentration (units/m^3)
q = emission rate (units/s)
u = wind speed (m/s)
σ_y = horizontal dispersion coefficient (m)
σ_z = vertical dispersion coefficient(m)
z = the height measured from the surface of the ground (m)
h = height of the source.
$V_1 = (V_d - V_g)/2$
V_d = dry deposition velocity of the particle (m/s)
V_g = gravitational settling velocity of the particle (m/s)
K = eddy diffusivity(m^2/s)

The profiles of wind velocity and eddy diffusivity at a given downwind distance are given by $u = u_1(\frac{z}{z_1})^m$ and $K = K_1(\frac{z}{z_1})^n$ respectively.

The downwind concentrations from a line source are obtained by integrating the Equation (1) for a point source. There are two choices while carrying out the integration depending on the choice of length of the line source.

The finite length (Y) equation given by Nimmatoori and Kumar [14] is adopted for calculating downwind concentrations. They obtained the Equation (2) by integrating Equation (1) from -Y/2 to Y/2.

$$C_{(x,y,z)} = \frac{q}{2\sqrt{2\pi}\sigma_z u}\exp\left\{\frac{-V_g(z-h)}{2K} - \frac{V_g^2\sigma_z^2}{8K^2}\right\}\left[\exp\left\{\frac{-(z-h)^2}{2\sigma_z^2}\right\} + \exp\left\{\frac{-(z+h)^2}{2\sigma_z^2}\right\} - \sqrt{2\pi}\frac{V_1\sigma_z}{K}\exp\left\{\frac{V_1(z+h)}{K} + \frac{V_1^2\sigma_z^2}{2K^2}\right\} erfc\left\{\frac{V_1\sigma_z}{\sqrt{2}K} + \frac{z+h}{\sqrt{2}\sigma_z}\right\}\right]\left[\mathrm{erf}\left(\frac{\frac{Y}{2}}{\sqrt{2}\sigma_y}\right) - \mathrm{erf}\left(\frac{-\frac{Y}{2}}{\sqrt{2}\sigma_y}\right)\right] \quad (2)$$

An infinite length source equation was derived from Equation (1) and is given as Equation (3) for computing ground level concentrations.

$$C_{(x,y,z)} = \frac{q}{\sqrt{2\pi}\sigma_z u}\exp\left\{\frac{-V_g(z-h)}{2K} - \frac{V_g^2\sigma_z^2}{8K^2}\right\}\left[\exp\left\{\frac{-(z-h)^2}{2\sigma_z^2}\right\} + \exp\left\{\frac{-(z+h)^2}{2\sigma_z^2}\right\} - \sqrt{2\pi}\frac{V_1\sigma_z}{K}\exp\left\{\frac{V_1(z+h)}{K} + \frac{V_1^2\sigma_z^2}{2K^2}\right\} erfc\left\{\frac{V_1\sigma_z}{\sqrt{2}K} + \frac{z+h}{\sqrt{2}\sigma_z}\right\}\right] \quad (3)$$

The expressions for the horizontal and vertical dispersion coefficients for stable conditions are given as Equation (4) and Equation (5); and for unstable conditions are given as Equation (6) and Equation (7). These equations are based on the work of Snyder et al. [15] and include an additional term m_t to account for the additional vertical spread due to the vehicular turbulence as suggested by Madiraju and Kumar [16].

$$\sigma_z = a\frac{u_*}{U_e}x\frac{1}{\left(1+b_s\frac{u_*}{U_e}\left(\frac{x}{L}\right)^{\frac{2}{3}}\right)} + m_t \quad (4)$$

$$\sigma_y = c\frac{\sigma_v}{u_*}\sigma_z\left(1 + d_s\frac{\sigma_z}{|L|}\right) \quad (5)$$

$$\sigma_z = \mathrm{a}\frac{u_*}{U_e}x\left(1 + b_u\frac{xu_*}{LU_e}\right) + m_t \quad (6)$$

$$\sigma_y = c\frac{\sigma_v}{u_*}\sigma_z\left(1 + d_u\frac{\sigma_z}{|L|}\right)^{-\frac{1}{2}} \quad (7)$$

where, u_* is the surface friction velocity, U_e is the effective wind speed, L is the Monin-Obukhov length, m_t is vertical spread due to the turbulence created by the vehicles.

m_t is computed using the formulation given by Madiraju and Kumar [16] : m_t= (1.7*H)/2.15, where H is the height of the vehicle.

The values of the parameters: a, c, b_s, d_s b_u, and d_u are also taken from Snyder et al [15]. These coefficients depend on the atmospheric stability conditions.

Note that the K is assumed to be constant with downwind distance 'x' in Equation (3) during its derivation. The value of K is determined by the Equation (8) considered from Rao [17]; and Nimmatoori and Kumar [14].

$$K = \frac{\sigma_Z^2 u_1}{2x} \quad (8)$$

Use of Equation (8) at different downwind distances indicates that K is a function of x. It is assumed that the model will perform better if the value of K is updated at each downwind distance.

The dry deposition velocity (V_d) and gravitational settling velocity (V_g) of the particles are computed using the algorithms used in the AERMOD by USEPA [18]. The expressions are given as Equations (9) and (10)

$$V_d = \frac{1}{R_a + R_p + R_a R_p V_g} + V_g \quad (9)$$

where,

R_a = Aerodynamic resistance (s/m)

R_p = Quasi-laminar sublayer resistance

$$V_g = \frac{(\rho - \rho_{air}) g d_p^2 C_2}{18\mu} S_{CF} \quad (10)$$

where,

P = particle density (g/cm³),

ρ_{air} = air density (g/cm³),

d_p = particle diameter (μm),

g = acceleration due to gravity (m/s²),

μ = absolute viscosity of air (g/cm/s),

C_2 = air unit's conversion constant (cm²/μm²), and

S_{CF} = slip correction factor (dimensionless).

3. Application of the model

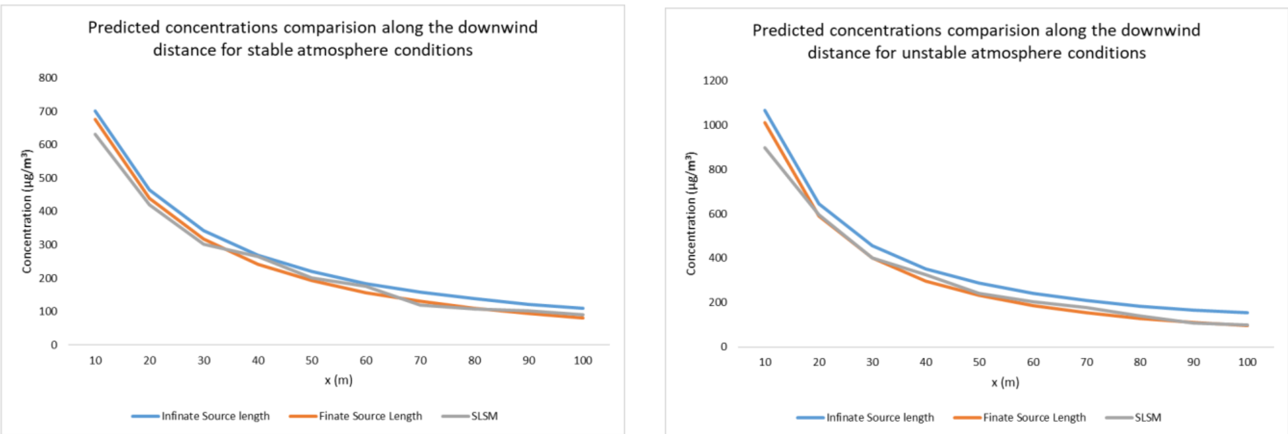
The developed model is applied as follows depending on the availability of particle size profile for emitted PM.

1. Emission data with given particle size profile: If the input data available to run simulation to predict the ground level concentration of the PM include the details on distribution of the particle sizes then the formulation provided in the Equation (2) and Equation (3) is first applied to each range of particle size distribution. The total particulate concentration (C_{TP}) will be sum of concentrations for each size range.
2. Emission data with no particle size distribution: If the input data available to run simulation to predict the ground level concentration of the PM does not include the detailed distribution of the particle sizes then the formulation provided in the Equation (2) and Equation (3) is used.

4. Model results

A test case was developed using data collected from the literature to perform the simulations. The source information, meteorological data, and the surrounding terrain input data was considered from the Snyder et al [15], [19] and Nimmatoori and Kumar [14], [20]. The atmospheric stability input parameters such as Monin-Obukhov length (L), friction velocity (u_*), and convective velocity (w_*) are considered from the field data used by Snyder et al. They are needed to compute the R_a and R_p in the Equation (9). All the other input parameters were considered from the AERMOD User's Guide by USEPA [18], [21] .

The model results are generated for the SLINE PM 1.0 model using the Equation (2) for the finite length source of length 1 kilometer and Equation (3) for an infinite length source. These results are compared in Figure 1 with the concentrations calculated using a simple line source model (SLSM) given in the textbook by Wark et al [22].



(a) (b)

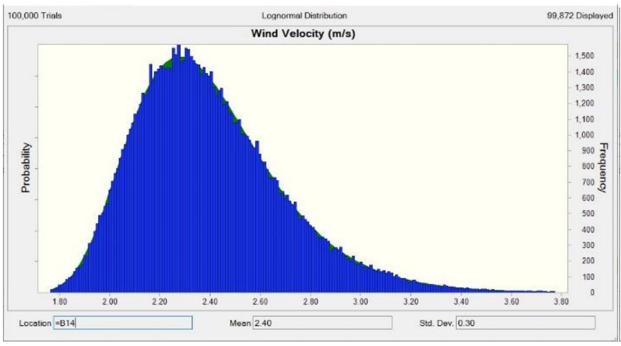
Figure 1. Comparison of simulated concentrations using finite, infinite and SLSM models.

The particle size in exhaust gases varies from 0.23 – 10 μm. The concentrations in the Figure 1 represent the total particulate concentration (summation of all the PM sizes). Figure 1 (a) represents the test case results under stable atmosphere condition and Figure 1 (b) represents the test case results for the unstable atmospheric conditions. The concentrations for different downwind distances up to 100 m from the source are shown.

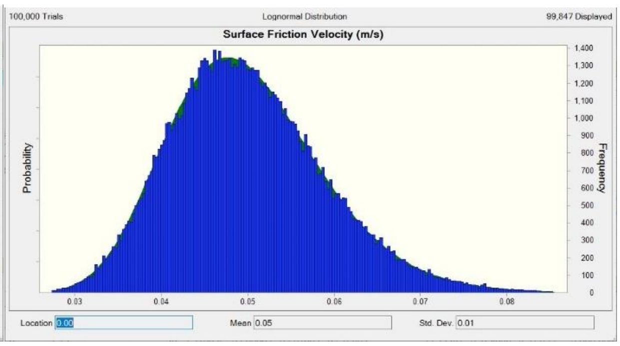
As expected, the concentration of the pollutants is decreasing with the incremental downwind distance. However, it was observed from the computed concentrations for the infinite length source model are more than the concentrations of the PM predicted by the finite length source model. The finite length source model results are closer to the values of the SLSM model. Future model evaluations with the field data will clarify the choice of the model.

5. Sensitivity

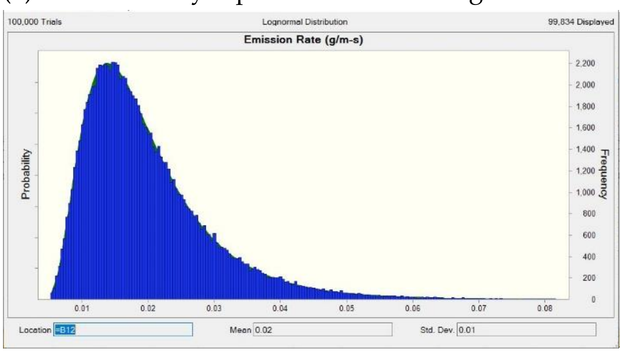
The sensitivity analysis of a dispersion model is the quantification of uncertainty in the model output concentrations based on its input variables/parameters. Currently, many tools are available to perform sensitivity analysis. In this study, the sensitivity analysis was performed on SLINE PM 1.0 using the Crystal Ball Software (version 11.1.2.4) **[23]** . The software allows to study the sensitivity by simultaneously varying all the input variables. Two test cases were considered in this study to assess the sensitivity of the input parameters/variables for the SLINE PM 1.0 representing each atmospheric stability. The selected input variables/parameters required for running SLINE PM 1.0 include emission rate of the pollutant (q), wind velocity at reference height (u_1), the coefficient a, coefficient b_s (only for stable conditions), coefficient b_u (only for unstable conditions), surface friction velocity u_*. The maximum and minimum values for these variables were chosen based on the different distributions (e.g.: normal distribution, lognormal distribution) used for each input. The distributions were selected based on the preliminary conducted on the literature.

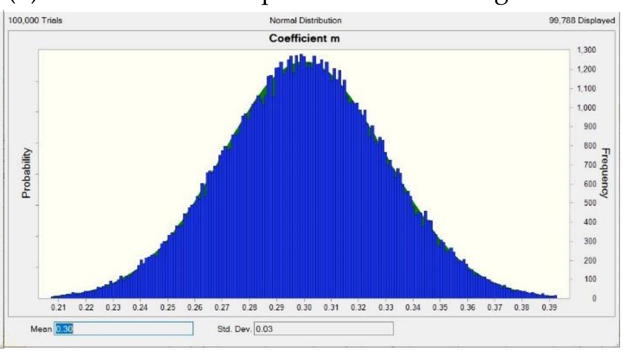


(a) Wind velocity input distribution range

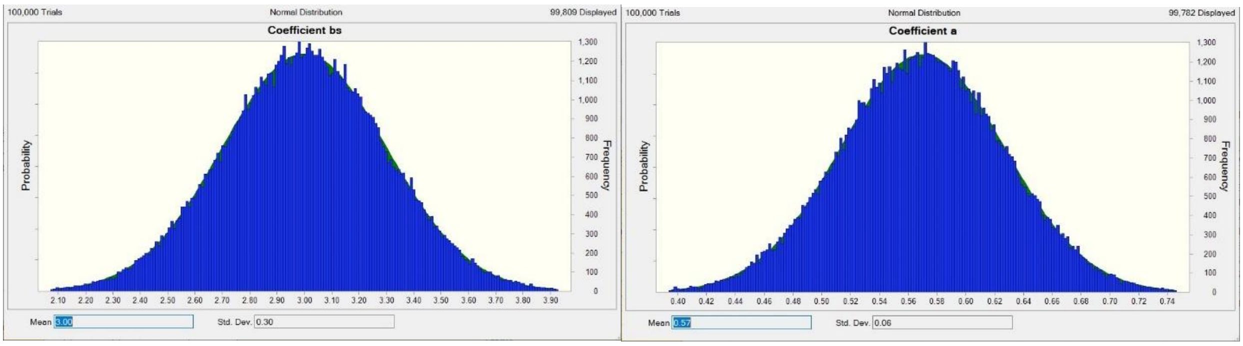


(b) Surface Friction input distribution range



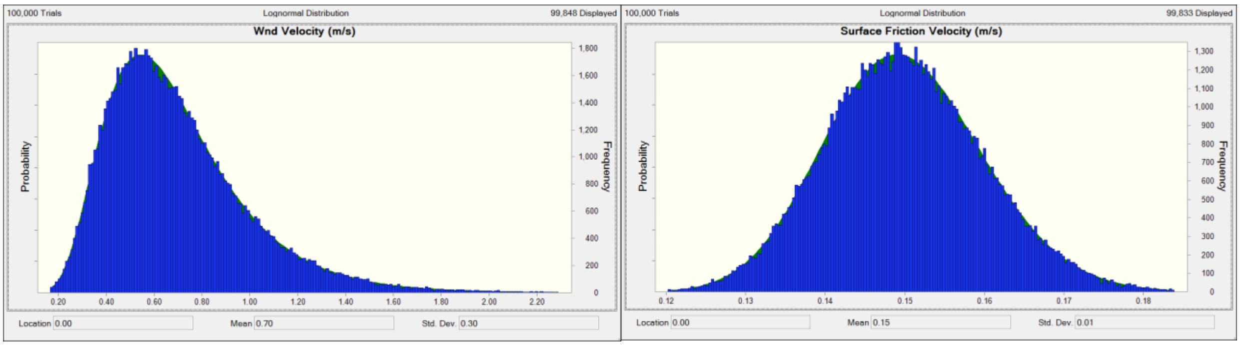


(c) Emission Rate input distribution range (d) Coefficient m input distribution range

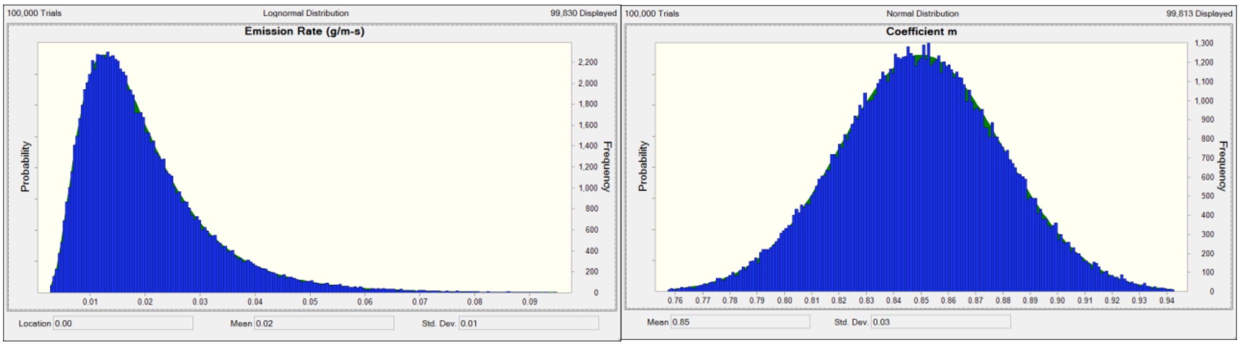


(e) Coefficient *m* input distribution range (f) Coefficient *a* input distribution range

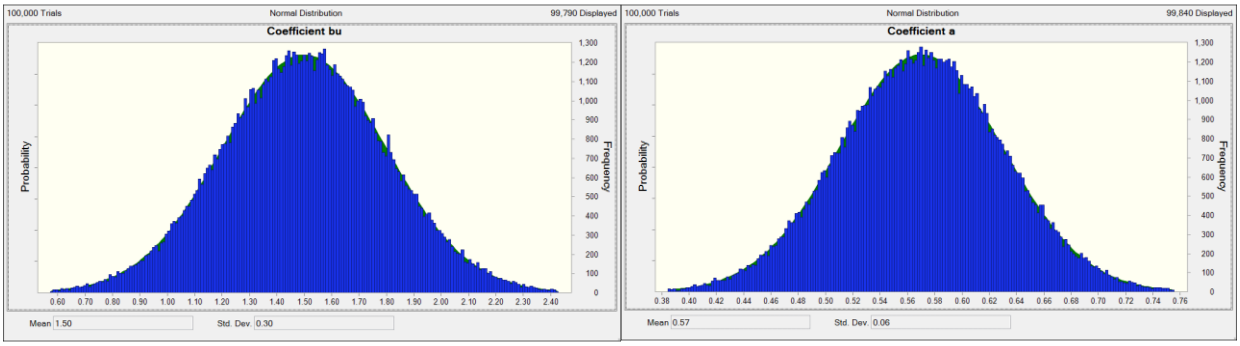
Figure 2. The independent input variables distribution rage considered for the sensitivity analysis for stable conditions.



(a) Wind velocity input distribution range (b) Surface Friction input distribution range

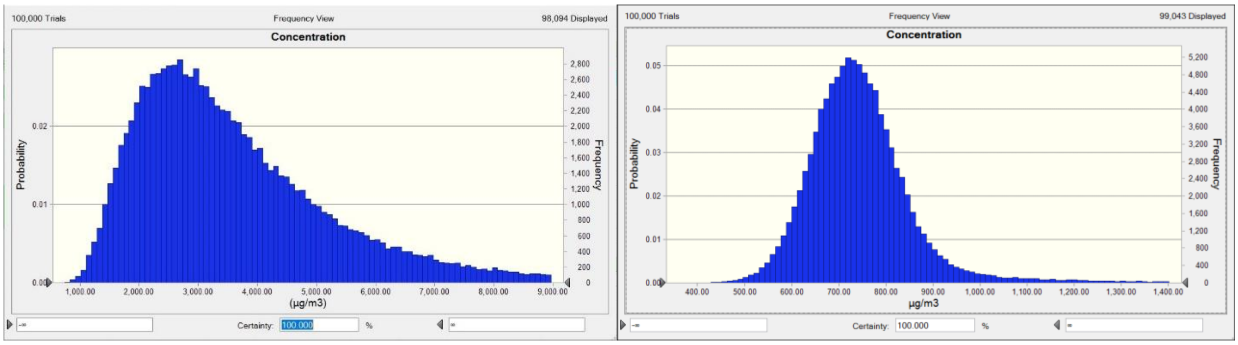


(c) Emission Rate input distribution range (d) Coefficient m input distribution range

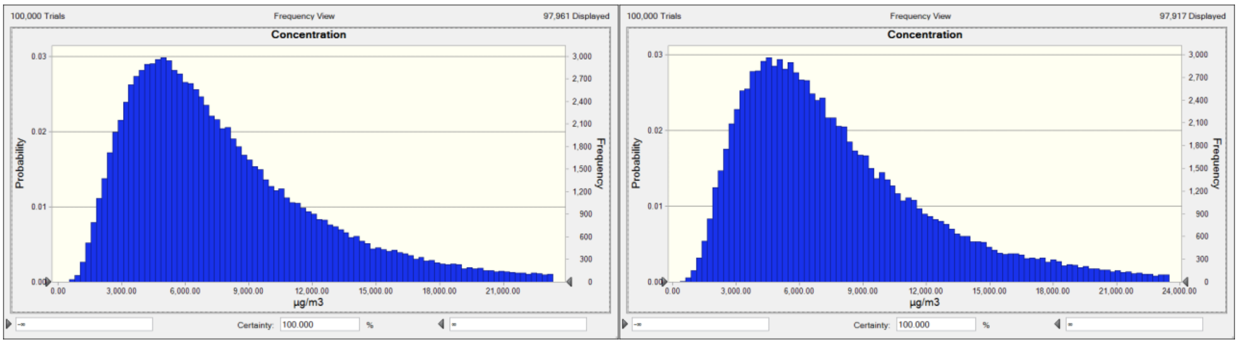


(e) Coefficient *m* input distribution range (f) Coefficient *a* input distribution range

Figure 3. The independent input variables distribution rage considered for the sensitivity analysis for unstable conditions.

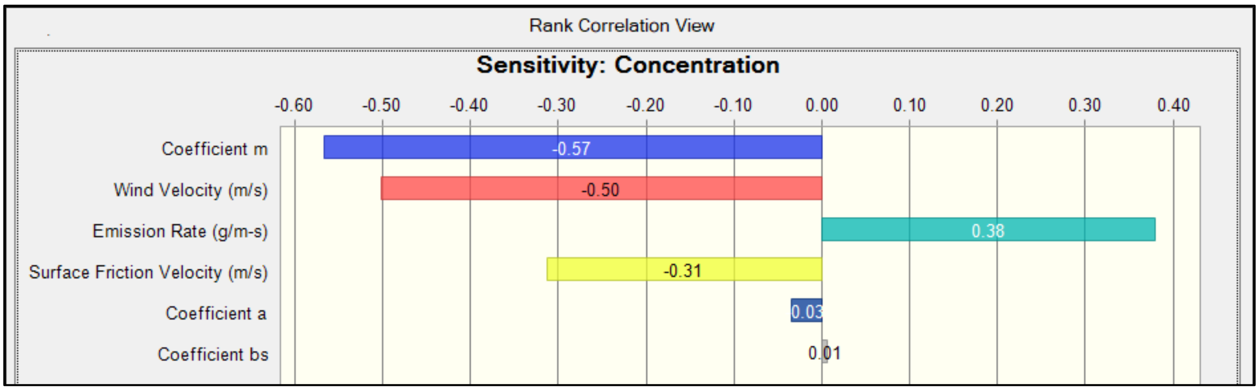


(a) Infinite – Stable Condition (b) Finite –Stable Condition

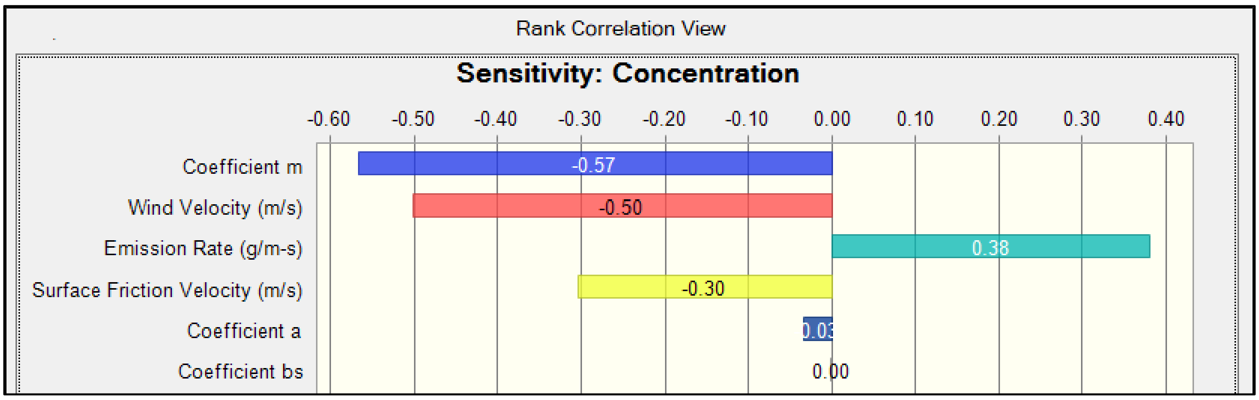


(c) Infinite – Unstable Condition (d) Finite – Unstable Condition

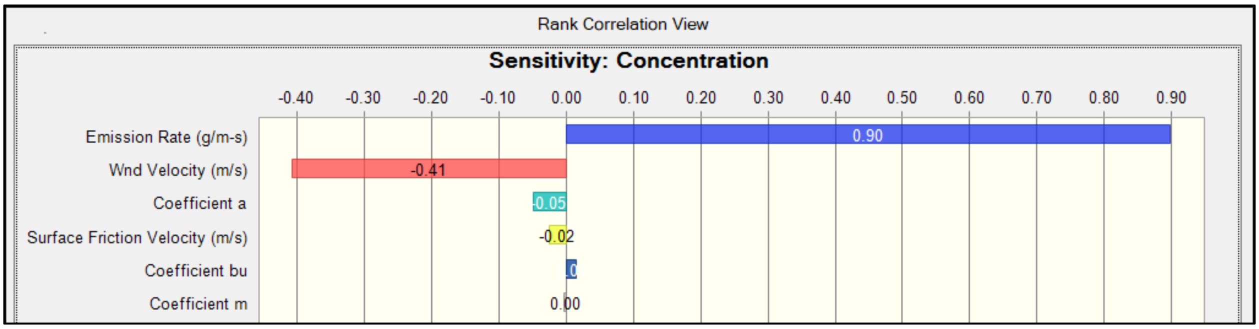
Figure 4. The simulated concentration distribution for infinite and finite length source respectively for stable atmospheric conditions.



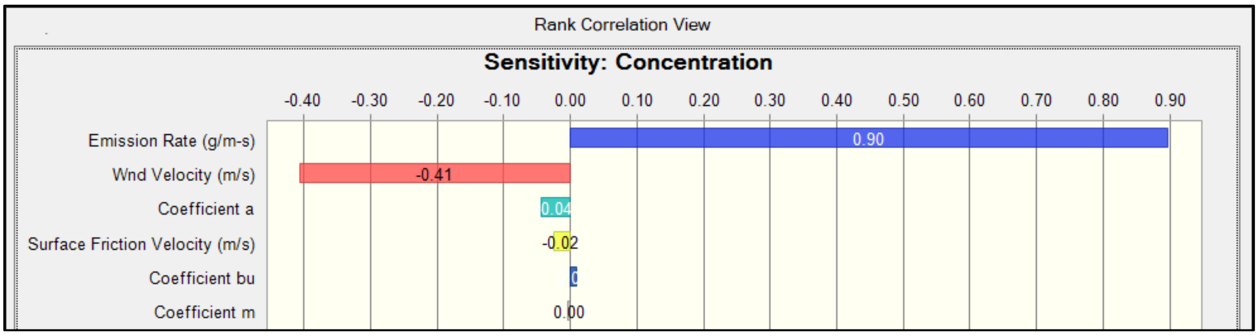
(a) Sensitivity analysis results for the Infinite length source for stable condition.



(b) Sensitivity analysis results for the finite length source for stable condition



(c) Sensitivity analysis results for the Infinite length source for unstable condition



(d) Sensitivity analysis results for the finite length source for unstable condition

Figure 5. The sensitivity analysis results using Crystal Ball (version 11.1.2.4).

The simulations were executed for each input variable/parameter in the pre-defined ranges by running the 100,000 trials. The distribution of the variables in the considered range for both stable and unstable conditions is represented in Figures 2 and 3. The concertation simulations were also computed for the 100,000 trials to identify the sensitivity that the SLINE PM 1.0 model shows towards the considered input variables/parameters.

The sensitivity results were computed using the Crystal Ball software (version 11.1.2.4) and are shown in Figure 4. The results are displayed in terms of the rank correlation coefficient. The rank correlation is always in the interval [-1, 1] and is invariant under any monotonic increasing transformation of the data. In the current sensitivity analysis, the rank correlation is used to assess the level of significance of the relation between the input variable/parameters and the predicted concentration. The "-/+" signs denote the negative or positive correlation and the value represents the significance of correlation **[24]**.

Figures 5 (a) and 5 (b) indicate that the sensitivity to compute downwind concentrations are very similar for all the variables considered under stable condition. These results show that the model SLINE PM 1.0 is most sensitive to the coefficient *m*, followed by the reference wind velocity (u_1). The model is moderately sensitive to the emission rate (q) and surface friction velocity (u_*); and almost insensitive to the coefficient a and coefficient b_s. Thus, the concentrations predicted by SLINE PM1.0 is sensitive to wind velocity and emission rate. One would expect this result for a typical dispersion model.

Figures 5 (c) and 5 (d) show that the sensitivity to compute downwind ground level concentrations are similar for all the variables under unstable condition. The model is most sensitive to the emission rate (q), followed by reference wind velocity (u_1) for both infinite and finite-length sources. This model is slightly sensitive to the coefficient a and surface friction velocity (u_*) and almost insensitive to the coefficient b_u and coefficient m .

Overall, the sensitivity analysis determines the effect of the variation of the input parameters on final concentrations obtained using the SLINE PM 1.0 model. In general, the analysis shows that emission rate (q) is positively corelated and velocity is negatively corelated. The surprising result is that the variables related to dispersion coefficients show very little sensitivity. This result is different than the one reported by Harsha and Kumar **[16], [25]–[27]** using ASTM method and Sensitivity–Index method. The primary reason for different conclusion is that the Crystal Ball simultaneously changes all the variables like real life situations to determine the sensitivity.

6. Conclusions

Overall, this study presents the development of SLINE PM 1.0, an analytical line source dispersion model to predict ground level concentrations for PM in different particle size ranges. Separate dispersion equations are presented for the infinite and finite length sources. The total concentrations computed using the developed equations were compared with a simple line source model SLSM available in the textbook.

The model sensitivity is determined using the Crystal Ball software (version 11.1.2.4). Rank correlation coefficient is used to identify the sensitivity of the SLINE PM 1.0 model to the input variables: emission rate of the pollutant (q), wind velocity at reference height (u_1), the coefficient a, coefficient b_s (only for stable conditions), coefficient b_u (only for unstable conditions), surface friction velocity u_*, and the exponent of power-profile. The sensitivity analysis results indicate that the SLINE PM 1.0 model is highly sensitive to the emission rate and wind velocity.

The model should be evaluated using the data from field studies.

Supplementary Materials: Not Applicable

Author Contributions: Conceptualization, A.K., S.V.H.M.; Investigation, A.K., S.V.H.M.; Methodology, A.K., S.V.H.M.; Project administration, A.K.; Supervision, A.K.; Validation, A.K.; Writing—Original draft, S.V.H.M.; Writing—Review & editing, A.K. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

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