

# Lagrangian Particle Method for Local Scale Dispersion Modeling

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**Abstract.** A deterministic model is developed for radioactive dispersion analysis based on random-walk Lagrangian Particle Dispersion Method (LPDM). A diagnostic 3-dimensional mass-consistent wind-field with a capability to handle complex topography can be used to provide input for particle advection. Turbulent diffusion process of particles is determined based on empirical lateral and linear vertical relationships. Surface-level concentration is calculated for constant unit release from elevated point source. A series of 60-second segmented groups of particles are released in 3600 seconds total duration. Averaged surface-level concentration within a 5 meter surface layer is obtained and compared with available analytical solution. Results from LPDM shows good agreement with the analytical result for vertically constant and varying wind field with the same atmospheric stability.

## 1. Introduction

Atmospheric dispersion study is performed to assess how pollutant are dispersed in the atmosphere given the variation in space and time of meteorological condition and source-term. It is important to be able to know pollutant concentration and deposition at certain times and receptor locations to mitigate the impact. In many cases, pollutant concentration can be calculated using the advection-diffusion provided in equation (1).

$$\begin{aligned} \frac{\partial \bar{C}}{\partial t} = & -\bar{u} \frac{\partial \bar{C}}{\partial x} - \bar{v} \frac{\partial \bar{C}}{\partial y} - \bar{w} \frac{\partial \bar{C}}{\partial z} + \frac{\partial}{\partial x} \left( K_x \frac{\partial \bar{C}}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial \bar{C}}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial \bar{C}}{\partial z} \right) \\ & + w_s \frac{\partial \bar{C}}{\partial z} - \Lambda \bar{C} - \lambda \bar{C} + Q \end{aligned} \quad (1)$$

Parameter  $\bar{C}$  is the average concentration,  $\bar{u}, \bar{v}, \bar{w}$  are wind components in x,y,z directions,  $K_x, K_y, K_z$  are turbulent diffusion coefficients for x,y,z and  $w_s$  is the gravitational settling velocity.  $\Lambda$  is the depletion coefficient,  $\lambda$  is the decay constant, and  $Q$  is the source-term. Depletion may occur as part of the particles are deposited to the ground in the event of rain (rainout or washout).

Analytical and numerical solutions to advection-diffusion equation (1) are available. In a 3-dimensional domain, analytical solution is generally solved for very specific case, such as



provided by the Gaussian model, where turbulent diffusion is parameterized as a function of distance and Pasquill-Gifford stability classes. This model, however, is justified for only a short distance from the source[1]. The solution assumes that wind speed is vertically uniform over a flat terrain. Source geometry is usually a point source and the release is in steady-state condition. In a more realistic situations where there are spatial variations of wind and diffusivity as well as the presence of other processes like dry and wet deposition as well as radioactive decay or other chemical process, analytical solution can be hard to obtain.

In this situation, Lagrangian Particle Dispersion Method (LPDM) can be employed to provide solution to equation (1) by incorporating a 3-dimensional wind-field[2] to provide spatially varying wind speed and diffusion coefficient. Various relationships for dispersion coefficient  $K$  can be used in the advection-diffusion equation as a reference to obtain pollutant distribution in the atmosphere.

The objective of this paper is to investigate the fitness of LPDM in radioactive pollutant concentration estimation in the local-scale, a downwind distance of a few kilometers from the source. Linear vertical dispersion coefficient and empirical lateral coefficients with Pasquill-Gifford stability criteria are used. Averaged surface level is calculated and compared to the existing analytical solution to assess the performance of this method.

## 2. Lagrangian Particle Dispersion Method

Lagrangian Particle Dispersion Method (LPDM) is run by tracking a number of fictitious particles released into a flow field. LPDM uses stochastic differential equation to explain the similar process as the advection-diffusion equation in Lagrangian framework as proposed in Ermak[3]. Stochastic differential equation for the movement of such particle  $i$  in three dimension is:

$$dx_i = \bar{u}dt + (2K_x)^{\frac{1}{2}} dW_x \quad (2)$$

$$dy_i = \bar{v}dt + (2K_y)^{\frac{1}{2}} dW_y \quad (3)$$

$$dz_i = \bar{w}dt + (2K_z)^{\frac{1}{2}} dW_z + \frac{\partial K_z}{\partial z} \quad (4)$$

$dW_{x,y,z}$  are random numbers with zero average and variance  $dt$ , namely  $d\bar{W} = 0$  and  $d\bar{W}^2 = dt$ . In equation (2) and (3) it is assumed that turbulence is homogeneous in  $x$  and  $y$  directions. The above equations can be integrated with time to obtain particle path which represent the movement of each individual particle. A large number of particles are released and each particle can be labeled with a certain characteristic such as mass or radioactivity level. Concentration at time  $t$  can be calculated from locations of particles and their characteristic.

Implementation of random-walk method for vertical direction is explained below. The equation for horizontal direction has the same form but without the differential form of turbulent or eddy diffusivity ( $\partial K_z / \partial z$ ). Ermak et al., [3] proposed that the height of a particle  $i$  after one time step  $z_{i+1}$  is a summation of four terms, namely the initial height of the particle  $z_i$ , movement by wind  $\bar{w}\Delta t$ , average diffusive movement  $\Delta z_i^*$  and random diffusive movement  $\Delta z_i'$ :

$$z_{i+1} = z_i + \bar{w}\Delta t + \Delta z_i^* + \Delta z_i' \quad (5)$$

Average diffusive movement is represented as follows:

$$\Delta z_i^* = \left( \frac{\partial K_z}{\partial z} \right)_i \Delta t_i \quad (6)$$

Random diffusive movement has the following average and variance:

$$\langle \Delta z_i' \rangle = 0 \quad (7)$$

$$\langle \Delta z_i'^2 \rangle = 2K_{zi}\Delta t_i + \left( \frac{\partial K_z}{\partial z} \right)^2 \Delta t_i^2 \equiv \sigma_{zi}^2 \quad (8)$$

Random diffusive movement  $\Delta z'_i$  is obtained using uniform distribution function:

$$P(\Delta z'_i) = \begin{cases} \frac{1}{2\sqrt{3}\sigma_{zi}} & \text{if } -\sqrt{3}\sigma_{zi} < \Delta z'_i < \sqrt{3}\sigma_{zi} \\ 0 & \text{others} \end{cases} \quad (9)$$

Hence  $\Delta z'_i$  is given by:

$$\Delta z'_i = 2\sqrt{3}\sigma_{zi}(r - 0.5) \quad (10)$$

Variable  $r$  is a random number from a pseudorandom number generator with a range of [0,1]. Relationship between  $\sigma_{xjyzi}$  and  $K_x, K_y, K_z$  is given in equation (8). Similarly, the horizontal random diffusive movement in the lateral direction  $y$  is given by:

$$\Delta y'_i = 2\sqrt{3}\sigma_{yi}(r - 0.5) \quad (11)$$

$$\langle \Delta y_i'^2 \rangle = 2K_{yi}\Delta t_i \equiv \sigma_{yi}^2 \quad (12)$$

In this case, horizontal random diffusive movement along the center of the plume in the  $x$  direction is assumed to be zero since in most cases it is much less than the advective movement  $\bar{u}\Delta t$  except in calm condition.

**Table 1.** Values for  $p_y$  and  $q_y$  for various conditions.

Emission height	Stability class	Coefficients p and q for $\sigma_y$		Classification
		$p_y$	$q_y$	
50 m	A	0.87	0.81	Extremely unstable
50 m	B	0.87	0.81	Unstable
50 m	C	0.72	0.78	Slightly unstable
50 m	D	0.62	0.77	Neutral
50 m	E	1.69	0.62	Slightly stable
50 m	F	5.38	0.58	Stable
100 m	A	0.23	1.00	Extremely unstable
100 m	B	0.23	0.97	Unstable
100 m	C	0.22	0.94	Slightly unstable
100 m	D	0.22	0.91	Neutral
100 m	E	1.69	0.62	Slightly stable
100 m	F	5.38	0.58	Stable

Stability is determined based on temperature lapse rate and wind speed at height  $z$  is determined from speed at wind monitor height and surface roughness. Vogt [2] developed a set of values for  $\sigma_y$  using the following formulae ( $x$  is the downwind distance up to 10 km, the validity limit):

$$\sigma_y = p_y x^{q_y} \quad (13)$$

$K_y$  is provided by the following relationship:

$$K_y = \frac{1}{2} \frac{d}{dt} \sigma_y^2 \quad (14)$$

The values of  $p_y, q_y$  for the different classes of atmospheric stability for emission heights of 50m and 100m are given in Table below (A=unstable, D=neutral, F stable):

### 3. Analytical Solution

Analytical solution for equation (1) for vertically varying wind-field is given in Brown [4] and Huang [5] for a point source at height  $z$  and vertical wind profile of the form  $v(z) = az^p$ . Vertical dispersion parameter has the form  $K(z) = K_1 z^n$  for which analytical solution is presented in Huang [5] for  $n = 0$  and terminal velocity of particles  $v_s = 0$  and  $v_s \neq 0$ . The power law form for wind profile and linear dispersion parameter is consistent with several field experiments as can be found in Brown et al. [4]. Lateral or horizontal dispersion parameters can be obtained from Pasquill-Gifford relations (13). Terminal velocity of particle  $v_s$  is ignored in this case because the particle is assumed to be buoyant and passive.

$$\bar{C} = \frac{Q_1}{\sqrt{2\pi}\sigma_y} \exp\left[-\frac{(y - y_z)^2}{2\sigma_y^2}\right] \times \exp\left[-\frac{a(z^\alpha + h_z^\alpha)}{b\alpha^2 x}\right] \frac{(zh_z)^{\frac{1-n}{2}}}{b\alpha x} \times I_{-\nu}\left[\frac{2a(zh_z)^{\frac{\alpha}{2}}}{b\alpha^2 x}\right] \quad (15)$$

Parameters  $\alpha$  and  $\nu$  are obtained by  $\alpha = 2 + p - n$  and  $\nu = (1 - n)/\alpha$ . Location of point source is at  $(0, y_z, h_s)$  and  $I_{-\nu}$  is a Bessel function with of  $-\nu$  order. The Pasquill-Gifford curves can be used to estimate the lateral spread  $\sigma_y(x)$ .

Comparison between analytical and numerical solution is provided for linear turbulent diffusion ( $n = 1$ ) in both uniform vertical wind profile ( $p = 0$ ) and vertical wind profile as a function of height. Vertical turbulent diffusion coefficient is a non-linear function of height.

### 4. Methodology

Lagrangian particle dispersion is facilitated by dispersing fictitious massless particles in a number of plumes each carrying 1200 particles in 60 second duration. The total source strength of the dispersed particle is 1. A total simulation time of 3600 seconds is used to accommodate plume travel up to several kilometers. Flat topography and constant as well as vertically varying ( $v(z) = az^p$ ) wind fields are used. The value for  $p$  may vary from 0.15 to 0.6 for neutral to stable atmosphere[5] using the following relation:

$$v(z) = v_{10} \left(\frac{z}{10}\right)^p \quad (16)$$

taking into reference the wind speed at 10 meters. In this paper, the vertical wind profiles are provided by  $v(z) = 30$  and  $v(z) = 30z^{0.2}$ .

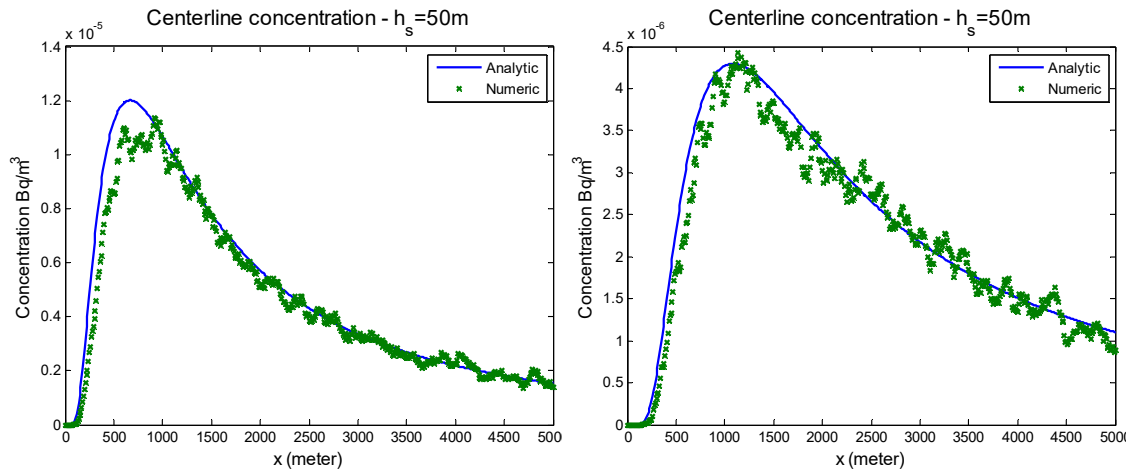
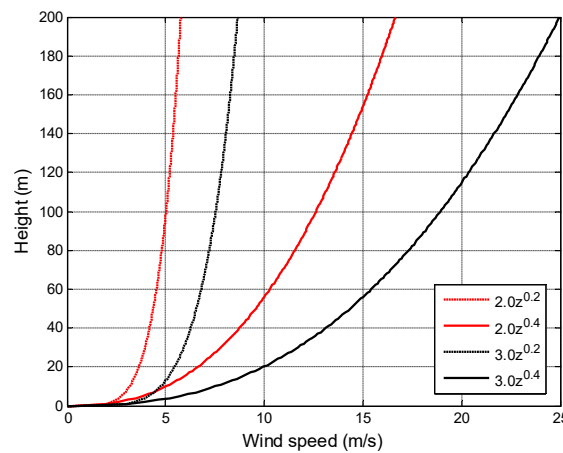
Linear vertical dispersion coefficient of the form  $K(z) = K_1 z^n$  is used for  $K_1 = 01$  and  $n = 10$ . Lateral dispersion coefficient is given as  $\sigma_y(x) = p_y x^{q_y}$  for unstable, neutral and stable atmospheric condition. Dispersion in  $x$  direction is ignored because the value is usually much smaller than the advection term.

Concentration for the LPDM is calculated for the first 5 meter surface layer and then compared to the average value of concentrations for 0 to 5 meters for the analytical solution in equation (15). Model grid is of 1000 m x 2000 m x 2000 m size in grid interval of  $\Delta x$ ,  $\Delta y$  and  $\Delta z$  each of 10 meters. The grids are arranged such that the location of peak concentration and ground-level concentration can be contained. Release point is located at (0,500,50) and (0,500,100). Constant particle time step,  $\Delta t$ , is chosen in such a way that particles do not jump more than 1 grid distance at each step.

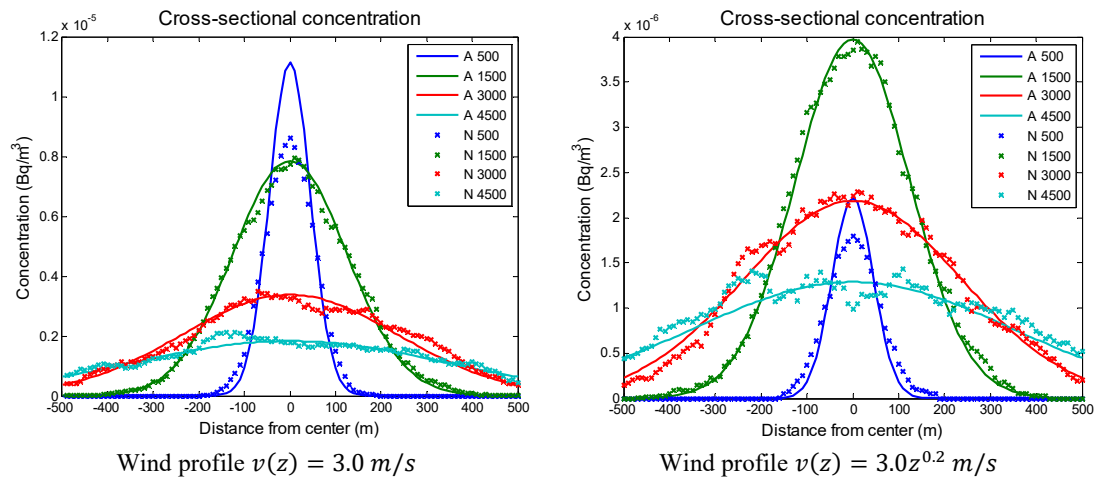
### 5. Result and Discussion

Verification with analytical solution is performed for linear diffusivity coefficient with respect to height  $z$  of  $K(z) = 01z$  and constant vertical wind speed profile of 3.0 and for variable wind speed  $v(z) = 30z^{0.2}$ . Steady-state source strength is 1 Bq/s with a release height  $h_s = 50$  m on a flat terrain. Concentration is calculated for ground-level (up to 5 meters above ground) using kernel density estimation. Analytical solutions are also averaged within the same level.

Simulation is done for 3600 seconds with a time-step  $\Delta t$  of 0.75 second for the best result. Puffs with 60 seconds duration each containing 1200 particles are used, equivalent to a total of 72,000 particles for the entire duration of the simulation. The 3600-second simulation time is adequate to capture the location and magnitude of peak concentration.

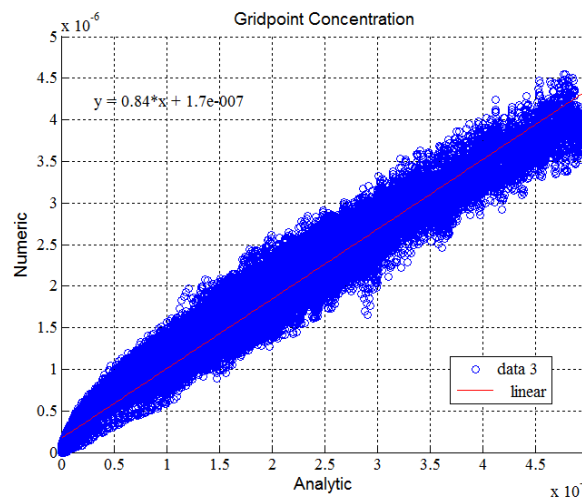
Wind profile  $v(z) = 3.0$ Wind profile  $v(z) = 3.0z^{0.2}$ **Figure 1.** Centerline concentration profiles for various wind conditions**Figure 2.** Vertical wind-speed profile

Examples of centerline concentration are provided in Figure 1 for constant wind speeds of 3 and  $v(z) = 3.0z^{0.2}$  m/s respectively. Good agreement is obtained for all the cases above, particularly for higher wind speed cases given as the example. However, for lower wind speed, the peak concentration is slightly lower although still within one order of magnitude. This lower concentration is caused by faster expansion of the plume to the lateral direction as can be seen from Figure 2, where at closer distance from the source, the base of the curve is wider, thus reducing the peak. Diehl et.al. [7] reduced the lateral expansion by setting gradual expansion of horizontal diffusion coefficient from  $K_H/8$  at the source up to  $K_H$  at  $x = h/0.65$  where  $h$  is the release height. Figures 3 shows the cross-section profile for  $x=500, 1500, 3500$  and  $4500$ m.



**Figure 3.** Cross-sectional concentration for various wind condition

Scatter plot of numerical and analytical solution for selected receptor points are provided in Figure 4. The obtained values for numerical analysis is slightly lower at grid points using  $\Delta t = 0.75$  second. These values are sensitive to the time step and therefore it should be determined specifically for the grid interval used. If the time step is too small, the concentration value tends to be higher at grid points.



**Figure 4.** Scatter-plot of grid-point concentrations ( $\text{Bq/m}^3$ ).

## 6. Conclusion

The Lagrangian Particle Dispersion Method has been able to reproduce ground level concentration within a downwind distance of 5 kilometers for spatially varying dispersion coefficient and wind speed in various atmospheric stability condition.

Centerline and cross-sectional concentration profiles indicate that the numerical solution can represent analytical solution quite well. The difference in the peak concentration in the case of slower wind-speed is mainly due to lateral dispersion in the numerical method although both solutions agree within one order of magnitude. Smoother concentration profile can be improved with more particles.

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