

Solution of the diffusion equation using Adomain decomposition

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Abstract: The objective is to estimate 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 release 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.

1 Introduction

The Adomian decomposition method (ADM) has been applied in wide class of stochastic and deterministic problems in many interesting mathematics and physics areas [1]. Adomain gave a review of the decomposition method in [2]. The numerical solution of sixth order boundary value problem by ADM is found by [3]. The Adomians decomposition and wavelet - Galerkin methods is used to solve integro- differential equations by [4]. The Sine -Galerkin and the modified decomposition methods is used for two - point boundary -value problems by [5].

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.

2 Numerical Method

Time dependent advection - diffusion equation is written as [6].

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} (K_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y} (K_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z} (K_z \frac{\partial c}{\partial z}) \quad (1)$$

where c is the average concentration of air pollution ($\mu\text{g}/\text{m}^3$). 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 (m^2/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:

$$u \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} (K_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z} (K_z \frac{\partial c}{\partial z}) \quad (2)$$

Assuming that $k_y = k_z = k(x)$, integrating the equation 2 with respect to y , we obtain the normalized crosswind integrated concentration $c_y(x,z)$ of contaminant at a point (x,z) of the atmospheric advection-diffusion equation is written in the form as [7]:

$$\frac{\partial^2 c_y(x,z)}{\partial z^2} = \frac{u \partial c_y(x,z)}{K \partial x} \quad (3)$$

Equation 3 is subjected to the following boundary condition 1-It is assumed that the pollutants are absorbed at the ground surface i.e.

$$k \frac{\partial c_y(x,z)}{\partial z} = -v_g c_y(x,z) \quad \text{at } z = 0 \quad (i)$$

where v_g is the deposition velocity (m/s).

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

$$k \frac{\partial c_y(x,z)}{\partial z} = 0 \quad \text{at } z = h \quad (ii)$$

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3-The mass continuity is written in the form

$$u c_y(x, z) = Q \delta(z - h) \quad \text{at } x = 0 \quad (\text{iii})$$

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.

$$c_y(x, z) = 0 \quad \text{at } z = \infty \quad (\text{iv})$$

In equation 3, we take $A = \frac{u}{k}$ and Equation 3 can be solved using Adomain decompositions method as follows:

$$L_{zz} c_y(x, z) = A L_x c_y(x, z)$$

$$\text{where } L_{zz} = \frac{\partial^2}{\partial z^2}, L_x = \frac{\partial}{\partial x}$$

Multiplying both sides of the above equation by L_{zz}^{-1} (inverse), one gets:

$$c_y(x, z) = c_0 + A L_{zz}^{-1} L_x c_y(x, z)$$

$$L_{zz}^{-1} = \int_0^z \int_0^z (c_0 + A L_{zz}^{-1} L_x c_y(x, z)) dz dz \quad (4)$$

Assuming that

$$C_0 = M(x) + zN(x) \quad (5)$$

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

$$c_{n+1} = A \int_0^z \int_0^z \frac{\partial c_n}{\partial x} dz dz \quad (6)$$

Put $n = 0$

$$\begin{aligned} c_1 &= A \int_0^z \int_0^z \frac{\partial c_0}{\partial x} dz dz \\ &= A \int_0^z \int_0^z \left(\frac{\partial M}{\partial x} + z \frac{\partial N}{\partial x} \right) dz dz \quad (7) \\ &= A \frac{\partial M}{\partial x} \frac{z^2}{2!} + A \frac{\partial N}{\partial x} \frac{z^3}{3!} dz dz \end{aligned}$$

Assuming the solution has the form

$$W_n = \sum_0^{\infty} c_n$$

$$\begin{aligned} W_1 &= c_0 + c_1 \\ &= M(x) + zN(x) + A \frac{\partial M}{\partial x} \frac{z^2}{2!} + A \frac{\partial N}{\partial x} \frac{z^3}{3!} \quad (8) \end{aligned}$$

By differentiating the equation 8 with respect to z and multiplying by k_z , we obtain that:

$$K_z \frac{\partial W_1}{\partial z} = K_z N(x) + A z K_z \frac{\partial M}{\partial x} + A \frac{z^2}{2!} K_z A \frac{\partial N}{\partial x} \quad (9)$$

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

$$K_z \frac{\partial W_1}{\partial z} = K_z N(x) = M(x)$$

$$\therefore N(x) = \frac{-v_g}{K_z} M(x) \Rightarrow M(x) = -\frac{K_z}{v_g} N(x) \quad (10)$$

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

$$kN(x) + Ahk \frac{\partial M}{\partial x} + \frac{h^2}{2!} AK \frac{\partial N}{\partial x} = 0$$

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

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

$$kN(x) - Ahk \left(\frac{K}{v_g} \frac{\partial N}{\partial x} + \frac{N(x)}{v_g} \frac{\partial k}{\partial x} \right) + \frac{h^2}{2!} AK \frac{\partial N}{\partial x} = 0$$

$$\left[\frac{h^2 AK}{2!} - \frac{Ahk^2}{v_g} \right] \frac{\partial N}{\partial x} + \left[K - \frac{Ahk}{v_g} \frac{\partial k}{\partial x} \right] N(x) = 0 \Rightarrow$$

$$\left[\frac{h^2 k A v_g - 2 A h k^2}{2 v_g} \right] \frac{\partial N}{\partial x} = \left[\frac{Ahk \frac{\partial k}{\partial x} - k v_g}{v_g} \right] N(x) \quad \Rightarrow \quad (11)$$

$$\frac{\partial N}{N(x)} = \left[\frac{2A \frac{\partial k}{\partial x} - 2v_g}{Ah(hv_g - 2K)} \right] \partial x$$

Integrating the equation 11 from 0 to x , we obtain that:-

$$N(x) = N_0(x) e^{\left[\frac{2A \frac{\partial k}{\partial x} - 2v_g}{Ah(hv_g - 2K)} \right] x} \quad (12)$$

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

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

Substituting from $N_0(x)$ in equation 12, we get that:-

$$N(x) = \frac{Q}{u} \delta(z - h) e^{\left[\frac{2A \frac{\partial k}{\partial x} - 2v_g}{Ah(hv_g - 2K)} \right] x} \quad (13)$$

Substituting from two equations 10 and 13 in equation 5, we obtain that:-

$$c_0 = \frac{-K}{v_g} N(x) + zN(x) = \left[\frac{-K}{v_g} + z \right] N(x) = (z - B)N(x) \quad (14)$$

where $B = k/v_g$

$$\frac{\partial N}{\partial x} = N \left[2 \frac{2Ah \frac{\partial k}{\partial x} - 2v_g}{Ah(hv_g - 2K)} \right] \quad (15)$$

$$M = \frac{-k}{v_g} \frac{\partial N}{\partial x} \quad (16)$$

$$\frac{\partial M}{\partial x} = \frac{-kN}{v_g} \left[2 \frac{2Ah \frac{\partial k}{\partial x} - 2v_g}{Ah(hv_g - 2K)} \right] \quad (17)$$

Substituting equations (11) and (17) in equation (7), we obtain that:

$$c_1 = (AD) \left(\frac{z^3}{3!} - \frac{k}{v_g} \frac{z^2}{2!} \right) N \quad (18)$$

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

Similar, we get

$$c_2 = (AD)^2 \left(\frac{z^5}{5!} - \frac{k}{v_g} \frac{z^4}{4!} \right) N$$

$$c_3 = (AD)^3 \left(\frac{z^7}{7!} - \frac{k}{v_g} \frac{z^6}{6!} \right) N \quad (19)$$

$$c_4 = (AD)^4 \left(\frac{z^9}{9!} - \frac{k}{v_g} \frac{z^8}{8!} \right) N$$

the general solution:

$$\frac{\partial c_y(x,z)}{Q} = \frac{v_g}{u(hv_g - k)} e^{\frac{2(Ah \frac{\partial k}{\partial x} - v_g)x}{Ah(hv_g - 2k)}} \sum_0^n \left(\frac{2u(Ah \frac{\partial k}{\partial x} - v_g)x}{Ahk(hv_g - 2x)} \right)^i \left(\frac{-kz^{2i}}{v_g(2!)} + \frac{z^{2i+1}}{(2!+1)!} \right) \quad (20)$$

3 Results and discussion

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

$$u_{115} = u_{10} \left(\frac{z}{10} \right)^p \quad (21)$$

where :

u_{115} is the wind speed at 115m.

u_{10} is the wind speed at 10m.

z is the physical height.

p is parameter estimated by [8], 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 [8].

Stability Classes	Very unstable (A)	Moderately unstable (B)	Slightly unstable (C)	Neutral (D)	Slightly stable (E)	Moderately stable (F)
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 form from $k_1(x) = 0.04ux$ and the second method are referenced to [6] where k takes in the form:

$$k_z(x) = 0.16 \left(\frac{\sigma_w^2}{u} \right) x$$

where σ_w 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 Copenhagen.

Run no.	Stability	$u_{10}(m/s)$	$u_{115}(m/s)$	distance (x)(m)
1	A	2.1	3.34	1900
1	A	2.1	3.34	3270
2	C	4.9	10.71	2100
2	C	4.9	10.71	4200
3	B	2.4	4.01	1900
3	B	2.4	4.01	3700
3	B	2.4	4.01	5400
5	C	3.1	4.93	2100
5	C	3.1	4.93	4200
5	C	3.1	4.93	6100
6	C	7.2	11.45	2000
6	C	7.2	11.45	4200
6	C	7.2	11.45	5900
7	B	4.1	6.85	2000
7	B	4.1	6.85	4100
7	B	4.1	6.85	5300
8	D	4.2	8.74	1900
8	D	4.2	8.74	3600
8	D	4.2	8.74	5300
9	C	5.1	11.14	2100
9	C	5.1	11.14	4200
9	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 [9] and [10]. The tracer sulfur hexafluoride (SF6).

was released from a tower at a height of 115m without buoyancy. The values of different parameters such as stability, wind speed at 10m (U_{10}), wind speed at 115m(U_{115}), 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 C_y/Q and downwind distance.

4 Statistical method

Now, the statistical method is presented and comparison among analytical, statically and observed results will be offered [11]. The following standard statistical performance measures that characterize the agreement between model prediction ($Cp = C_{pred}/Q$) and observation ($Co = C_{obs}/Q$):

Table 3 Comparison between Observed, two numerical models normalized crosswind-integrated concentrations C_y/Q and downwind distance.

RUN NO.	Stability	down distance (m)	$C_y/Q * 10^{-3} (s/m^2)$		
			Numeric. model 1	Numeric. model 2	Observed
1	A	1900	3.59	2.08	6.48
1	A	3700	4.93	3.79	2.31
2	C	2100	7.36	4.03	5.38
2	C	4200	2.04	1.27	2.95
3	B	1900	1.05	1.32	8.20
3	B	3700	8.94	3.40	6.22
3	B	5400	1.20	6.25	4.30
5	C	2100	1.18	3.55	6.72
5	C	4200	1.69	8.75	5.84
5	C	6100	3.76	1.53	4.97
6	C	2000	2.02	2.82	3.96
6	C	4200	1.44	7.24	2.22
6	C	5900	5.31	1.18	1.83
7	B	2000	1.81	2.63	6.70
7	B	4100	1.46	6.09	3.25
7	B	5300	1.01	8.62	2.23
8	D	1900	5.14	7.11	4.16
8	D	3600	9.14	1.50	2.02
8	D	5300	4.32	2.42	1.52
9	C	2100	5.97	3.50	4.58
9	C	4200	1.05	7.70	3.11
9	C	6000	1.60	1.18	2.59

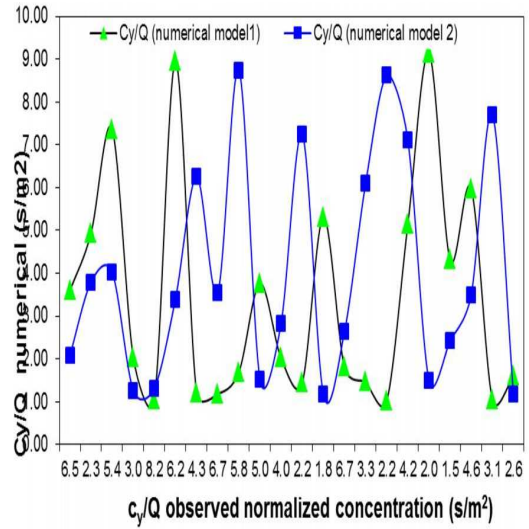


Fig. 2 The variation of the numerical predicted normalized crosswind concentrations via observed normalized crosswind concentrations.

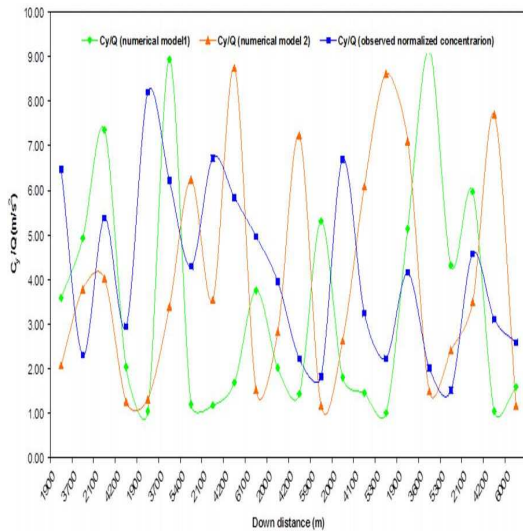


Fig. 1 Comparison between numerical cross observed normalized crosswind integrated concentration and downwind distance.

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

$$\text{Factor of Two (FAC2)} = 0.5 \leq \frac{C_p}{C_o} \leq 2.0$$

Where σ_p and σ_o are the standard deviations of C_p and C_o respectively. Here the over bars indicate the average over all measurements (N_m). A perfect model would have the following idealized performance:

$$NMSE = FB = 0 \text{ and } COR = FAC2 = 1.0$$

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

$$\text{Normalized Mean Square Error (NMSE)} = \frac{((\overline{C_p} - \overline{C_o})^2)}{((\overline{C_p C_o}))}$$

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

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.

5 Conclusion

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 (SF_6). In this model the vertical eddy diffusivity depends on the downwind distance and it is calculated using two methods $k_1(x) = 0.04ux$ and $k_2(x) = 0.16(\sigma_w/u)x$. 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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References

- [1] G. Adomain, Solving Frontier problems of physics. The Decomposition Method, Kluwer, Boston, 1994.
- [2] G. Adomain, J.Math.Anal.Appl. **135**, 501-544 (1988).
- [3] A. Wazwaz, Appl. Math. Comput. **118**, 311-325 (2001).
- [4] El-Sayed, M.Abdel-Aziz, Appl. Math. Comput. **139**, 151-159 (2003).
- [5] M. Elgamel, Appl. J. Comput. Phys. **223**, 369-383 (2007).
- [6] P.S. ARYA, Appl. J. Appl. Met. **34**, 1112-1122 (1995).
- [7] K.S.M. Essa, S. Maha EL-Qtaify, Meteorol. Atmo, Phys. **92**, 95-101 (2006).
- [8] J.S. Irwin, Atmospheric environment **13**, 191-194 (1979).
- [9] S. E. Gryning, E. Lyck, J. Climate Appl. Meteor. **23**, 651-660 (1984).
- [10] S.E. Gryning, A.A.M. Holtslag, J.S. Irwin, B. Sivertsen, Atmospheric environment **21(1)**, 79-89 (1987).
- [11] S.R. Hanna, Atmospheric environment **23**, 1385-1395 (1989).