Simulation of Dispersion of Pollutant by Eddy Field

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Abstract. This research studies the behavior of the dispersion of a pollutant cloud, through the simulation of an eddy field velocity. To do so, a mathematical model was developed, with base in the Monte Carlo simulations, in order to analyze all statistic aspects, present in this process. A computational program was developed, so that it can be possible to establish the behavior of the cloud size, in a scale close to the beginning of the process. The reason for that is justified by the difficulty that the Models, based in the Hydrodynamic Theory, has to manage some results in the beginning of the dispersion process. The results have shown that the model satisfy the objective of the research, as well it could be the first step to analyze the process of dispersion of pollutant in large scale.

KeyWords: Dispersion Analysis, Water Quality Model, Turbulent Diffusion.

1. Introduction

The process of diffusion and dispersion of pollutant, in a body of water, has become a very important topic to be study, in order to bring a better understanding, about their mechanism. The importance of this understanding is related with the necessity of a better control over all environmental impact, caused by the wastewater discharge, as well as some unexpected disaster that has been occurred, principally, with oil spill in ocean, bay, and river, around the world.

The great challenge to understand this phenomenon concerns with the difficulty to relate the dispersion process with the energy spectrum, present in all turbulent fields. As one knows, turbulence plays a very important game in all small or large scale, concerning with water quality problem. Actually, the means of incorporating turbulence into mathematical model has remained relatively simple. In many of the engineering problems, the effect of turbulent motions on the disturbance of properties is characterized by constant eddy diffusion coefficient, considering its simplicity.

This research establishes a different way to focus this problem. The idea is to develop a model, by Random Walk Method, associated with a turbulent

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field, and see the behavior of a pollutant cloud formatted by a set of particles, that was abandoned in some point (x_0, y_0) of the field.

The results have shown that the spectral energy, present in the turbulence field, plays a very important role in the process of dispersion of a pollutant cloud.

2. Mathematical Model

In order to study the Dispersion of Pollutant in a body of water, a mathematical model was developed. This model has, as base, the Random walk method, applied to a set of particles that is released in a point (x_0, y_0) of the domain. After that, by the random walk method, each new position of particle is calculated. This initial process is similar to that developed by the Molecular Diffusion. In this case all the Mathematical Simulation brings, as results, the spread of the particles in the same way to the Fickian process. However, this mathematical simulation works, in these studies, only in the very beginning of the process. When the pollutant cloud becomes large enough, comparing to the scale of the smallest wavelength of the eddy size, the random walk stops, and the dispersion will be governed by the eddy simulation. In such way it will be possible to establish the growth of the pollutant cloud with time.

In order to establish the random walk model, June (1986) showed that for a particle realized in the point $x_t = x_0 = n\Delta t$, your new position will be:

$$x^k = x^{k-1} + \Delta x^{k-1} = \sum_{n=0}^{k-1} \Delta x^n \tag{1}$$

$$y^k = y^{k-1} + \Delta y^{k-1} = \sum_{n=0}^{k-1} \Delta y^n \tag{2}$$

Where (x^k, y^k) represents the coordinates of the particle in the time interval of k order and (Δx, Δy) represents the random displacements between the time $n\Delta t$ and $(n-1)\Delta t$.

It is important to note that (Δx^n, Δy^n) are random numbers with normal probability density function with mean zero and variance equal to $2D\Delta t$.

To simulate the eddy velocity field, in order to stand the advection of the process, the Spectrum of Fourier was utilized, through the set of equations:

$$u_{x\,i} = a_i \cos\left(\left(\frac{2\pi}{\lambda_i}\right) y_i + \phi_{xi}\right) \tag{3}$$

$$v_{y_i} = a_i \cos\left(\frac{2\pi}{\lambda_i} x_i + \phi_{yi}\right) \tag{4}$$

Where:

x_i corresponds to a fix random direction in the plan x,y ;
y_i corresponds to a fix random direction in the plan x,y;
λ_ι represents the wavelength of the component velocity u_{xi};
a_i represents the amplitude of the wave (that is constant to a stationary wave, and time dependent for a non stationary wave);
ϕ_i = represents the plane angle (been random to each wave cycle the of the compound velocity field);
u_{xi} = represents the velocity field component in the direction x_i;
v_{yi} = represents the velocity field component in the direction y_i.

As point out Van Dam (1986) the simulation constitutes an infinite field of congruent eddies, contained in squares on an angle of 45^0 with (x,y) – axes.

It is important to note that all elements of the formulation of the model have random characteristics.

In this research, the amplitude of the wave, considering not stationary, will be calculated by the equation, proposed by Van Dam (1986):

$$a_i = a\left(1 + \cos\left(\frac{2\pi}{T}t + \psi\right)\right) \quad (5)$$

Where:

a is a constant;
T is the period of the wave;
ψ is a phase angle.

The velocity field described through this set of equations, satisfies the continuity equation, in a bi – dimensional plane defined by:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (6)$$

The advective displacements caused by the turbulent velocity field are calculated through the ordinary differential equations:

$$\frac{\partial x_i}{\partial t} = u_{xi} \quad (7)$$

$$\frac{\partial y_i}{\partial t} = v_{yi} \quad (8)$$

where (x_i, y_i) represents the coordinate of the particle i.

The solution of these equation were gotten by the 2^0 order Runge Kutta numerical method through the relations:

$$x_i^{n+1} = x_i^n + \frac{2}{3}kx_1 + \frac{1}{3}kx_2 \quad (9)$$

Where:

$$kx_1 = \Delta t u_{xi}^n \left(x_i^n , t_n \right) \tag{10}$$

$$kx_2 = \Delta t u_{xi}^n \left(x_i^n + \frac{3}{2} kx_1 , t_n + \frac{3}{2} \Delta t \right) \tag{11}$$

Where, x_i^{n+1} represents the coordinate of the particle I, in direction x and time $\Delta t(n+1)$.

Applying the same mechanism for the y_i direction, one has:

$$y_i^{n+1} = y_i^n + \frac{2}{3} ky_1 + \frac{1}{3} ky_2 \tag{12}$$

Where:

$$ky_1 = \Delta t v_{yi}^n \left(y_i^n , t_n \right) \tag{13}$$

$$ky_2 = \Delta t v_{yi}^n \left(y_i^n + \frac{3}{2} ky_1 , t_n + \frac{3}{2} \Delta t \right) \tag{14}$$

The spectrum of the field velocity can be defined by:

$$dE_k = E\left(k\right)dk \tag{15}$$

Where:

dE_k is the kinetic energy per unit of mass and unit of wavelength;
k is the number of waves.

Following Van Dam (1986), some theoretical form of E(k) is practically always of the simple type:

$$E(k) = c_k k^{-m} \tag{16}$$

in which c_k stands for various expressions, depending on the theory concerned. The best-known case is probably the kinetic energy spectrum that considers m=5/3. This theory leads the coefficient of turbulent diffusion to be defined as proportional to the $L^{4/3}$, where L is defined as a length scale. In this research, L will be used as the length of the pollutant cloud size, defined by:

$$L = \sqrt{\left(\left(\tau_x^2 \right)_i^{n+1} + \left(\tau_y^2 \right)_i^{n+1} \right)} \tag{17}$$

Where, τ_x, τ_y represent the standard deviation in the x_i and y_i.

The values of the turbulent diffusion coefficient, for any time in the process will be calculated by the expression:

$$K(L) = .01L^{4/3} \qquad (18)$$

Where L is expressed in cm and K(L) is getting in cm^2/s.

3. Analysis of the Results

In the present study, a set of simulations were made, in order to evaluate the behavior of all statistical parameters that exist in the dispersion processes, as it studied the growth of the o pollutant cloud with time. Also, the simulations have shown the behavior of the concentration with time, as they have shown the development of the turbulent diffusion coefficient for different length scale.

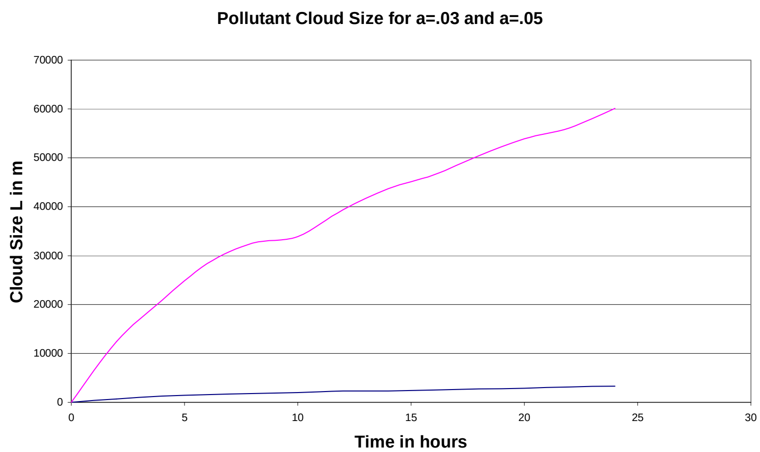

Figure 1 – Pollutant Cloud Size for different eddies.

The "Figure 1" shows the development of the pollutant cloud size as function of time, for different turbulent eddy intensity. The results have shown that, in the beginning of the process, the cloud size increases very fast. After that, this growth becomes smoother. Through the figure, also, it could be seen that, for a stronger eddy field, the cloud size becomes rapidly large, suggesting that the pollutant concentration decrease in the same scale.

The "Figure 2" shows the behavior of the concentration with time. There it could be seen that, the concentration decrease with time in the beginning of the process. After that the decreasing becomes smoother. These results are in agreement with the field observations.

Finally, "Figure 3" and "Figure 4" show the behavior of the turbulent diffusion coefficient with time for different intensity of the turbulence. As it can be seen, there is an important relation between the turbulent diffusion coefficient and the length scale of the eddy velocity field. Through the figures, it is possible to observer that, the more intensity is the turbulent field, the bigger will be the turbulent diffusion coefficient. Other important point that should be noted is that the behavior of this coefficient is function of the eddy scale.

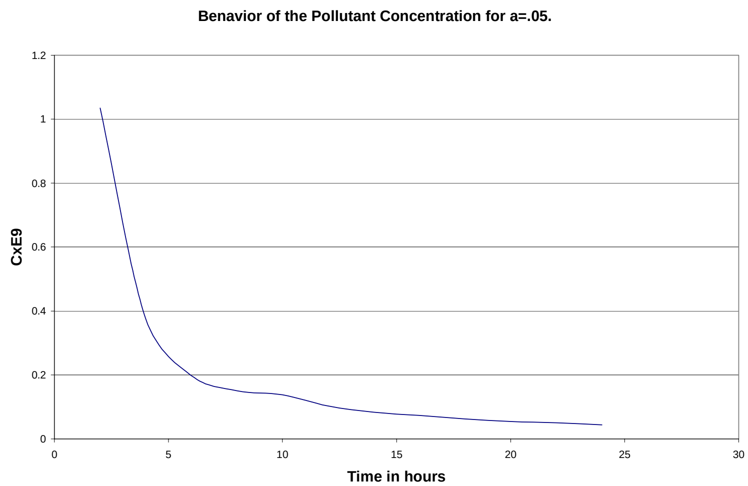

Figure 2 – Pollutant Concentration for a=.05 m/s^2.

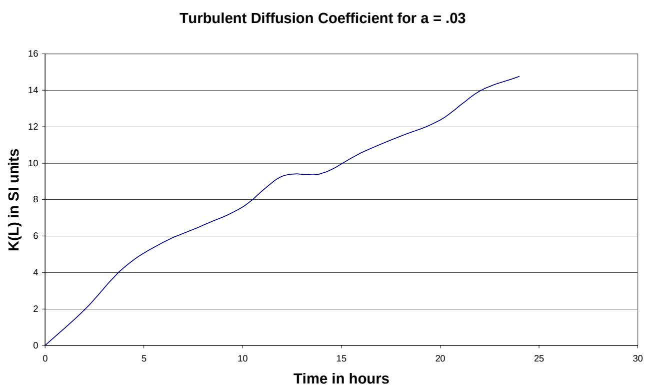

Figure 3 – Turbulent Diffusion Coefficient for a=0.03 m/s^2.

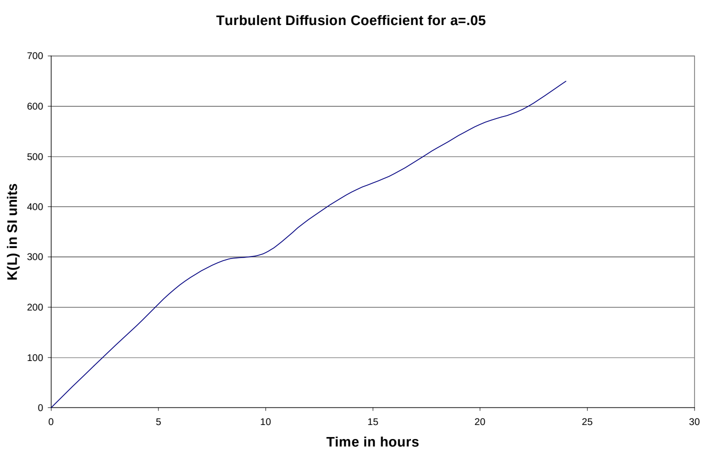

Figure 4 – Turbulent Diffusion Coefficient for a=.05 m^2/s.

4. Conclusions

After the analysis of the results, gotten from the mathematical simulation, one can conclude:

- The mathematical model satisfies the mean goal of the research.
- The pollutant cloud size is function of the eddy velocity field. Its behavior depends on the intensity of the Spectrum of Energy presents in all turbulent velocity fields.
- The concentration of the pollutant has the same behavior of the pollutant cloud size. Its values decrease rapidly with the intensity of the eddies in the turbulent velocity field.
- The simulation shows that the turbulent diffusion coefficient is function of the turbulent length scale. It shows yet that, for large length scale, this coefficient become large in the same way.

References

Bedford, K. W., & Babajimoponlos, C., 1980. Verifying Lake Transport Models With Special Statistics, *Journal of the Hydraulics Division*, vol. 106, nº HY1.

Fischer, H. B., 1979. *Mixing in Inland and Coastal Waters*, Academic Inc., London.

Lewis, R., 1997. *Dispersion in Estuaries and Coastal Waters.* John Wiley & Sons.

Jeng, S. W., & Holley E., 1986. *Two-Dimensional Random Walk Model for Pollutant Transport in Natural River*. Dissertation Presented to the Faculty of the Graduate School of the University of Texas, at Austin of the requirement for the Degree of Doctor of Philosophy.

Van Dam, G. C., 1986. *Eddy Simulation of Two-Dimensional Dispersion.* Nota GWAO-87022. Ministerie Van Verkeer in watertaat, Rijkswaterttaat, the Netherlands.