

Science and Technology for the Built Environment

ISSN: 2374-4731 (Print) 2374-474X (Online) Journal homepage: http://www.tandfonline.com/loi/uhvc21

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To cite this article: Jamiu Adetayo Adeniran, Dauda Olurotimi Araromi, Rafiu Olasunkanmi Yusuf, Lukuman Adekilekun Jimoda, Emmanuel Olusola Oke & Jacob Ademola Sonibare (2018): Analytical modeling of human exposure from short-term point source releases of aerosols from household spray products, Science and Technology for the Built Environment

To link to this article: https://doi.org/10.1080/23744731.2018.1499383

Accepted author version posted online: 11 Jul 2018.

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Analytical modeling of human exposure from short-term point source releases of aerosols from household spray products

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Abstract

Indoor air measurements of aerosols emitted from the use of household spray products are expensive and time-consuming. An analytical model was developed and incorporated into a graphical user interface to quantify exposure as a function of distance and time. The model considered point source dispersion with reflection from a wall and aerosol concentration decay due to air exchange rate and

deposition. Aerosol concentration decreased with respect to increase in time and distance from the release point. There was no significant difference between the developed model and experimental results. The developed model could be used to adequately predict indoor human exposure to aerosols as a function of distance and time.

Keywords: Indoor air, model, exposure, aerosols, spray product

Summary

A simple, inexpensive and fast model incorporated in a graphical user interface (GUI) was developed for predicting the fate of aerosols from spray product

Higher concentrations of aerosols were observed and predicted using the developed model in the proximity of the source location.

Modeled and experimental measurements were close

The developed model can be used to adequately predict the fate of aerosol released from household product as a function of distance and time at the same time.

The developed soft sensor could serve as guide to relevant stakeholders as regards policy formation and implementation.

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1.0 Introduction

Household spray products are used worldwide on daily basis. Studies have established that aerosols generated from the use of these products have deleterious health and environmental consequences

ranging from cancer to death (1-6). The use of household spray product in indoor environment can cause an increase in the concentrations of airborne gaseous and particulate matter(7-10). Pollutants in the indoor air are 1000 times more likely to be inhaled than pollutants in outdoor air due to the long resident times and room concentrations (11). Both indoor and outdoor sources contribute and affect the concentration and composition of particles in indoor environment.

Zhang and Chen (12)opined that the dispersion of aerosols over time in indoor space after release has to be predicted with reasonable accuracy in order to predict the exposure of individuals to the aerosols. Information on emission characteristics, such as emission factors or emission rates, of outdoor particle sources is usually more available than the indoor sources (13, 14). However, quantification of emissions from indoor sources is very important for the assessment of the total human exposure to particles. The concentration of indoor air pollutants is strongly influenced by the rate of transport and irreversible deposition onto surfaces in the indoor environment (15-19). The transport rate depends on movement of indoor air, and the molecular diffusivity of pollutants(20, 21).

The characteristics of air movement can change rapidly as ventilation systems turn on and off, windows open or close, and through convective air movement as a result of heat generated by people. Studies have sought to understand aerosol transport through mathematical modeling (22-24). and measurements (25) but these measurements are sparse, expensive and often time-consuming (26). Prediction of aerosols transport in the indoor environment is crucial to the welfare of consumers. Exposure models would be required to provide estimates of aerosol decay and exposure. Therefore, the aim of this study is to develop mathematical model to predict human exposure to aerosols released from household spray products as a function of distance and time.

2.0 Methodology

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Representative indoor Environment showing aerosol spraying and the corresponding concentration decay routes through deposition and air exchange rate is as depicted in Figure 1. It was assumed that concentration decay in x-direction applies to other directions.; particles concentration decay is due to fresh air ventilation $\propto (s^{-1})$ and deposition $\mathcal{K}$; Diffusion coefficient D is constant and Concentration at time t = 0, is constant.

Figure 1

The Initial distribution occupies a finite region such that the initial state is defined as

$$C = C_0, \qquad x > 0, \qquad t = 0 \qquad 1$$

The concentration C_o in the region $-L \leq x \leq L$ is maintained with the boundary Condition defined as

$$C = C_0, \qquad x = 0, \; t = 0 \qquad 2a$$

$$C = C_{e,} \qquad x = L, \qquad t = t_e \qquad 2b$$

From the first principle (Fick's law of diffusion)

$$J = -D\left(\frac{d}{dx}\right) C \qquad 3$$

where $\left(\frac{dC}{dx}\right)$ is the concentration gradient per unit length, J = Flux, and D is the diffusivity in $m^2/_S$

Taking the material balance across the elemental length change δx as a function of time (Figure 1).

$$\frac{\partial C}{\partial t} = \frac{\delta}{\delta x}[J(x) - J(x + dx)] = \frac{-\partial J}{\partial x} \qquad 4$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) \qquad 5$$

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$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad 6$$

Applying Equation 6 to concentration decay from a short-term release of aerosols from a spraying can in a room with length L, width W, and Height H, we obtain

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2}\right) - \left(\propto + \frac{Kd}{V}\right)C \qquad 7$$

where

C is particulates number concentration (particles/m^3); D is the diffusivity (m^2/s), k_d is the deposition velocity on surfaces (m/s); A is the surface area available for deposition (m^2); V is volume of the room (m^3)

$\mathcal{K}$ is defined as:

$\mathcal{K} = \frac{K_d A}{V}$;

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2}\right) - (\propto + \mathcal{K})t \qquad 8$$

Equation 8 is the equation for diffusion in one dimension when D is constant. The total amount of substance M diffusing in the room is given by:

$$M = \int_{-\infty}^{\infty} C dx\,, \qquad 9$$

and the concentration distribution for a instantaneous point source release (27):

$$C(x,t) = \frac{A}{t^{\frac{3}{2}}} e^{-(x^2/4Dt)} \qquad 10$$

If the concentration equation is that of Eqn 10:

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where

$$x^2/4Dt = \xi^2\,,\ dx = (4Dt)^{\frac{3}{2}}\,d\xi \qquad 11$$

Using these in Equation 6 gives

$$M = (4AD)^{\frac{3}{2}}\int_{-\infty}^{\infty}\exp(-\xi^2)d\xi\ =\ (4A\pi D)^{\frac{3}{2}} \qquad 12$$

Equation12 shows that the amount of substance diffusing remains constant and equal to the amount originally deposited in the plane $x = 0$. By using substitution for A from Equation 12 in Equation 10 to replace A, the following equation was obtained:

$$C(x,t) = \frac{M_{xo}}{(4\pi Dt)^{\frac{3}{2}}}e^{-(\alpha+\mathcal{K})t} \qquad 12$$

with reference to Figure 1, consider the diffusing substance in an element of width $d\xi$, to be the source of strength $C_0\ d\xi$. Then from Equation 10, the concentration at the source point, at distance ξ from the element, at time t is

$$C(\xi,t) = \frac{C_0\ d\xi}{(4\pi Dt)^{\frac{3}{2}}}\exp(-\xi^2/4Dt), \qquad 13$$

and the complete distribution due to initial distribution occupies the finite region with resulting initial state such that:

$$C = C_0\,, \qquad \xi > 0, \quad t = 0;\ C = C_0,,\ \xi = 0\,,\ t = 0 \qquad 14$$

The complete solution due to the initial distribution (Equation 14) is given by

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$$C(x,t) = \frac{C_0}{(4\pi Dt)^{\frac{3}{2}}}\int_{\xi}^{\infty} \exp(-\xi^2/4Dt)\, d\xi = \frac{C_0}{\pi^{\frac{3}{2}}}\int_{\xi/2\sqrt{(Dt)}}^{\infty} \exp(-\eta^2) d\eta, \qquad 15$$

where $\eta = \xi/2\sqrt{(Dt)}$

A standard mathematical function for which extensive tables are available is the error function, usually written as $erf\ z$ and is expressed as

$$\text{erf}\ z = \frac{2}{\pi^{\frac{3}{2}}}\int_0^z \exp(-\eta^2) d\eta \qquad 16$$

According to Crank(1975), this type of function has the following properties

$$erf(-z) = -erf\ z \quad , erf\ (0) = 0, \quad erf(\infty) = 1 \qquad 17$$

and

$$\frac{2}{\pi^{\frac{3}{2}}}\int_z^{\infty} \exp(-\eta^2)\, d\eta = \frac{2}{\pi^{\frac{3}{2}}}\int_0^{\infty} \exp(-\eta^2)\, d\eta - \frac{2}{\pi^{\frac{3}{2}}}\int_0^z \exp(-\eta^2)\, d\eta$$

$$1 - \text{erf}\ \ z = \text{erf}\, c\ \ z \qquad 18$$

where erf c is referred to as the error – function complement, the solution of (Equation 16) is usually written in form

$$C(x,t) = \frac{1}{2} C_0\, \text{erf}\ \ c\ \frac{x}{2\sqrt{(Dt)}} \qquad 19$$

The comprehensive tables of error functions are available in previous literature (27, 28)

For an instantaneous source in x-plane including the reflection term, we have

$$C(x,t) = \frac{M_{xo} e^{-(\propto+\mathcal{K})t}}{(4\pi Dt)^{3/2}} R_x \qquad 20$$

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where $C(x,t)$ is the indoor particulate number concentration (particles/m^3) at position x and time 't' in a room

M_{xo} = total number of particles released at source point (x_0)

The R_x term in Equation 20 which specifies the wall reflection term for a rectangular room is defined in previous studies (29, 30) as:

$$R_x = \sum_{i=-\infty}^{\infty} e^{-\frac{(x+2iL-x_0)^2}{4Dt}} + e^{-\frac{(x+2iL-x_0)^2}{4Dt}} \quad 21$$

Substituting Equation 20 in Equation 21, we have

$$C(x,t) = \frac{M_{xo}e^{-\left(\propto+\frac{k_dA}{V}\right)t}}{(4\pi Dt)^{3/2}} . \sum_{i=-\infty}^{\infty} e^{-\frac{(x+2iL-x_0)^2}{4Dt}} + e^{-\frac{(x+2iL-x_0)^2}{4Dt}} \quad 22$$

Recall, $\mathcal{K}$, deposition rate (/s), $\mathcal{K} = \frac{k_dA}{V}$

therefore,

$$C(x,t) = \frac{M_{xo}e^{-(\propto+k)t}}{(4\pi Dt)^{3/2}} . \sum_{i=-\infty}^{\infty} e^{-\frac{(x+2iL-x_0)^2}{4Dt}} + e^{-\frac{(x+2iL-x_0)^2}{4Dt}} \quad 23$$

The space term (R_x) was solved by expanding in negative exponentials considering reflection in both –x and + x direction, and integrating with respect to time, (t). The resulting solution is given as:

$$C(x,t) = \int_0^t \frac{M_{xo}e^{-(\propto+\mathcal{K})t}}{(4\pi Dt)^{3/2}} . \left[e^{-\left(\frac{(x-x_0)^2}{4Dt}\right)} + \sum_{i=1}^{2} e^{-\left(\frac{(x-x_i)^2}{4Dt}\right)}\right] dt \quad 24$$

Inhalation Exposure, IE, can then be described as:

$$IE = BR \int_0^t \frac{M_{xo}e^{-(\propto+\mathcal{K})t}}{(4\pi Dt)^{3/2}} . \left[e^{-\left(\frac{(x-x_0)^2}{4Dt}\right)} + \sum_{i=1}^{2} e^{-\left(\frac{(x-x_i)^2}{4Dt}\right)}\right] dt \quad 25$$

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Where BR is the breathing rate of a man which can be taken as 17 m^3/day

Equations 24 and 25 were solved using the recursive adaptive Simpson quadrature (quadv) in MATLAB 2012a. The flowchart for solving the developed model is as presented in Figure 2.

Figure 2

The model was validated using the percentage mean relative deviation modulus (MRDM) - %E as indicated in Equation 26

$$\%E = \sum \left| \frac{V_E - V_P}{V_E} \right| \quad 26$$

where V_E is the experimental value and V_P is the predicted value

Validation of the Developed Model

The description of the experimental room used for the validation of the developed model is in Figure 3 as presented in our previous study (8). Freshly calibrated Particle Counters (Model GT- 321) manufactured by MetOne Instruments Inc., USA were used to measure particulate matter (PM) number concentration of mass range of 0.3 – 5.0 µm. Each of the monitors has measuring time is 1 minutes per particle size with a flow rate of 0.1 cubic feet per minute and a concentration limit of 3,000,000 particles per cubic feet. Zero Count Filter PN G3111 was used to cater for the error that may arise from the counters. The experimental room has an area of 15.68 m^2 and a volume of 42.65 m^3. To cater for the error that may arise from the instantaneous release of aerosols, spray products were applied at the centre of the experimental room at the height of 2 m above the ground level while each of the samplers was placed at 1.5 m above the ground level. The monitors were arranged in series and placed at 0.5 m apart from one another. Particulate sizes of 0.5 and 2.0 µm were chosen as representative submicron

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and fine particles, respectively. This is because fine and submicron particles have been linked with deleterious health outcomes such as respiratory and cardiovascular diseases(31).

Figure 3: Description of the experimental room used for model validation

Source: Adeniran et al.(8)

3.0 Results and Discussion

The initial measured particulate concentrations were 7.57×10^6 and 4.48×10^5, respectively for 0.3 and 2.0 µm particles, respectively. The GUI interface was developed for the simulation (Figure 4). Figures 5a and b show the average inhaled concentration against time and distance, respectively. Aerosol diffusion in the indoor environment was expressed as a function of distance from the release point and time respectively. The results of the analytical model are similar to those obtained by Drivas, Valberg (29).

A comparison was made between the model predicted results and the Experimental results. Figures 6 and 7 show the close relationship observed between the predicted and experimental results for the change in concentration against time and distance. This is a good indication that the analytical model can be used to predict aerosol concentration profile with respect to time. The mean relative deviation error used to measure accuracy prediction were estimated as 1.2 and 1.26% for Figures 6 and 7, respectively.

MRDM of less than or equal to 10% indicates a good prediction of the experimental data and lower percentage indicates the model will predict better (32).The error lies in the 0.08 and 9.22 for the plot of concentration against time while the range of 0.04 -5.90 % were calculated for the plot of concentration against distance. These results show that the developed model can be used to predict the average concentration of particulates that can be inhaled as a result of the use of household spraying aerosol products. Higher concentration of aerosols was observed and predicted using the developed soft

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sensor in the proximity of the source location. As expected, concentration decreases with time and distance.

Figure 3

Figure 4

Figure 5a

Figure 5b

Figure 6

Figure 7

4.0 Conclusion

This study has developed a simple, inexpensive and fast model incorporated in a graphical user interface (GUI) for predicting the fate of aerosols from spray product as a function of distance and time in the indoor environment. Higher concentrations of aerosols were observed and predicted using the developed model in the proximity of the source location. The close agreement between the modeled and experimental measurements indicates that the developed model can be used to adequately predict the fate of aerosol released from household product as a function of distance and time at the same time. It is believed that the developed soft sensor could serve as guide to relevant stakeholders as regards policy formation and implementation. The graphical user interface could assist consumers in determining the concentration levels of aerosols from spray product.

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Indoor air quality problems associated with the use of spray products can be resolved efficiently and effectively by avoiding their use where practicable. Local exhaust could be used to effectively remove pollutants by removing the contaminated air outside. The ventilation system in buildings should be properly designed, operated and maintained as this will automatically dilute the concentration of pollutants faster with time and distance. Exposure to aerosols should be controlled by adjusting the time, amount and location of use to reduce potential exposures. Use of air cleaners should be encouraged in homes. Educating the general populace/ indoor occupants regarding indoor air quality is critical. People should be provided with information about contents and pollutants that may be emitted from consumer spraying products, use and proper operation of ventilation systems and strategies.

Water-based consumer products could be used instead of the propellant based ones. This will drastically reduce the exposure to volatile organic compounds. Insects control strategies such as indoor residual spraying and larviciding in which water-based chemical are used should be encouraged and subsidized by government.

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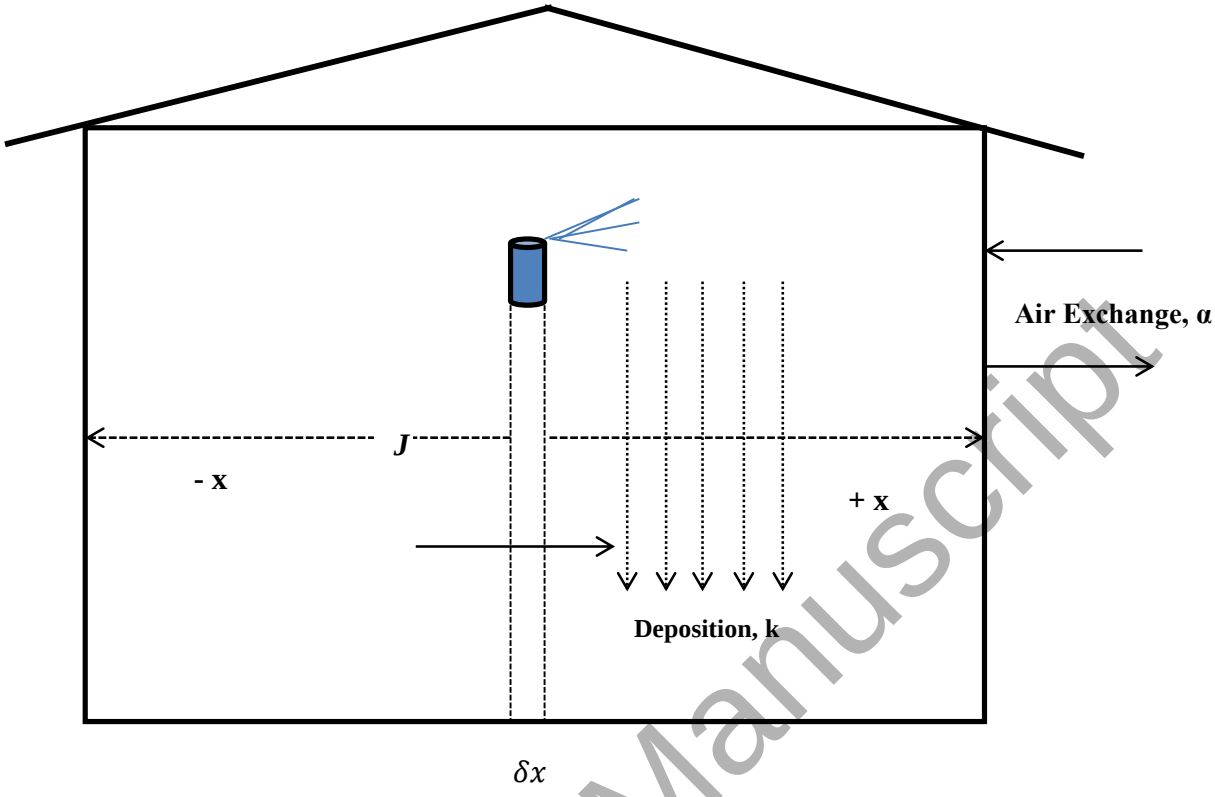
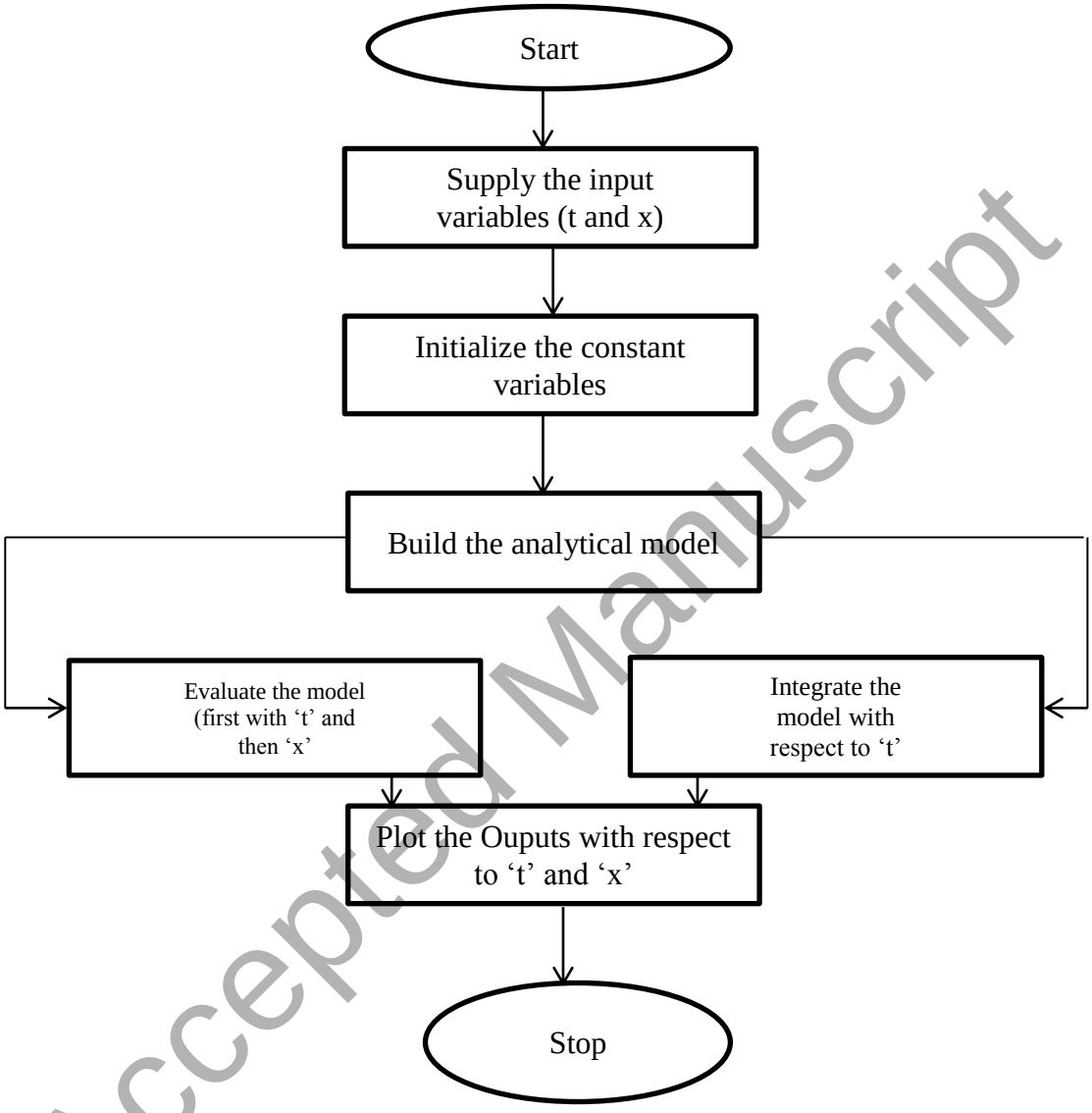


Figure 1: Representative indoor Environment showing aerosol spraying and the corresponding concentration decay routes through deposition and air exchange rate

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Figure 2: Flowchart for the implementation of the developed model

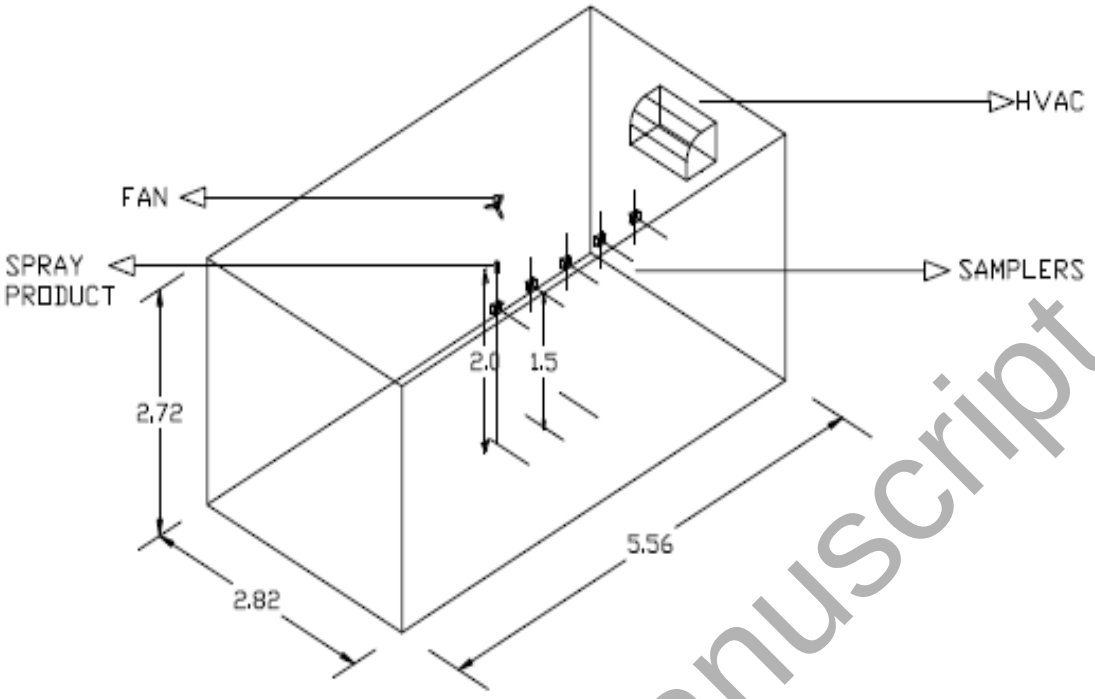


Figure 3: Description of the experimental room used for model validation

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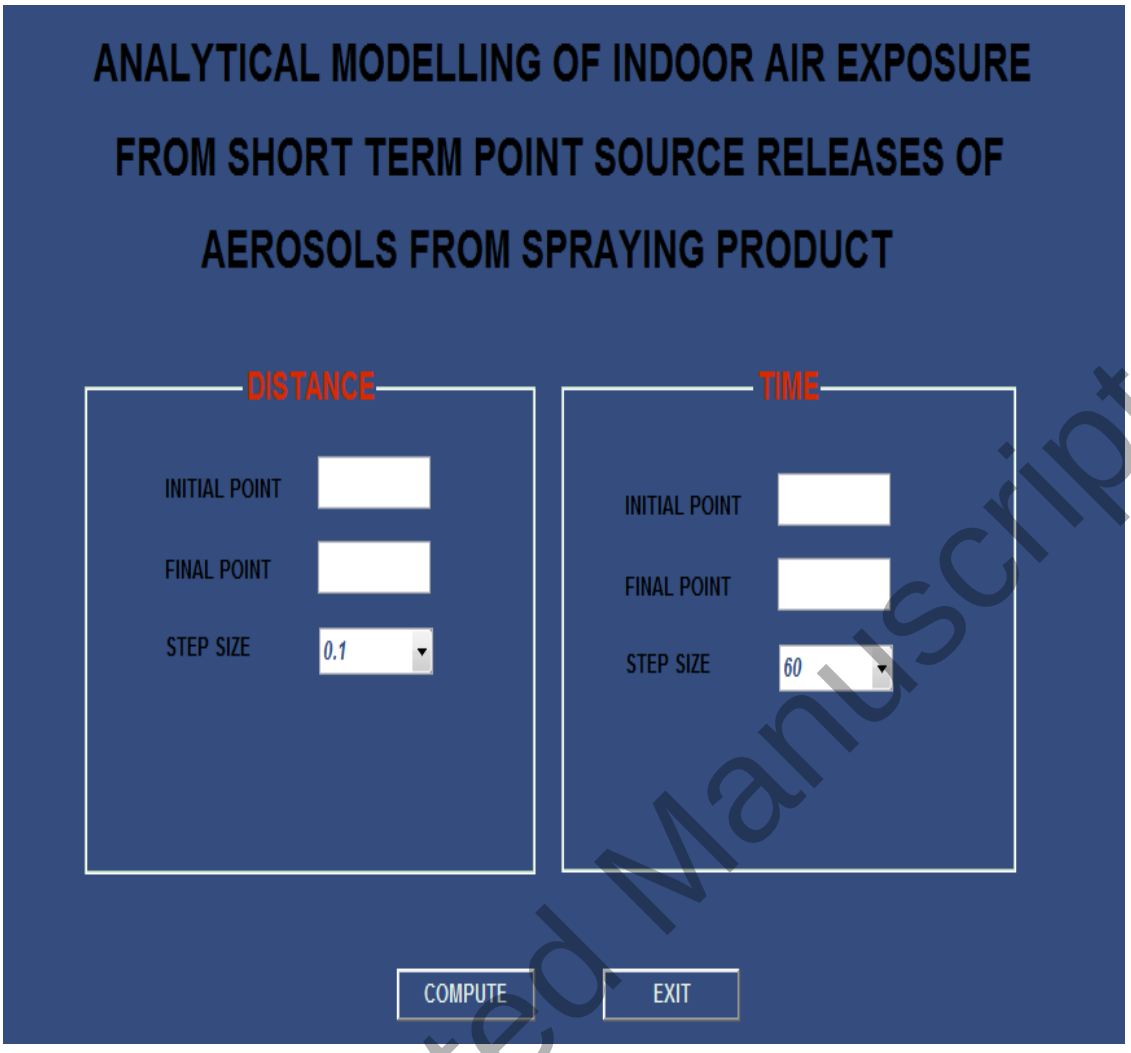


Figure 4: GUI interface for the exposure modeling

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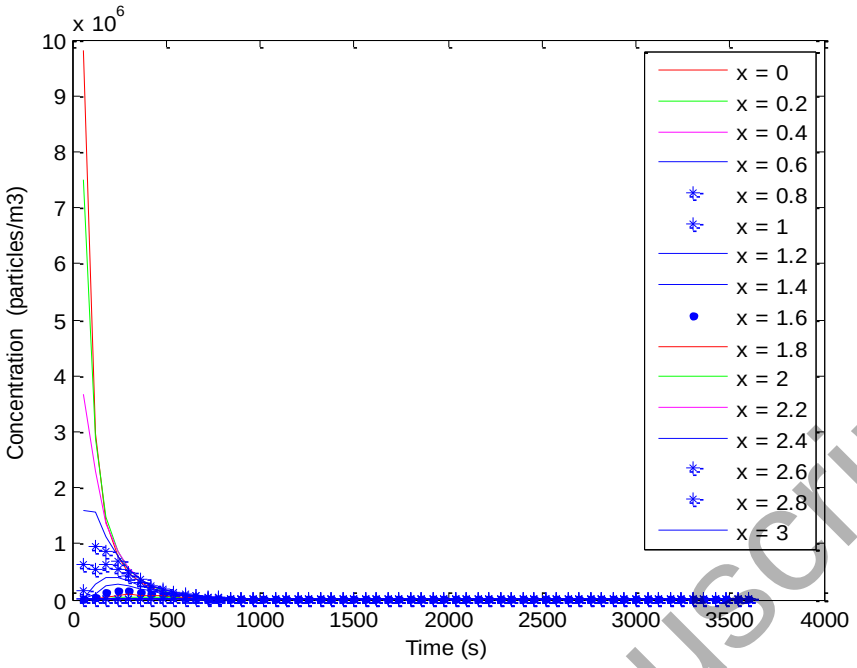


Figure 5a: Predicted Aerosol Concentration against time

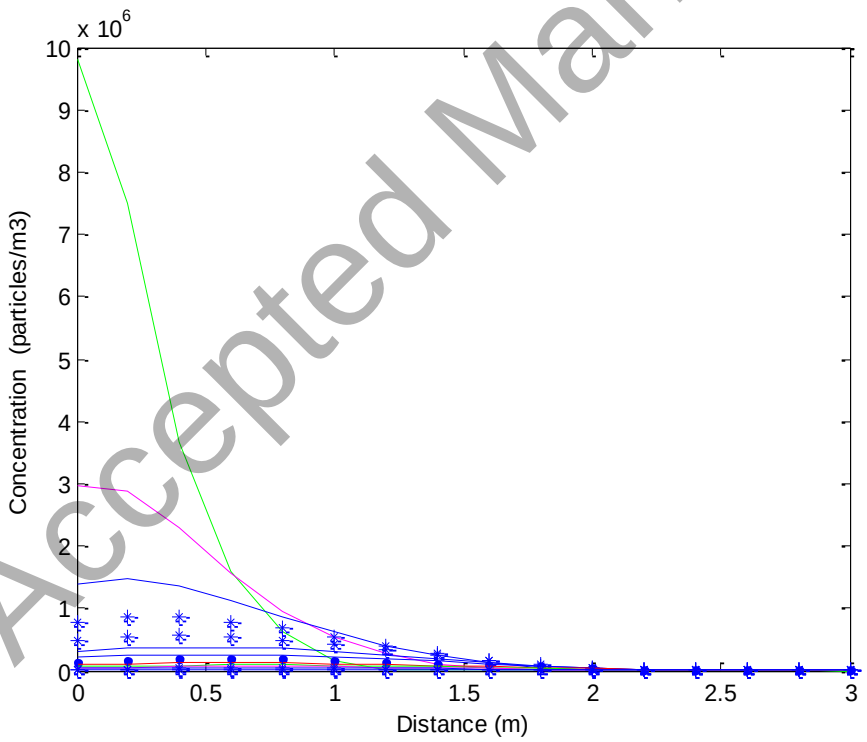


Figure 5b: Predicted Aerosol Concentration versus distance

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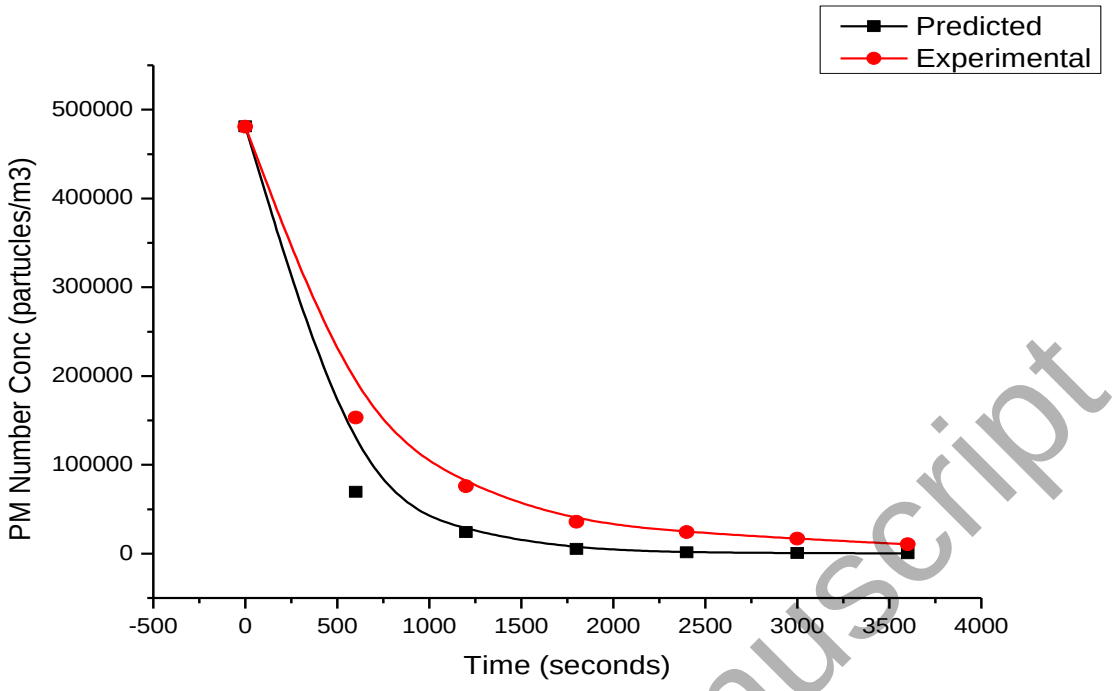


Figure 6: Concentration against Time Graph for Spray Product x = 1 m for 2 µm particle

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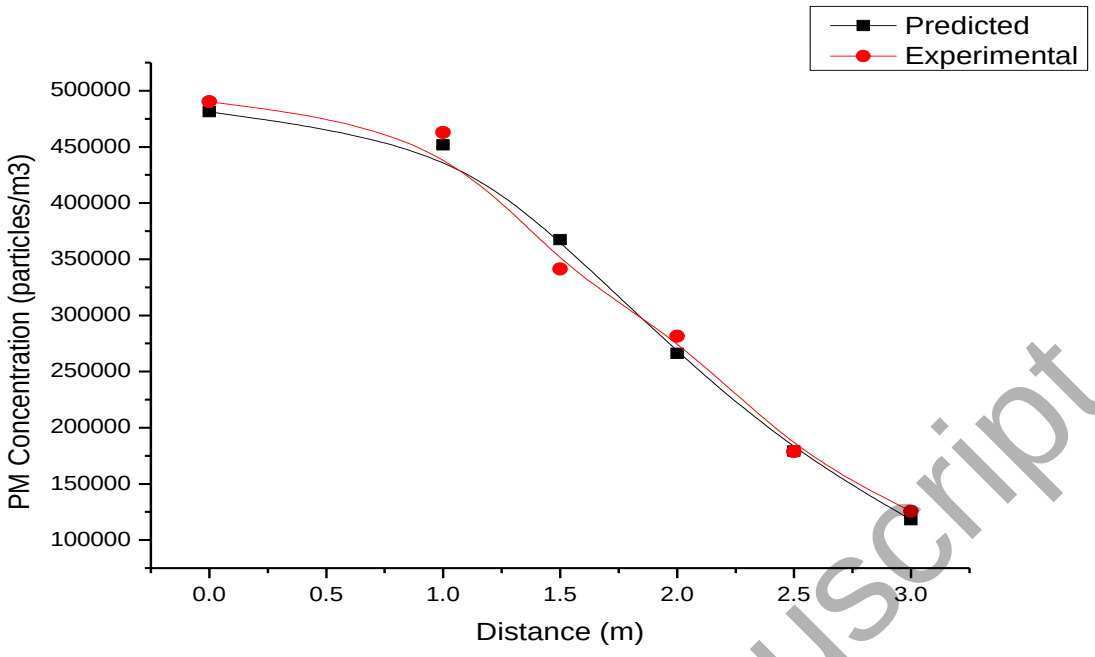


Figure 7: Concentration against Distance Graph for Spray Product at t = 0 s for 0.5 µm particle

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