Diffusion of the Air Pollutants Based on Random Walk

Siyuan He *

Department of Math, Pennsylvania State University, Eire, the United States

* Corresponding Author Email: Sqh6079@psu.edu

Abstract. As a matter of fact, air pollutants prediction serves as a key issue for environment analysis in recent years. In consideration of the stochastic motion of the air particles, it is crucial to implement numerical simulation tools to analyze the random effects. With this in mind, random walk is utilized as a typical scheme to simulate the diffusion process incorporated with concepts of Monte Carlo simulations. On this basis, this paper will present a systematical analysis for simulation of pollution diffusion by means of random walk. To be specific, the calculation principle, formulae and process will be demonstrated. Subsequently, the simulation results will be given in the meantime. In addition, the application scenarios will be discussed and illustrate. At the same time, the evaluations of the results will also be presented and the current limitations will be estimated with suggestions for further research. Overall, these results shed light on guiding further exploration of air pollution.

Keywords: Air pollutant; diffusion; random walk.

1. Introduction

Nowadays, with cities developing and technology growing, the air pollution becomes more and more severe. According to WHO, air pollution is contamination of the indoor or outdoor environment by any agent in either chemical, physical or biological forms that changes the natural characteristics of the atmosphere. The primary research about the air pollution were mainly about the harms it may do to the creatures on the Earth. For example, as former researchers estimated, air pollution can contribute to about 500,000 lung cancer deaths and 1.6 million COPD deaths, but it may also account for 19% of all cardiovascular deaths and 21% of all stroke deaths [1]. In order to minimize the harm caused by the air pollution, scholars and researchers did a mass of investigations to estimate and forecast the dispersion of air pollution. Take Ádám Leeloss's review of air pollution as an example. In the review, the author listed different models used for estimating the dispersion of air pollutants, such as Gaussian, Lagrangian, Rluerian and CFD models [2].

All of these models can successfully estimate the spread of pollutants [2]. However, they function differently based on the detection range. For example, the CFD model works better in the range of less than 1km while the Eulerian model works better in the range of 100-1000 km [2]. In 2015, scientists like Sara Janhäll found the impact of urban vegetation to the dispersion of air pollutants. In the review, she indicated that local air pollution levels will be increased by the reduced mixing in trafficked street canyons on adding large trees, whereas low vegetation which near sources can help solve the air pollution problems in the way of increasing deposition [3]. This can add some new parameters to the present air pollution forecast models since the probability of dispersion of the air pollutants can be influenced by the surrounding environment. Just as Suwen Zhou indicated in her article, the wind tunnel method, which is one of the main methods to estimate the dispersion of air pollution, can provide stable wind direction and speed conditions, and can also control stable emission sources [4].

However, wind tunnel experiments cannot simulate the influence of solar radiation and other thermal effects on air flow and pollutant diffusion changes [4]. For example, the ENVI-met model simplifies the plant model into a column shape instead of refining the branch structure of plants [5]. Whereas, the model method can strictly control the setting of weather factors, traffic factors, street and building factors and plant factors, and can be used to study the influence of specific input parameters on pollutant concentration in street canyons. In addition, the model method can also simulate the trajectory of fluid, so as to simulate the diffusion process of pollutants [4]. In short, the model method can not only obtain continuous and dynamic simulation results, but also quantify the influence of various influencing factors on pollutant concentration. Compared with the wind tunnel method, it is more economical in scientific research, so it is more and more favored. Thus, in this investigation, it will also choose to use the model method.In this article, aiming to set up a model which can predict the extent of air pollution. According to the Brownian motion, any of various physical phenomena in which some quantity is constantly undergoing small, random fluctuations [6]. In other words, the pollutant particles are undergoing random movement all the time. Because of the randomness of the pollutant movement, a 2-dimensional random walk model is introduced in this investigation. This article tries to set up an estimation model to the air pollution with respect to the Lagrange coefficient and to some extent of a basic 2-dimensional random walk. Then some simulation of this model will be conducted to check the accuracy. Finally, this study will analyze and evaluate the model based on the present limitation and potential future development of it.

2. Basic Descriptions

The processes of change in nature can be roughly divided into two categories. One is that its change process has a definite form, or has an inevitable change law, in mathematical language, its change process can be described by one or several definite functions of time t, this kind of process is called deterministic process. For example, when a capacitor is discharged through an electrical resistance, the change in the potential difference between the two ends of the capacitor with time is a deterministic function. The other kind of process has no definite change form, that is, there is no definite change rule for its measurement results each time. In mathematical language, the process of change of such things cannot be described by one or several definite functions of time t, and this kind of process is called stochastic process. Then one can provide a more precise definition of the stochastic process. In a two-dimensional random walk, the random walker can choose four different directions to move: forward, backward, left and right. The most common application of two-dimensional random walk is to calculate the probability of the walker to return to the original point after N steps. In this case, it is assumed that the number of steps $N = 2n$. Russian mathematician Andrey Andreyevich Markov studied and proposed a general law model that can explain natural changes with mathematical methods, named Markov Chain. Markov chain is a random process that transitions from one state to another in the state space, which requires "memoryless", that is, the probability distribution of the next state can only be determined by the current state, and the events preceding it have nothing to do with it in the time series. This particular type of "memorylessness" is called the Markov property [7]. Since the walker's next destination is only determined by his present position. In this case, the random walk model has the Markov property. Then the probability of a two-dimensional departure from origin and return to origin is that:

$$U_{2n} = \sum_{k=0}^{n} \frac{(2n)!}{k!k!(n-k)!(n-k)!} \cdot \left(\frac{1}{4}\right)^{2n} \tag{1}$$

There can be some extent of the basic 2-dimensional random walk. If a walker starts at point $(0,0)$, The general solution for the probability of it to stop at point (a, b) will be given as following. It is assumed that the walker needs to go right for k steps, then it should go left for $k + a$ steps, move upward for j steps, then it has to move downwards for $j + b$ steps. The equation of the solution is:

$$U_n = \left(\frac{1}{4}\right)^n \sum_{k=0}^{n} \frac{n!}{\left(\frac{n-b-a-2k}{2}\right)!\left(\frac{n-a+b-2k}{2}\right)!k!(k+a)!} \tag{2}$$

3. Setting Model

In 1921, The Lagrange method was proposed to study the turbulent diffusion of a single particle by Taylor, which laid the theoretical basis of turbulence diffusion [8]. The motion of many particles in turbulent flow can only be regarded as continuous, but this does not prevent the discussion of the motion path of a specified flow mass point in turbulent flow [8]. The basic idea of the Lagrange method is to study the motion law of a single particle in a flow field [9]. In an open environment that has a wind speed at a uniform velocity u, a pollutant particle is dropped instantly at the origin point at $t = 0$. Take the moving coordinate system that moves with the flow. In other words, the diffusion process is studied by tracking the center of the fluid cluster according to the Lagrange view. If the turbulent field itself is uniformly isotropic, then the pollutant will show a normal distribution with the original point as the center. The x direction displacement at moment t is $x(t) = \int_0^t v'(t_1)dt_1$, where the $v(t)$ is. In this investigation, one sets up the random walk model. The basic principle of the random walk model is to use the release of a large number of labeled particles to characterize the continuous discharge of pollutants so that they can be transported in the atmosphere [10]. At the same time, a series of random bit shifts are used to simulate turbulent diffusion and track their motion trajectory. Finally, the overall distribution of these particles in time and space is calculated to obtain the law of pollutant diffusion [9]. Then, one can get that the dispersion of the pollutant in x-direction:

$$f_x = R_x\sqrt{2K_x\Delta t} \tag{3}$$

Here, the R_x is a standard normally distributed random number with a mean of 0 and a variance of 1 with the range of $(-1, 1)$. Δt is a time step. Therefore, the new position of the particle at x-direction is:

$$x_{end} = x_{old} + \int udt + R_x\sqrt{2K_x\Delta t} \tag{4}$$

The coordinate at y-direction works the same as the x-direction. Supposing one releases N labeled particles, the coordinate of the i-th labeled particle at moment $t = n\Delta t$ is (x_i^n, y_i^n), then the new coordinate of it at moment $t = (n+1)\Delta t$ is (x_i^{n+1}, y_i^{n+1}) can be displayed. After one introduce the random variables R_x and R_y. Supposing the amount of the pollutant is Q, the number of labeled particles are N, then after counting the number of particles per grid cell at moment t, the instant concentration of pollutant can be obtained:

$$C_{i,j,k} = \frac{nQ}{N\Delta V} \tag{5}$$

Here, the i, j, k represent the number of grid and ΔV is the volume of the grid. As long as one got the average value of wind speed at horizontal and vertical direction, determine K_x and K_y, the spatial distribution of the particles can be determined.

4. Simulation

The pollutant is dropped into a closed box and the air flow speed in the environment is u. The start moment is $t = 0$. Take the moving coordinate system that moves with the flow. In other words, the diffusion process of a fluid cluster is studied by tracking the particularity in it according to Lagrange's view. If the turbulence characteristics are uniformly isotropic, then the pollutant at moment t will show up as expanded in a spherical symmetry with the center of the moving coordinate system (seen from Fig. 1) [11].

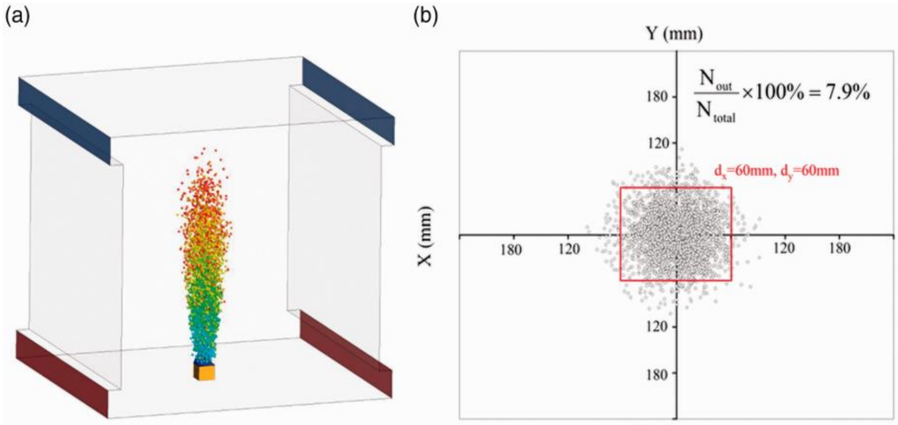

Fig. 1 The state of the air pollutant moving in space (a), and a perfect spherical symmetry with horizontal dispersion of 7.9% within a grid of width and length of $60mm$ (b).

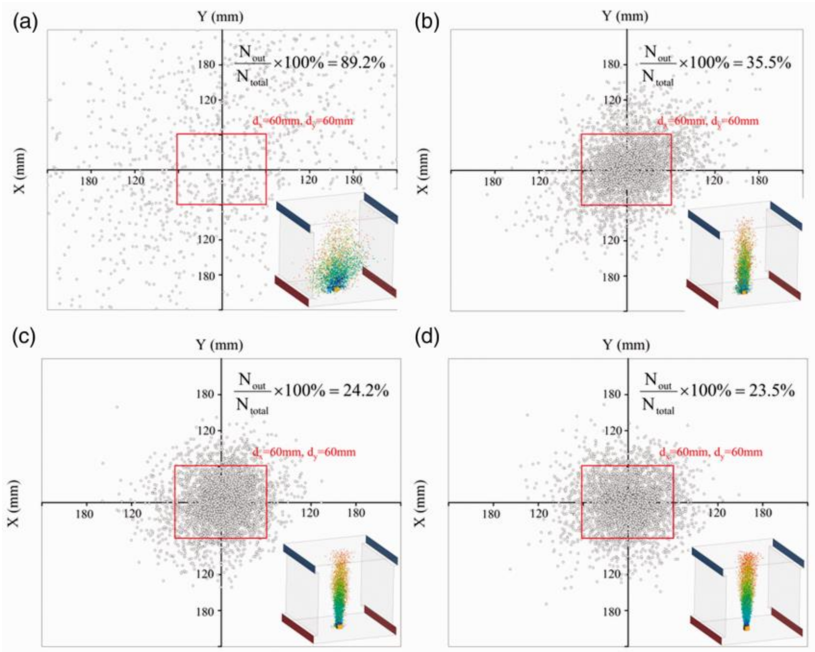

Fig. 2 Simulation results.

In order to simulate the accuracy of the model, different sized pollutant particles are investigated as given in Fig. 2 [11]. In this simulation, an average diameter of 0.1, 0.2, 0.3 and 0.5μm pollutant particles are put in four exactly the same boxes and wait for $600\Delta t$, the dispersion of the particles is displayed on the graph. One can find out that no matter what size of particles is, the dispersion of the particles will always be a normal distribution with spherical symmetry and the only difference is the length of displacement. One can see that a larger sized pollutant particle is less likely to undergo long dispersion, which means the R_x and R_y are closer to 0 instead of the two boundaries 1 and -1. Seen from Fig. 2, the result obtained from the model one used in the article is exactly the same as the experiment the other researchers did. As a result, the result of the calculation got from the model is convincing.

5. Application

The model can also be applied in some real cases to approximate the dispersion of air pollutants. For example, in the case of estimating the concentration of the pollutant particles in the atmospheric boundary layer in China [12], Peng and his team set up a random walk model and used the model to do the calculation. They took the field experiment and collected the data at the level of 4000 m and height of 75 m. The result they gathered from the experiment is shown in Fig. 3.

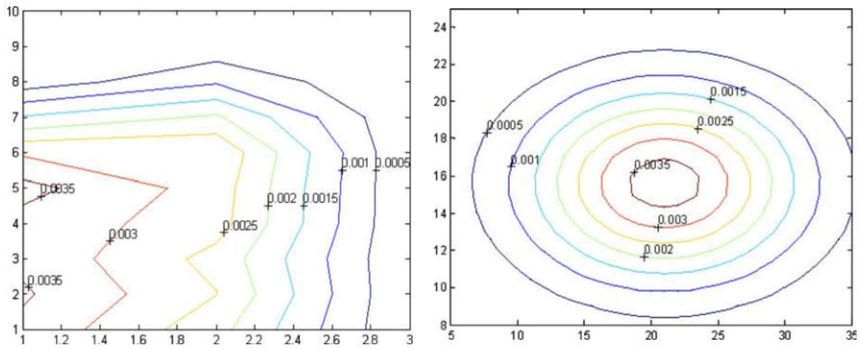

Fig. 3 Pollution distribution.

Seen from the Fig. 3, the pollutant shows a normal distribution, and this also follows the result of the model used in this investigation. This can show that the result of the 2-dimensional random walk model `set up is accurate. In the researcher’s article, they not only use the 2-dimensional random walk model but also the Gaussian model [12]. In order to use the Gaussian model, they checked the atmospheric boundary since different atmospheric boundary layers can have different calculation results [12]. As for the result of the Gaussian model shown on the figure above, the spherical symmetry is more obvious. This also helps prove that the result obtained from the 2-dimensional random walk model is accurate. The model can not only estimate the dispersion of air pollutants. Once the parameters of the equations are changed, the random walk model can also estimate the dispersion of the water pollutants since water has some similar property like the air. As shown in Fig. 4, the dispersion of water pollutants is presented. He also used the random walk model. The result also turned out that the water pollutant concentration has a normal distribution. This indirectly indicated that the random walk model used for estimating the dispersion of air pollutants will also have a result of having the pollutant concentration distribution as normal distribution.

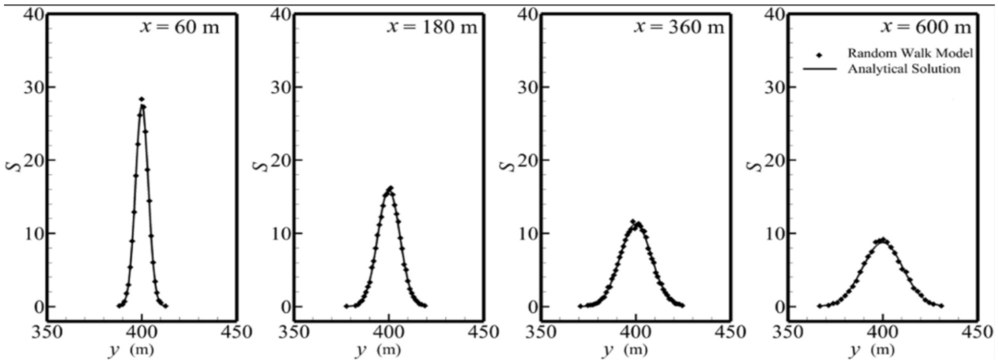

Fig. 4 Pollution simulation results.

6. Evaluations

Even though there are a lot of random walk models to estimate the dispersion of the pollutant in the environment, there are still some problems remaining in the model’s people use. For example, the accuracy of the estimation is mostly dependent on the approximate value of the parameters. Once the approximation of the parameters can be developed, the accuracy of the model can be improved. What’s more, this model used in the article lacks the support of the data of field experiments, which is a little bit unconvincing. The model can only estimate the dispersion of the air pollutant in open fields without buildings and vegetation. With the increasing complication of the surrounding environment, it would be harder to do the approximation to the parameters above and this would cause the errors of estimating the dispersion of air pollutants. The main reason for this is that if the environment becomes more complicated, it is necessary to change the probability of the random walking pollutant particle to go to the next stop. For example, if there is vegetation nearby, it is less likely that the pollutant will be spread to this specific area.

In the future, there is still a lot of improvement for the limitations found in this investigation. Firstly, the way of estimating the horizontal and vertical turbulent diffusion coefficient needs to be discovered more deeply. What's more, if possible, some field experiments can be conducted to prove that the model can work for multiple cases. In real cases, more parameters need to be taken into consideration during the process of setting up the model, such as the roughness of the surface area, the cover ratio of the vegetation, and the temperature of the surrounding environment. These factors may have an influence on the dispersion of the air pollutant particles and thus impact the accuracy of the result obtained from the model. Last but not least, there are quite a lot of other excellent models like CFD models for estimating the movement of particles. In the further investigation, maybe some comparison between the model one set up and the model set up by other researchers can be conducted.

7. Conclusion

To sum up, the investigation aims to set up a 2-dimensional random walk model to estimate the dispersion of air pollutant particles with the usage of Lagrange coefficient. The rule of the dispersion of the pollutants obtained from the model is that no matter what size the particles are, they will finally show up as a spherical symmetry and the concentration of the pollutant has a normal distribution. Even though the model can estimate the dispersion of pollutants well theoretically, it still lacks the field experiment so that it can be proved to be practical in multiple cases. In the future, maybe some comparison with other useful estimating models can be conducted to discover more limitations and advantages of the model set up in this investigation. Hoping with this model, the estimation of the air pollutants can be easier and thus save people's time to take action against the pollution.

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