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Solution of the diffusion equation using Adomain decomposition

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ABSTRACT: The objective is estimated the concentration of air pollution, by solving the atmospheric diffusion equation (ADE) using Adomain decomposition method. The solution depends on eddy diffusivity profile (K) and wind speed at the released point (u). We solve the ADE numerically in two dimensions using Adomain decomposition method, then, compared our results with observed data.

Keywords: Adomain decomposition/ eddy diffusivity/ atmospheric diffusion equation.

INTRODUCTION

The Adomian decomposition method (ADM) has been applied in wide class of stochastic and deterministic problems in many interesting mathematics and physics areas (Adomain ,1994). Adomain gave a review of the decomposition method in (Adomain, 1988). Bellomo and Monaco(1985) have used ADM in solving random nonlinear differential equations, Wazwaz (2001) found the numerical solution of sixth order boundary value problem by ADM, El-Sayed and Abdel – Aziz (2003) compared between Adomians decomposition method and wavelet – Galerkin method for solving integro- differential equations. El-gamel (2007) compared between the Sine –Galerkin and the modified decomposition methods for two – point boundary –value problems.

In this paper, advection diffusion equation was solved in two dimensional space (x,z) using Adomian decomposition method to obtain the normalized crosswind integrated concentration employing numerical form. Two forms models of the eddy diffusivities as well as the wind speed at the released point were used in the solution. Two calculated models were compared with observed data measured at Copenhagen in Denmark my using statistical technique.

Numerical Method

Time dependent advection – diffusion equation is written as (Arya, 1995)

 $\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} \left(k_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial c}{\partial z} \right) \quad (1)$

where:

c is the average concentration of air pollution (μ g/m3).

u is the wind speed (m/s).

 K_x , k_y and k_z are the eddy diffusivities coefficients along x, y and z axes respectively (m2/s).

For steady state, taking dc /dt=0 and the diffusion in the x-axis direction is assumed to be zero compared with the advective in the same directions, hence:

$$u\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(k_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z\frac{\partial c}{\partial z}\right)$$

(2)

Assuming that $k_y = k_z = k(x)$, integrating the equation (2) with respect to y, we obtain the normalized crosswind integrated concentration cy (x, z) of contaminant at a point (x, z) of the atmospheric advection–diffusion equation is written in the form (Essa et al. 2006):

$$\frac{\partial^2 c_{y(x,z)}}{\partial z^2} = \frac{u \partial c_{y(x,z)}}{\partial z^2}$$

 $\overline{\partial z^2} - \overline{\partial x^2}$ Equation (3) is subjected to the following boundary condition (3)

1-It is assumed that the pollutants are absorbed at the ground surface i.e. where v_g is the deposition velocity (m/s).

$$k \frac{\partial c_{y}(x,z)}{\partial z} = -v_{g}c_{y}(x,z) \qquad \text{at } z = 0 \quad (i)$$

2-The flux at the top of the mixing layer can be given by

$$k \frac{\partial c_{\perp}(x,z)}{\partial z} = 0 \qquad \text{at } z = h$$
(ii)
3-The mass continuity is written in the form:-

u c_y (x,z) =Q δ (z-h) at x=0 (iii) where δ is Dirac delta function, Q is the source strength and h is mixing height.

4-The concentration of the pollutant tends to zero at large distance of the source, i.e. $c_y(x,z) = 0$ at $z = \infty$ (iv) In equation (3), we take A=u/K and Equation (3) can be solved using Adomain decompositions method as follows:

$$\begin{split} L_{zz} c_{y} \left(x, z \right) &= A L_{x} c_{y} \left(x, z \right) \\ where \quad L_{zz} = \frac{\partial^{2}}{\partial z^{2}}, L_{x} = \frac{\partial}{\partial x} \\ \text{Multiplying both sides of the above equation by L^{-1} }_{zz} (inverse), one gets: \\ c_{y} \left(x, z \right) &= c_{0} + A \ L_{zz}^{-1} \ L_{x} \ c_{y} (x, z) \\ L_{zz}^{-1} &= \int_{z}^{z} \int_{0}^{z} (c_{0} + A \ L_{zz}^{-1} \ L_{x} \ c_{y} (x, z)) dz dz \\ \text{Assuming that:-} \\ C_{0} = M(x) + z \ N(x) \end{split}$$
(4a)

where M and N are unknown functions which will be determined from boundary conditions, using equation (4) to get the general solution in the from:-

 $c_{n+1} = A \int_0^z \int_0^z \frac{\partial c_n}{\partial x} dz \, dz \tag{5}$

Put n=0

$$c_{1} = A \int_{0}^{z} \int_{0}^{z} \frac{\partial c_{0}}{\partial x} \partial z \, \partial z = A \int_{0}^{z} \int_{0}^{z} \left(\frac{\partial M}{\partial x} + z \, \frac{\partial N}{\partial x} \right) \partial z \, \partial z = A \frac{\partial M}{\partial x} \frac{z^{2}}{2!} + A \frac{\partial N}{\partial x} \frac{z^{3}}{3!}$$
(6)

Assuming the solution has the form:-

$$W_n = \sum_{n=0}^{\infty} c_n$$

$$W_1 = c_0 + c_1 = M(x) + z N(x) + A \frac{\partial M}{\partial x} \frac{z^2}{2!} + A \frac{\partial N}{\partial x} \frac{z^3}{3!}$$
(7)

By differentiating the equation (7) with respect to z and multiplying by k_z , we obtain that:

$$k_{z} \frac{\partial W_{1}}{\partial z} = k_{z} N(x) + Az k_{z} \frac{\partial M}{\partial x} + A \frac{z^{2}}{2!} k_{z} \frac{\partial N}{\partial x}$$
(8)

Using the boundary condition (i) at z=0, we obtain that: -

$$k_{z} \frac{\partial W_{1}}{\partial z} = k_{z} N(x) = -v_{g} M(x)$$

$$\therefore N(x) = \frac{-v_{g}}{k_{z}} M(x) \Longrightarrow M(x) = -\frac{k_{z}}{v_{g}} N(x)$$
(9)

Using the boundary condition (ii) at z=h, we obtain that: -

$$k N(x) + A h k \frac{\partial M}{\partial x} + \frac{h^2}{2!} A k \frac{\partial N}{\partial x} = 0$$

$$\therefore M(x) = \frac{-k}{v_g} N(x)$$

$$\therefore \frac{\partial M(x)}{\partial x} = \frac{-k}{v_g} \frac{\partial N}{\partial x} - \frac{N(x)}{v_g} \frac{\partial k}{\partial x}$$

$$k N (x) - A h k \left(\frac{k}{v_{g}} \frac{\partial N}{\partial x} + \frac{N (x)}{v_{g}} \frac{\partial k}{\partial x}\right) + \frac{h^{2}}{2!} A k \frac{\partial N}{\partial x} = 0$$

$$\left[\frac{h^{2} A k}{2!} - \frac{A h k^{2}}{v_{g}}\right] \frac{\partial N}{\partial x} + \left[k - \frac{A h k}{v_{g}} \frac{\partial k}{\partial x}\right] N (x) = 0 \Rightarrow$$

$$\left[\frac{h^{2} k A v_{g} - 2A h k^{2}}{2v_{g}}\right] \frac{\partial N}{\partial x} = \left[\frac{A h k \frac{\partial k}{\partial x} - k v_{g}}{v_{g}}\right] N (x) \Rightarrow$$

$$\frac{\partial N}{N (x)} = \left(\frac{2A \frac{\partial k}{\partial x} - 2v_{g}}{A h (h v_{g} - 2k)}\right) \partial x \qquad (9a)$$

Integrating the equation (9a) from 0 to x, we obtain that:-

$$N(x) = N_0(x) e^{\frac{(2A\frac{\partial x}{\partial x} - 2v_g)}{hA(hAv_g - 2k)^x}}$$
(10)

Using the boundary condition (iii), we get that:-

$$N_0(x) = \frac{Q}{u}\delta(z-h)$$

Substituting from $N_0(x)$ in equation (10), we get that:-

$$N(x) = \frac{Q}{u} \delta(z-h) e^{\frac{2\left(\frac{\lambda h}{\partial x} - v_B}\right)x}{\frac{\lambda h}{h(h_B - 2k)}}}$$
(11)

Substituting from two equations (9) and (11) in equation (4a), we obtain that:-

$$c_{0} = \frac{-k}{v_{g}} N(x) + z N(x) = \left(\frac{-k}{v_{g}} + z\right) N(x) = (z - B) N(x)$$
(12)

Where B=k/vg

$$\therefore \frac{\partial N}{\partial x} = N \left(\frac{2 \left(A h \frac{\partial k}{\partial x} - v_g \right)}{A h \left(h v_g - 2 k \right)} \right)$$

$$M = \frac{-k \partial N}{A h \left(h v_g - 2 k \right)}$$
(13)

$$M = \frac{1}{v_g} \frac{\partial x}{\partial x}$$
$$\therefore \frac{\partial M}{\partial x} = \frac{-kN}{v_g} \left(\frac{2\left(Ah\frac{\partial k}{\partial x} - v_g\right)}{Ah(hv_g - 2k)} \right)$$
(14)

Substituting equations (9a) and (14) in equation (6), we obtain that :-

$$c_{1} = (AD) \left(\frac{z^{3}}{3!} - \frac{k}{v_{g}} \frac{z^{2}}{2!} \right) N$$
(15)

Where Similar, we get

$$D = N \left(\frac{2 \left(Ah \frac{\partial k}{\partial x} - v_g \right)}{Ah \left(hv_g - 2k \right)} \right)$$

The general solution: $c_{2} = (A D)^{2} \left(\frac{z^{5}}{5!} - \frac{k}{v_{s}} \frac{z^{4}}{4!}\right) N$ $c_{3} = (A D)^{3} \left(\frac{z^{7}}{7!} - \frac{k}{v_{s}} \frac{z^{6}}{6!}\right) N$ $c_4 = (A D)^4 \left(\frac{z^9}{9!} - \frac{k}{v_g} \frac{z^8}{8!}\right) N$

(16)

$$\frac{c_{y}(x,z)}{Q} = \frac{v_{g}}{u(hv_{g}-k)}e^{\frac{2\left(Ak\frac{\partial k}{\partial x}-v_{g}\right)x}{Ah(hv_{g}-2k)}} \left[\sum_{0}^{n} \left(\frac{2u\left(Ah\frac{\partial k}{\partial x}-v_{g}\right)x}{Ahk\left(hv_{g}-2x\right)}\right)^{l} \left(\frac{-kz^{2l}}{v_{g}\left(2!\right)}+\frac{z^{2l+1}}{\left(2!+1\right)!}\right)\right]$$
(17)

RESULTS AND DISCUSSION

(27)

Where:-

We can obtain the wind speed at source height 115m as follows:

$$u_{115} = u_{10} \left(\frac{z}{10}\right)^p$$

U115 is the wind speed at 115m.

U10 is the wind speed at 10m height.

z is the physical height.

p is a parameter estimated by Irwin (1979), which is related to stability classes, is given in Table (1).

| Table 1. Estimates of the power (p) in urban areas for six Stability Classes based on information by Irwin (1979b) | | | | | | | | |
|--|-------------------|--------------|----------------------------------|-------------|--|-----------------------|--|--|
| Stability | Very Unstable (A) | Moderately | Slightly unstable (C) | Neutral (D) | Slightly stable (E) | Moderately Stable (F) | | |
| Classes | , | Unstable (B) | U , V , V , | | 0, | , | | |
| Urban p | 0.19 | 0.21 | 0.32 | 0.30 | 0.36 | 0.46 | | |

In the present model, we used two methods for the calculation of the eddy diffusivity depends on the downwind distance (x). The first method taking k in the from $k_1(x) = 0.04ux$ and the second method are referenced to (Arya, 1995) where k takes in the form:-

$$k_{z}\left(x\right) = 0.16 \left(\frac{\sigma_{w}^{2}}{u}\right) x$$

Where σw is the standard deviation of the vertical velocity.

Table 2. Values of wind speed at 10 m and 115 m and downwind distance through unstable and neutral stabilities in northern part of

| Run no. | Stability | u 10 (m/s) | U115 (m/s) [| Distance (x) (m) |
|---------|-------------------------|------------|--------------|------------------|
| 1 | Very unstable (A) | 2.1 | 3.34 | 1900 |
| 1 | Very unstable (A) | 2.1 | 3.34 | 3700 |
| 2 | Slightly unstable (C) | 4.9 | 10.71 | 2100 |
| 2 | Slightly unstable (C) | 4.9 | 10.71 | 4200 |
| 3 | Moderately unstable (B) | 2.4 | 4.01 | 1900 |
| 3 | Moderately unstable (B) | 2.4 | 4.01 | 3700 |
| 3 | Moderately unstable (B) | 2.4 | 4.01 | 5400 |
| 5 | Slightly unstable (C) | 3.1 | 4.93 | 2100 |
| 5 | Slightly unstable (C) | 3.1 | 4.93 | 4200 |
| 5 | Slightly unstable (C) | 3.1 | 4.93 | 6100 |
| 6 | Slightly unstable (C) | 7.2 | 11.45 | 2000 |
| 6 | Slightly unstable (C) | 7.2 | 11.45 | 4200 |
| 6 | Slightly unstable (C) | 7.2 | 11.45 | 5900 |
| 7 | Moderately unstable (B) | 4.1 | 6.85 | 2000 |
| 7 | Moderately unstable (B) | 4.1 | 6.85 | 4100 |
| 7 | Moderately unstable (B) | 4.1 | 6.85 | 5300 |
| 8 | Neutral (D) | 4.2 | 8.74 | 1900 |
| 8 | Neutral (D) | 4.2 | 8.74 | 3600 |
| 8 | Neutral (D) | 4.2 | 8.74 | 5300 |
| 9 | Slightly unstable (C) | 5.1 | 11.14 | 2100 |
| 9 | Slightly unstable (C) | 5.1 | 11.14 | 4200 |
| 9 | Slightly unstable (C) | 5.1 | 11.14 | 6000 |

The used data set was observed from the atmospheric diffusion experiments conducted at the northern part of Copenhagen, Denmark, under unstable conditions (Gryning and Lyck, 1984; Gryning et al., 1987). The tracer sulfur hexafluoride (SF6)

| Table 3. Com | parison between | Observed, | two numerical | models nori | malized c | crosswind-int | tegrated | concentrations | Cy/Q | and down | wind d | listance |
|--------------|-----------------|-----------|---------------|-------------|-----------|---------------|----------|----------------|------|----------|--------|----------|
| | | | | | | | | (10 1 (a/m2)) | | | | |

| | Stability | Down distance (m) | Cy/Q 10-4 (s/m2) | | | | |
|--------|-------------------------|---------------------|-------------------|-------------------|----------|--|--|
| un no. | Stability | Down distance (III) | Numerical model 1 | Numerical model 2 | Observed | | |
| 1 | Very unstable (A) | 1900 | 3.59 | 2.08 | 6.48 | | |
| 1 | Very unstable (A) | 3700 | 4.93 | 3.79 | 2.31 | | |
| 2 | Slightly unstable (C) | 2100 | 7.36 | 4.03 | 5.38 | | |
| 2 | Slightly unstable (C) | 4200 | 2.04 | 1.27 | 2.95 | | |
| 3 | Moderately unstable (B) | 1900 | 1.05 | 1.32 | 8.2 | | |
| 3 | Moderately unstable (B) | 3700 | 8.94 | 3.40 | 6.22 | | |
| 3 | Moderately unstable (B) | 5400 | 1.20 | 6.25 | 4.3 | | |
| 5 | Slightly unstable (C) | 2100 | 1.18 | 3.55 | 6.72 | | |
| 5 | Slightly unstable (C) | 4200 | 1.69 | 8.75 | 5.84 | | |
| 5 | Slightly unstable (C) | 6100 | 3.76 | 1.53 | 4.97 | | |
| 6 | Slightly unstable (C) | 2000 | 2.02 | 2.83 | 3.96 | | |
| 6 | Slightly unstable (C) | 4200 | 1.44 | 7.24 | 2.22 | | |
| 6 | Slightly unstable (C) | 5900 | 5.31 | 1.18 | 1.83 | | |
| 7 | Moderately unstable (B) | 2000 | 1.81 | 2.63 | 6.7 | | |
| 7 | Moderately unstable (B) | 4100 | 1.46 | 6.09 | 3.25 | | |
| 7 | Moderately unstable (B) | 5300 | 1.01 | 8.62 | 2.23 | | |
| 8 | Neutral (D) | 1900 | 5.14 | 7.11 | 4.16 | | |
| 8 | Neutral (D) | 3600 | 9.14 | 1.50 | 2.02 | | |
| 8 | Neutral (D) | 5300 | 4.32 | 2.42 | 1.52 | | |
| 9 | Slightly unstable (C) | 2100 | 5.97 | 3.50 | 4.58 | | |
| 9 | Slightly unstable (C) | 4200 | 1.05 | 7.70 | 3.11 | | |
| 9 | Slightly unstable (C) | 6000 | 1.60 | 1.18 | 2.59 | | |

Was released from a tower at a height of 115m without buoyancy. The values of different parameters such as stability, wind speed at 10m (U10), wind speed at 115m (U115), and downwind distance during the experiment are represented in (Table 2).

Table (3); shows the observed, two analytical models, and two numerical normalized crosswind-integrated concentrations Cy/Q and downwind distance.



Figure 1. Comparison between numerical cross observed normalized crosswind integrated concentration and downwind distance



Figure 2. The variation of the numerical predicted normalized crosswind concentrations via observed normalized crosswind concentrations

Fig. (1), shows that the variation of numerical and observed normalized crosswind concentrations data downwind distances. We find that numerical model 1 have points agree with the observed data, while the others points are over predicated.

Fig. (2) Show comparison between numerical model 1, 2 and observed normalized crosswind integrated concentrations. We find that numerical model 1 agree with observed data than numerical model 2, while numerical model 2 has most points are over predicted with the observed data.

Statistical method

Now, the statistical method is presented and comparison among analytical, statically and observed results will be offered (Hanna 1989). The following standard statistical performance measures that characterize the agreement between model prediction (Cp=Cpred/Q) and observation (Co=Cobs/Q):

Normalized Mean Square Error (NMSE) =
$$\frac{(C_p - C_o)}{(C_p C_o)}$$

Fractional Bias (FB) = $\frac{(\overline{C_o} - \overline{C_p})}{[0.5(\overline{C_o} + \overline{C_p})]}$

Correlation Coefficient (COR) = $\frac{1}{N_m} \sum_{i=1}^{N_m} (C_{pi} - \overline{C_p}) \times \frac{(C_{oi} - \overline{C_o})}{(\sigma_p \sigma_o)}$

Factor of Two (FAC2) = $0.5 \le \frac{C_p}{C_0} \le 2.0$

Where σp and σo are the standard deviations of Cp and Co respectively. Here the over bars indicate the average over all measurements (Nm). A perfect model would have the following idealized performance: NMSE = FB = 0 and COR = FAC2 = 1.0

Table 4. Comparison between our different models according to standard statistical performance measure

| Models | NMSE | FB | COR | FAC2 |
|-------------------|------|------|--------|------|
| Numerical model 1 | 0.66 | 0.04 | - 0.11 | 1.19 |
| Numerical model 2 | 0.79 | 0.19 | - 0.08 | 1.09 |

From the statistical method, we find that the two models are factors of 2 with observed data. Regarding to NMSE, numerical model 1 is better than numerical model 2. The numerical model 1 is also the best regarding to FB. The correlations of numerical model 1 and model 2 are equal -0.11 and -0.08 respectively.

CONCULSION

We have used numerical solution of two- dimensional atmospheric diffusion equation by Adomain decomposition method to calculate normalized crosswind concentrations for continuous emits sulfur hexafluoride (SF6). In this model the vertical eddy diffusivity depends on the downwind distance and it is calculated using two methods $k_1(x) = 0.04$ u x and $k_2(x) = 0.16$ (σ_w/u) x.

Graphically, we can observe that numerical models 1 and two have most points inside a factor of two with the observed data.

From the statistical method, we find that the two models are factors of 2 (FAC2)

Regarding to NMSE, numerical models 1 and two are better with observed data. Also the numerical models 1 and 2 are the best regarding to FB. The correlations of numerical model 1 and model 2 are equal -0.11 and -0.08 respectively.

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