ISSN 2348-1218 (print)
International Journal of Interdisciplinary Research and Innovations ISSN 2348-1226 (online)
Vol. 7, Issue 2, pp: (563-570), Month: April - June 2019, Available at: www.researchpublish.com

NEighbor hood Separation Techniques for solving Advection Diffusion problems

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Abstract: **It has been realized in the last few decades that ocean and other natural water bodies cannot receive infinitely large volumes of waste materials. Further the growing need in recent years for the water quality conservation requires monitoring and controlling the entry of these wastes and keeping their concentration below safe levels in the receiving waters. These have lead to studies to improve current understanding of the diffusion process and for prediction of how much the natural water bodies can disperse and absorb pollutants without causing permanent damage to the ecological system. The accuracy of predictions from mathematical models depend on how well the physical processes are modeled by the governing equations and how good are the methods to solve these problems. In this study an alternative numerical scheme named NEighborhood Separation Technique has been applied to solve advection diffusion problems**

Keywords: **Advection-Diffusion –Numericl schemes- NEighborhood Separation Technique.**

I. INTRODUCTION

In the past 20 years, tremendous amounts of research has been done in developing and utilizing modern high-resolution methods for approximating solutions of hyperbolic systems of conservation laws. Among these methods, the flux-corrected transport (FCT) method [1 –6] and the total variation diminishing (TVD) schemes [7 –10] are commonly used discretization schemes of this class. Modelling of transport problems becomes a great challenge in fluid mechanics. Even though conventional first-order finite difference methods (e.g. first-order upstream and Lax–Friedrichs schemes) are monotonic and stable, they are also powerfully dissipative. The solutions of conventional first-order finite difference methods are often found to be inaacurate. In the past 30 years, large number of research has been done in developing and makes use of modern high-resolution methods for approximating the result of hyperbolic systems of conservation laws. Among these methods, the flux-corrected transport (FCT) method [1 –6] and the total variation diminishing (TVD) schemes [7 –10] are commonly used discretization schemes of this class.

II. NEIGHBORHOOD SEPARATION TECHNIQUE (NEST)

An alternative numerical scheme, called the Neighborhood Separation Technique (NEST), proposed by [11] to solve advection-dispersion problems, has been presented and solved one dimensional problems.

This scheme uses Lagrangian method to model both diffusion and advection, unlike the mixed Euler–Lagrangian approaches,

- requires far less computations compared to Lagrangian methods,
- numerically solves the equation defining the Fick's first law, and relates the mass flux due to molecular or turbulent mixing to the average particle separation speed,
- is mass conservative and free from numerical diffusion, and
- can be applied to a wide variety of advection-diffusion problems.

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In this approach a dispersing patch is represented by a cluster of small patches, and the mass of each patch is set proportional to the dispersing material in each patch and it remains constant with time in the case of conservative dispersing substance. With time, these patches get separated further and further away through the process of molecular or turbulent dispersion. The mass flux due to dispersion defined by Fick's law is related to the average particle separation speed. The speed of separation of these patches from their neighbors and the extent of separation in small incremental time steps are estimated**.** In this approach the advective movements of these patches are independently estimated given the mean flow field.

A. ***Basics of NEST***

To make the explanation simpler, we will discuss here only the basics of NEST for one-dimensional diffusion problem. Consider two neighbouring dispersing patches or segments in a flow field between three points along the x-axis shown in Fig.1. The concentrations of the dispersing substance at these points or nodes be C_1, C_2 and C_3 respectively. Then the Fick's first Law in the finite difference form can be approximated as,

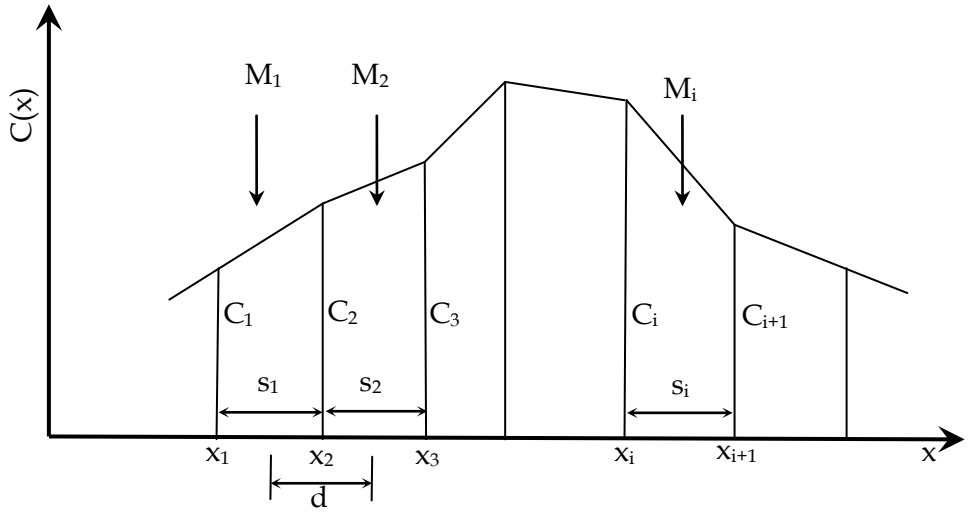

Fig 1: Discretized concentration distribution

$$q \equiv u_d C_2 = -\varepsilon \frac{C_3 - C_1}{(s_1 + s_2)} \quad \text{.....(1)}$$

where q, the mass flux of dispersing substance along the x-direction across the section at the point 2 per unit area is expressed as a product of the concentration C_2 at the node 2 and the average separation speed u_d due to dispersion process. ε is the dispersion coefficient, $s_1 \equiv (x_2 - x_1)$ and $s_2 \equiv (x_3 - x_2)$. Eqn. (5.31) can also be approximated in terms of the dispersing masses in the two segments as follows,

$$q \equiv u_d \frac{(M_1 + M_2)}{2d} = -\varepsilon \frac{M_2 / s_2 - M_1 / s_1}{d} \quad \text{.....(2)}$$

where $M_1 = (C_1 + C_2)s_1 / 2$ and $M_2 = (C_2 + C_3)s_2 / 2$ are the masses of the dispersing substances in the left and right segments respectively, and $d = (s_1+s_2)/2$.

Then the average separation speed of the dispersing substance becomes,

$$u_d = -2\varepsilon \frac{M_2 / s_2 - M_1 / s_1}{(M_1 + M_2)} \quad \text{.....(3)}$$

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Here u_d can be considered as the Lagrangian average separation speed of the interface at the node two, or the above relation can be interpreted as a Lagrangian equivalent of Fick's first Law of diffusion. This gives the displacement of the central node as,

$$\Delta x_2 = -2\varepsilon\Delta t \frac{M_2/s_2 - M_1/s_1}{(M_1 + M_2)} \quad \text{.....(4)}$$

Expressing Δx_2 in terms of the masses of the dispersing substance in neighboring patches is preferable, since the mass of the dispersing substance between two neighboring nodes remains constant with time. The displacement of the nodes due to the advective movements are independently estimated given the mean flow field, and added to Δx_2. Now given the initial concentration distribution, C_i^o, the displacement Δx_i of all the nodes after an incremental time Δt can be estimated. Then the spacing between the nodes can be updated

Since the spacing between the nodes change with time, the concentration distribution also changes. But the mass between any two nodes during the evolution of the patch remains constant with time. Hence in the i-th segment at time $n\Delta t$, we have,

$$(C_i^n + C_{i+1}^n)s_i^n/2 = M_i \quad \text{.....(5))}$$

where C_i^n is the concentration of the dispersing substance at the i-th node and s_i^n is the i-th segment length at time $n\Delta t$ (Fig. 4.3). Note that M_i, the mass of the dispersing substance between nodes remains constant with time. Writing down the above relation for the chosen m segments in the solution domain we get the matrix relation,

$$\begin{bmatrix} 1 & 1 & 0 & & & & \\ 0 & 1 & 1 & & & & \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ & & & & 1 & 1 & 0 \\ & & & & 0 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} C_1^n \\ C_2^n \\ . \\ . \\ . \\ C_m^n \\ C_{m+1}^n \end{bmatrix} = \begin{bmatrix} M_1/s_1^n \\ M_2/s_2^n \\ . \\ . \\ . \\ M_m/s_m^n \end{bmatrix} \quad \text{.....(6)}$$

The above matrix equation can be solved for C_i^n, given the boundary conditions. The performance of this technique has been demonstrated by Wong *et al.* through simulations of a few one and two dimensional dispersion problems and field dispersion problems. But more extreme test cases and field dispersion problems need to be simulated using this approach to understand the versatility of this method.

B. Results and discussion:

NEighbhorhood Separation Techniques: This Technique is used to solve the advection –diffusion for a one dimensional flow. The steps followed in this method are given below

1. For pure diffusion problems, using Eulerian formulation and Fick's law, $\frac{\partial c}{\partial t} = E\frac{\partial^2 c}{\partial x^2}$, Where E is assumed constant. Solution of this equation for an instantaneous release of mass M of a substance at x=0 and t=0 is given by,

$$C(x,t) = \frac{M}{\sqrt{4\pi Et}}\exp\left[\frac{-x^2}{4Et}\right] \qquad \text{Then} \quad \int C(x,t)dx = M \ ,$$

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$\sigma^2 = \frac{1}{M}\int x^2 C(x,t)dx$, $\sigma^2 = 2Et$

2 .This concentration distribution can be considered as a dispersion of a finite number of discrete particles and the probability of finding a particle at x and t is related to the concentration distribution,

$$p(x,t)dx = p(x,t) = \frac{C(x,t)}{M}dx$$

The mean square of separation of all pairs of particles can be shown to be

$\bar{s}^2 = 2\sigma^2 = 4Et$

$s = \sqrt{\bar{s}^2} = \sqrt{4Et}$ and $u = \frac{ds}{dt} = \frac{E}{s}$

3. Dispersing patch originating from number of instantaneous point sources is given by

$\sigma^2 = 2E(t+t_0)$ and $\sigma = 2Et_0$

$\bar{s}^2 = 2\sigma^2 = 4E(t+t_0)$, $s = 2\sqrt{E(t+t_0)}^1$ and $u = ds/dt = E/s$.

Any concentration profile can be considered as super position of concentration originating several points.

4. Particle separation rule:

Any concentration profile can be considered as super position of concentration originating several point sources.

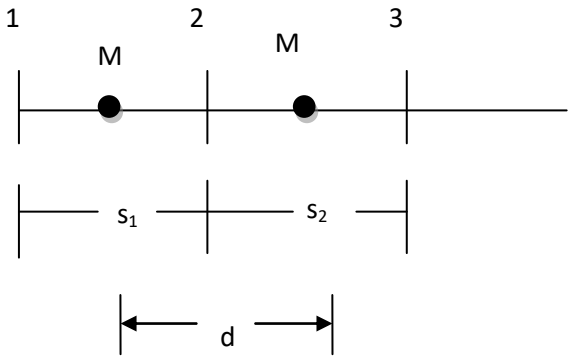
$$\frac{particle\ \ seperation\ rule}{diffussion\ of\ a\ series of\ 'n'\ \ particles}$$

$$u_i = E\left(\frac{1}{s_{i-1}} - \frac{1}{s_i}\right)$$

5. Fick's Law

$$q = u\frac{M}{d} = \frac{-E\,dc}{dx} = E\left(\frac{M}{s_1} - \frac{M}{s_2}\right)$$

$$u = E\left(\frac{1}{s_1} - \frac{1}{s_2}\right)$$



Fick's law is equivalent to the particle separation rule.

The particle separation rule can be interpreted as a langrangian equivalence of Fick's law of diffusion.

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6. One dimensional advection diffusion problem $\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}=E\frac{\partial^2 c}{\partial x^2}$

In the NEST method displacement of dispersing particles are calculated as follows

$$\Delta x = u\Delta t + E\Delta t\left(\frac{1}{s_n}-\frac{1}{s_{n+1}}\right)$$

7. Test cases to be solved :(a) 1-d pure diffusion problem $c(x,0)=\exp\left(\frac{-x^2}{\sigma^2}\right)$

$\sigma = 264m$

200 equal mess particles can be considered

$E=\frac{2m^2}{s}$ $assume\ E\Delta t < 1/2$ Estimate the distribution at t=4800sec and t= 9600sec.

(b).1-D advection diffusion problem

$c(x,0)=\exp\left(\frac{-x^2}{\sigma^2}\right)$ 200 equal mass particles can be considered

$\sigma = 264m$

$E=\frac{2m^2}{s}$ $,u=0.5m/s$

Estimate the distribution at t = 6000s & 12000s. For 1-D Advancing front Problem is solved by changing the time interval Δ t value.

Numerical results:

The proposed NEighborhood Separation Techniques is solved for a number of advection dominated problems. The scheme is used to advect a Gaussian concentration distribution for the consistent flow at a constant velocity of u=1m/s. For 100 particles of equal mass, the sharp Gaussian distribution is described, when c(x,0)=1.0exp(-x2/σ2),σ=264m .The computed concentration distribution for time t=6000secs and 12000 seconds along with the analytical solution is shown in figure Figure.1. For pure advection case the Langrangian scheme creates little problem but generally this models the advection exactly.The scheme is asked to advect a Gaussian concentration distribution at a constant velocity of u = 0.5 m/s in a uniform flow. The sharp Gaussian distribution, c(x,0) =1.0exp(-x^2/σ^2),σ =264m is described by 200 equal mass particles with the same standard deviation. Figure .1 shows the computed concentration distribution at t = 6000 s and 12000 s along with the exact solution.

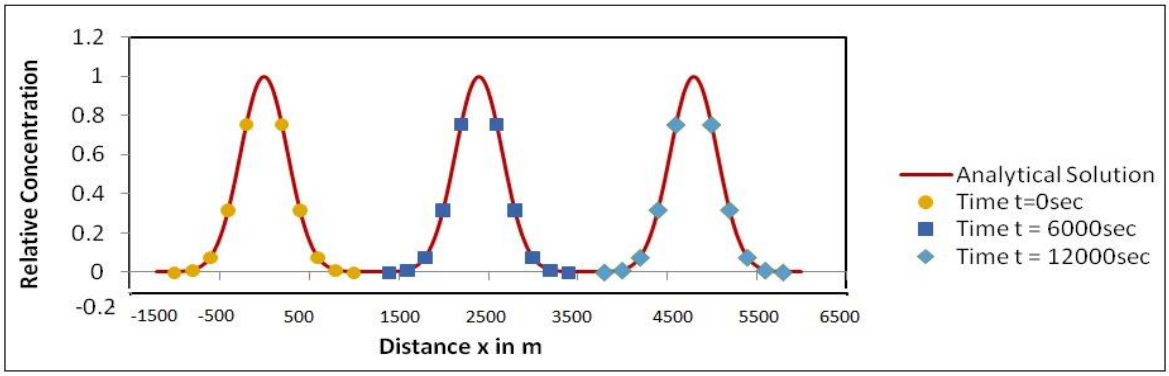

Figure 1: Pure advection simulation (u=1m/s)

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The numerical solution of the pure diffusion equation for $E=2m^2/_s$, and $E\Delta t/s^2=0.5$ is shown in figure.2. Numerical solution is shown for a constant particle size; the time step is set following compatibility requirement as shown by the equations, The performance of the method by different time steps using the numerical solution at time t=12000seconds and the time variation of the location of the centre of the particle are shown.

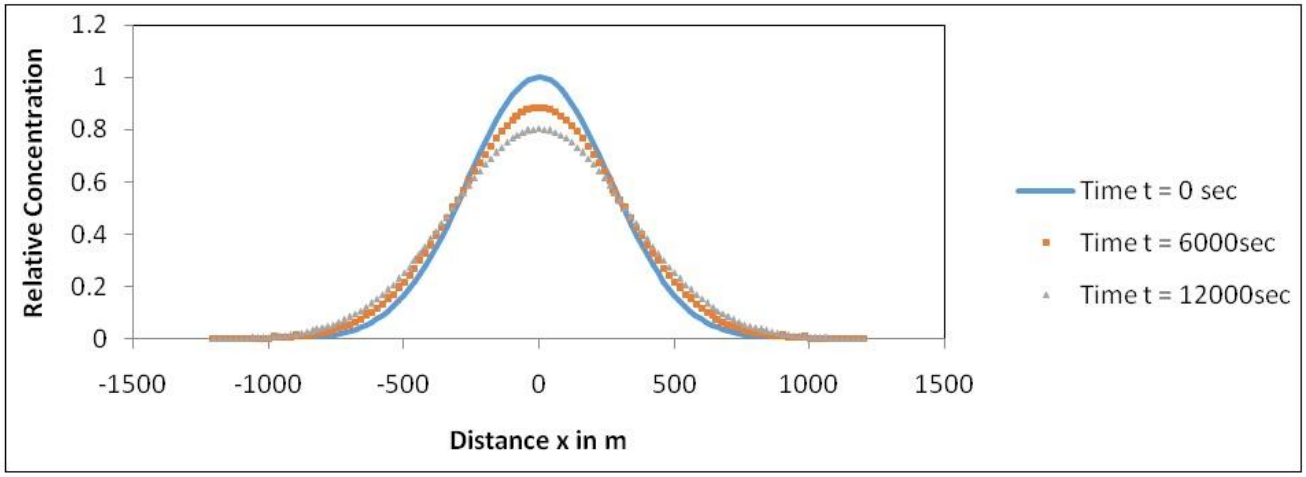

Figure 2: Pure Diffusion using Neighbhor hood Separation Technique (NEST), $E=2m^2/_s$

The results show that the scheme has small violation of the stability when E value increases and the rquirement does not destroy the calculation instantly, even though oscillations in the results about the exact solution can be seen. Root mean square error of the numerical solution is 0.0089. The performances of the model for two different time steps are shown in figure 3 and 4.

The results of the particle separation method is compared with the solution of the same problem at t=12000seconds using the random walk method. To achieve similar accuracy by random walk method, the particle required is generally larger by one to two orders of magnitude. Because the method is capable to model advection and diffusion individually, there is small problem when the entire advective- diffusion is modelled as shown in figure.4

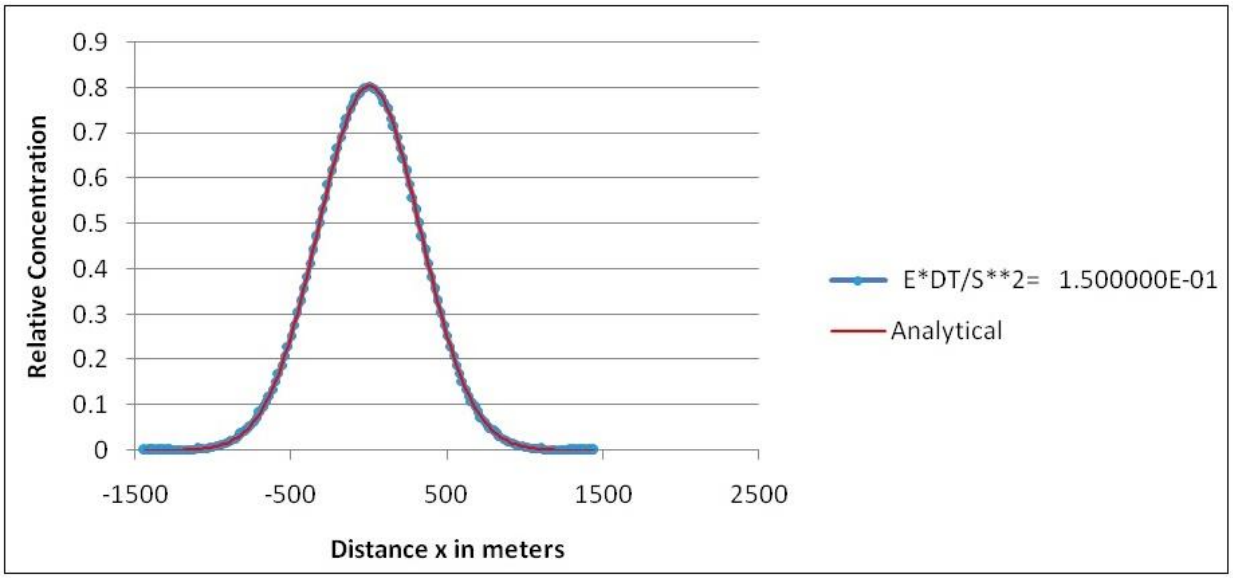

Figure 3: Numerical solution of pure diffusion. Concentration profile at t=12000seconds and $E\Delta t/s^2=0.15$

Figure.5 represents, the advection and diffusion modelling for different time interval and it shows there a little problem since it is capable of solving advection and diffusion separately. For high Peclet numbers, when the concentration gradients near the front, it is difficult to simulate precisely in most of the Eulerian schemes. Due to random particle fluctuation, it is hard to maintain an exact constant concentration for Random walk model. These problems were not found in the present scheme because there are no spatial grids which rely upon to capture the concentration distribution.

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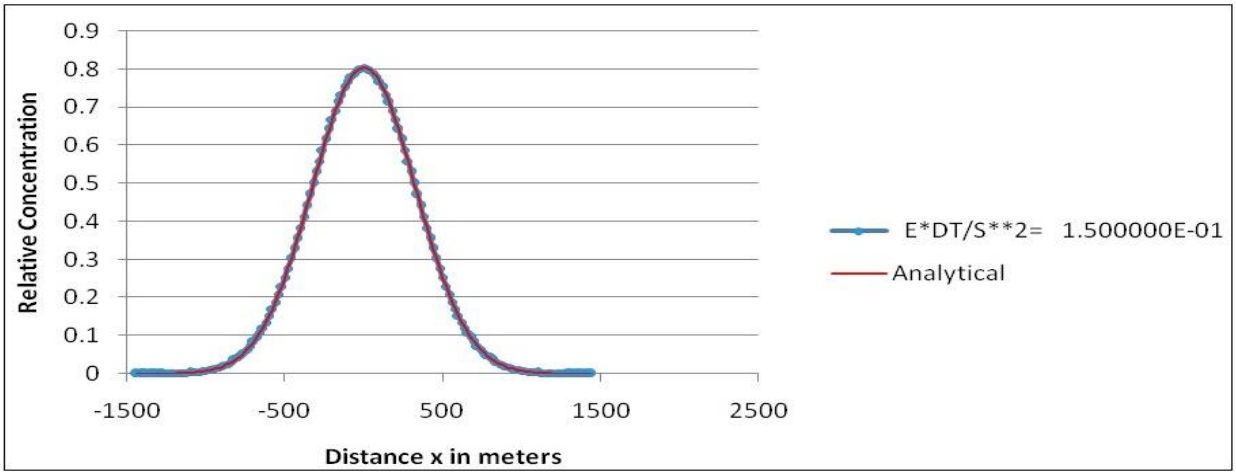

Figure 4: Numerical solution of pure diffusion. Concentration profile at t=12000 seconds and $E\Delta t/s^2=0.6$

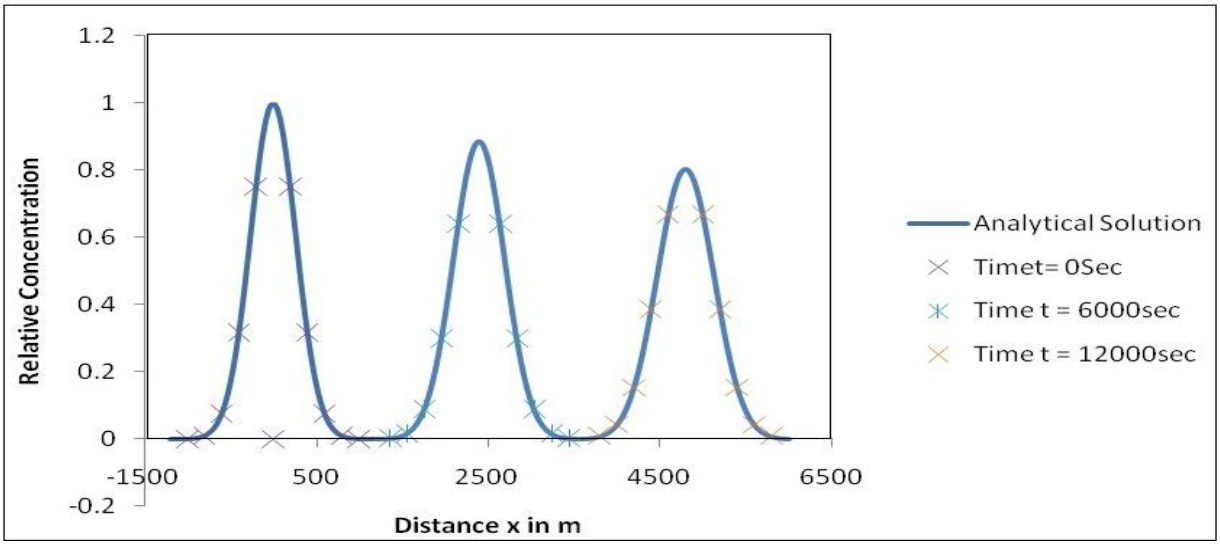

Figure 5: Simulation of advective –diffusion.

III. CONCLUSION

The main advantage of the Neighborhood separation technique is that, it has the ability to model particle attributes with a small number of langragian particles. This method is generally used to solve Advection–Diffusion problem without causing oscillations. The additional advantage of this method is that, it can able to solve Advection dominated problems, where other methods are not able to give accurate deterministic results without causing numerical diffusion. Also, when the stability parameter is increased to some extent, by changing the values of $E\Delta t/S^2$, it gives a good result. This method simulates the diffusion process via an equivalent macroscopic motion. It can able to model the diffusion process deterministically and accurately in a particle model by means of the Langragian implementation of Fick's law. It can be concluded that, it requires less number of particles compared to random walk method and it can be used to model the ecological problems.

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