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MATHEMATICAL MODELING AND SOLUTION OF ADVECTION-DIFFUSION EQUATION

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ABSTRACT

In this paper, we first develop advection-diffusion equation by considering mass conservation in a fixed control volume. Firstly, we consider the one dimensional situation where there is advection but no diffusion and we also described Gaussian plume model for the variation of concentration of air pollutants, from an elevated source in presence of wind, in steady state.

Keywords: *Solution of advection diffusion equation.*

AMS Mathematics subject classification (2010): *76Rxx, 76Sxx, 76Txx, 97M60.*

1. INTRODUCTION

The air pollution dispersion is a complex problem. It covers the pollutant transport and diffusion in the atmosphere. The transport of pollutant occurs in a large variety of environmental, agricultural and industrial processes. Accurate prediction of the transport of these pollutants is crucial to the effective management of these processes. The transport of these pollutants can be adequately described by the advection-diffusion equation. The problems related to environment such as deforestation, release of toxic materials, solid waste disposals, air pollution and many more, have attracted attention much greater than ever before. The pollutant dispersion in the atmosphere depends on pollutant features, meteorological, emission and terrain conditions. Physical and mathematical models are developed to describe the air pollution dispersion. Physical models are small scale representations of the atmospheric flow carried out in wind tunnels.

The advection-diffusion equation arises in a number of physical problems in engineering including migration of contaminants in a stream, smoke plume in atmosphere, dispersion of chemicals in reactors, tracer dispersion in a porous medium, etc.

The mass transport is the transport of solute in a solvent. The solute is dissolve and the solvent is the dissolver. Generally, the liquids are classified as solvent because they plays an important role in industry. In environmental applications, these solvents are solutes and water or air is usually the solvents. Also advection-diffusion arises in a number of biological transport problems in which a bulk fluid like water transports a solute or even a drug with concentration. The substance being transported can be either dissolved or particulate substances.

Air quality is an important social issue. Acid rain is a regional problem, affected by industrial by-products of toxic gas; it pollutes the ground and damages vegetation. In urban areas it is the ozone concentration that is considered to be the biggest health hazard. Air quality is mathematical description of atmospheric transport, diffusion, and chemical reaction of pollutants. The unknown variables are concentrations of chemical species in air. The aim in developing and studying such models is to be able to predict how peak concentrations will change in response to prescribed changes in meteorology and in the source of pollution. Ozone air quality modeling has been one of the main areas of emphasis in the United States in the last twenty years; it is of particular interest to the automobile industry. In this chapter we consider the modeling of transport and diffusion of single chemical, say ozone, ignoring the various underlying processes.

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Since the pioneering work of Roberts [15] and Sutton [16], analytical and approximate solutions for the atmospheric dispersion problem have been derived under a wide range of simplifying assumptions, as well as various boundary conditions and parameter dependencies. These analytical solutions are especially useful to engineers and environmental scientists who study pollutant transport, since they allow parameter sensitivity and source estimation studies to be performed. The simplest of these exact solutions is called the Gaussian plume, corresponding to a continuous point source that emits contaminants into a unidirectional wind blowing in a domain of infinite extent. This Gaussian plume solution, along with numerous variants, has been incorporated into industry-standard software packages that are used for monitoring and regulatory purposes. Gaussian plume models have been applied extensively in the study of emissions from large industrial operations as well as a variety of other applications including ash release from volcanic eruptions [23]; seed, pollen, and insect dispersal [24, 4, 27]; and odor propagation from livestock facilities [21]. The same approach (with slight modifications) may also be used to describe the flow of gas or liquid in porous soils and rocks, with applications to oil reservoirs, groundwater, and pollutant transport in aquifers, etc. [20, 9]. There has been a great deal of recent interest in applications relating to nuclear and biological contaminant release [8, 13], for which the importance of analytical approaches is nicely summed up in a review article by Settles: "plume dispersion modeling is central to homeland security" [7].

Analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena [18]. Many operative models (using an analytical formula for the air pollution concentration) adopt empirical algorithms for describing dry deposition. The Gaussian plume equation was modified to include source depletion models [5, 17]. The solutions proposed by [6, 19, 25] also retained the framework of invariant wind speed and eddies with height (as the Gaussian approach). More recent analytical solutions of the advection–diffusion equation with dry deposition at the ground have utilized height-dependent wind speed and eddy diffusivities [3, 12, 14]. However, these solutions are restricted to the specific case in which the source is located at the ground level and/or with restrictions to the wind speed and eddy diffusivity vertical profiles.

In this paper, we first develop advection-diffusion equation by considering mass conservation in a fixed control volume, we also described Gaussian plume model for the variation of concentration of air pollutants, *C*, from an elevated source in presence of wind, in steady state (Stockie, 2011) [26].

2. Derivation of advection-diffusion equation:

We will develop the diffusion equation by considering mass conservation in a fixed control volume. The mass conservation equation can be written as [2, 10]

$$Flux\ rate\ in\ - Flux\ rate\ out\ + Source\ rate - Sink\ rate = Accumulation\ rate. \tag{2.1}$$

We will use the rectangular control volume for the development of mass conservation (diffusion) equation.

2.1. Diffusive flux rate and Convective flux rate:

In the development of advection-diffusion equation, we have need of two types of flux rates one is diffusive flux rates and other is convective flux rates. The molecules of fluid "at rest" are still moving because of their internal energy. They are vibrating, in a solid, the molecules are held in a lattice. In a gas or liquid they are not, so they move around because of this vibration. Since the molecules are vibrating in all directions, the movement appears to be random. The molecules are generally much farther apart in gases, so the diffusivity of a compound in a gas is significantly larger than in liquid. Fick's law is a physically meaningful mathematical description of diffusion that is based on the analogy to heat conduction (Fick, 1855). Fick's law state two rule. (1) Diffusion occurs in the direction from high concentration to low concentration. (2) The rate of diffusion is proportional to the difference in the concentration. Let us consider one side of our control volume, normal to the x axis, with an area A_x, shown in figure 3.1. Fick's law describes the diffusive flux rate as

$$\text{Diffusive flux rate} = -D\frac{\partial C}{\partial x}\ A_x \tag{2.1.1}$$

where C is concentration of the solute, D is the diffusion coefficient of the solute in the solvent (water), which relates to how fast and how far the tracer molecules are moving to and fro, and $\frac{\partial C}{\partial x}$ is the gradient of concentration with respect to x, or the slope of x. Thus the diffusive flux rate depends on the diffusion coefficient and the gradient of concentration with distance.

The convective flux rate into our control volume is simply the chemical mass carried in by convection. If we consider the box as a control volume, except with a velocity component u in the x direction, the convective flux rate into the box from the left hand side is

$$\begin{bmatrix} Convective \\ fiux\ rate \end{bmatrix} = \begin{bmatrix} Velocity\ component \\ normal\ to\ surface \end{bmatrix} \times [Surface\ area] \times\ [Concentration] \tag{2.1.2}$$

$$Convective\ flux\ rate = u\ A_x\ C \tag{2.1.3}$$

where u is the component of velocity in the x- direction and A_x is the surface area normal to the x axis on then side of the box. All six sides of our box would have a convective flux through them, just as they would have a diffusive flux.

2.2. Accumulation, Source and sink rate:
The rate of accumulation is the change of chemical mass per unit time, or Rate of accumulation is given as

$$Rate\ of\ accumulation = \overline{V}\,\frac{\partial C}{\partial t} \tag{2.2.1}$$

where $\bar{V}$ is the volume of the box. The solute chemical can appear or disappear through chemical reaction. For both cases the source and sink rates are given as

$$\text{Source - Sink rate} = S\overline{V} \tag{2.2.2}$$

where S is the net source/sink rate per unit volume.

2.3. Mass balance on control volume
A mass balance on one compound in our box is based on the principle that whatever comes in must do one of three things: (1) be accumulated in the box, (2) flux out off another side, or (3) react in the source/sink terms. We will begin by assigning lengths to the sides of our box $dx, dy\ and\ dz$, as shown in Figure Then, for simplicity in this mass balance, we will arbitrarily designate thr flux as positive in the $+\,x$- direction, $+\,y$- direction, and $+\,z$- direction. The x- direction flux, so designed then, two flux terms in equation (2.1) become

$$\text{Flux rate in + Difference in flux rate = Flux rate out;} \tag{2.3.1}$$

or because a difference can be equated to a gradient times distance over which the gradient is applied,

$$\text{Flux rate out - Flux rate in = Gradient in flux rate} \times \text{Distance} \tag{2.3.2}$$

Equation (2.3.2) can thus be applied along each spatial component as

$$Flux\ rate\ (out - in)_x = \frac{\partial}{\partial x}\ (flux\ rate)dx \tag{2.3.3}$$

$$Flux\ rate\ (out - in)_y = \frac{\partial}{\partial x}\ (flux\ rate)dy \tag{2.3.4}$$

$$Flux\ rate\ (out - in)_z = \frac{\partial}{\partial x}\ (flux\ rate)dz \tag{2.3.5}$$

We will discuss the convective and diffusive flux rates separately, because they are separated in the final advection-diffusion equation, and it is convenient to make that break now. The x- component of the convective flux rate is equal to the x- component of the velocity u, times the concentration, C, times the area of our box normal to the x- axis. Therefore, in term of the convective rates, equation (2.3.3) becomes

$$Convective\ fiux\ rate(out - in)_x = \frac{\partial}{\partial x}\ (u\ C\ A_x)dx = \frac{\partial}{\partial x}\ (u\ C\ )dx\ dy\ dz \tag{2.3.6}$$

Because the normal area, $A_x = dy\ dz$ of our box does not change with x, it can be pulled out of the partial with respect to x. This is done in the second part of equation (2.3.6). The same can be done with the y- and z- components of convective flux rate.

$$Convective\ fiux\ rate(out - in)_y = \frac{\partial}{\partial x}\ \left(v\ C\ A_y\right)dy = \frac{\partial}{\partial x}\ (\ vC\ )dx\ dy\ dz \tag{2.3.7}$$

$$Convective\ fiux\ rate(out - in)_z = \frac{\partial}{\partial x}\ (\ w\ C\ A_Z\ )dx = \frac{\partial}{\partial x}\ (\ w\ C\ )dx\ dy\ dz \tag{2.3.8}$$

Finally, adding equations (2.3.6), (2.3.7) and (2.3.8) results in the total net convective flux rate

$$Net\ convective\ fiux\ rate = \left[\frac{\partial}{\partial x}\ (\ u\ C\ ) + \frac{\partial}{\partial y}\ (\ v\ C\ ) + \frac{\partial}{\partial z}\ (\ w\ C\ )\right]\ dx\ dy\ dz \tag{2.3.9}$$

For net diffusive flux rate in the x- direction, equation (2.3.3) becomes

$$Diffusive\ flux\ rate\ (\ out - in)_x = \frac{\partial}{\partial x}\ \left(-D\frac{\partial C}{\partial x}\ A_x\right)dx = \frac{\partial}{\partial x}\ \left(-D\frac{\partial C}{\partial x}\right)dx\ dy\ dz \tag{2.3.10}$$

Write out the diffusive flux rate in the y and z - direction on a separate sheet of paper. The result is similar to equation (2.3.10).

$$Diffusive\ flux\ rate\ (\ out - in)_y = \frac{\partial}{\partial y}\ \left(-D\frac{\partial C}{\partial y}\ A_y\right)dy = \frac{\partial}{\partial y}\ \left(-D\frac{\partial C}{\partial y}\right)dx\ dy\ dz \tag{2.3.11}$$

$$Diffusive\ flux\ rate\ (\ out - in)_z = \frac{\partial}{\partial z}\ \left(-D\frac{\partial C}{\partial z}\ A_z\right)dz = \frac{\partial}{\partial z}\ \left(-D\frac{\partial C}{\partial z}\right)dx\ dy\ dz \tag{2.3.12}$$

Finally, we can add equation (2.3.10) to (2.3.12) to write an equation describing the net diffusive flux rate (out-in) out of the control volume:

$$Net\ diffusive\ flux\ rate = -\left[\frac{\partial}{\partial x}\left(\ D\ \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\ D\ \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\ D\ \frac{\partial C}{\partial z}\right)\right]dx\ dy\ dz \tag{2.3.13}$$

The diffusion coefficient is often not a function of distance, such that equation (2.3.13) can be further simplified by putting the constant value diffusion coefficient in front of the partial derivative. However, we will also be substituting turbulent diffusion and dispersion coefficients for D when appropriate to certain applications, and they are not always constant in all directions. Therefore, we will leave the diffusion coefficient inside the brackets. We can now combine equations (2.1), (2.2.1), (2.2.2), (2.3.9) and (2.3.13) into a mass balance on our box for Cartesian coordinates. After dividing by $\vec{V} = dx\, dy\, dz$ and moving the diffusive flux terms to the right-handed side, this mass balance is

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(u\, C) + \frac{\partial}{\partial y}(v\, C) + \frac{\partial}{\partial z}(w\, C) = \left[\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D\,\frac{\partial C}{\partial z}\right)\right] + S \tag{2.3.14}$$

If the flow is assumed to be incompressible, the incompressible flow assumption is most always accurate for water in environmental applications and is often a good assumption for air. Then by using continuity equation, the above equation reduces to

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) + S \tag{2.3.15}$$

Then we can consider the particular case of equation of above equation without convective term. Then equation reduces to diffusion equation in three dimensions without any source. General solutions of the diffusion equation can be obtained for a various initial and boundary conditions provided the diffusion coefficient is constant

3. AIR QUALITY MATHEMATICAL MODELING

Advection is essentially the effect of the wind "blowing" the fumes in a given direction without significantly dispersing them. A good example is a distant cloud moving with a fixed velocity in a given direction without apparently altering its size or shape.

3.1. The mathematical air quality model:

We denote by c the concentration of one species, it is function of position (x_1, x_2, x_3) and of time t. The species is being transported by the wind, whose velocity $\vec{u} = \vec{u}(x_1, x_2, x_3, t)$ is assumed to be known. Particles of the species are also diffusing locally, they tend to move from areas of high concentration to areas of low concentration. If diffusion is ignored then the transport equation is [1]

$$\frac{\partial c}{\partial x} + \nabla.(\vec{u}c) = 0. \tag{3.1}$$

This is in some contexts also called the continuity equation. If we integrate (3.1) over any bounded domain D in R^3 we get

$$\frac{\boldsymbol{d}}{\boldsymbol{dt}} \iiint \boldsymbol{c}(x_1, x_2, x_3, t)\, \boldsymbol{d}x_1 \boldsymbol{d}x_2 \boldsymbol{d}x_3 \text{ } over\ D = \int\int c\,\vec{u}.\vec{n}dS \text{ } over\ \partial D, \tag{3.2}$$

where ∂D is the boundary of D and $\vec{n}$ is the outward unit normal to ∂D. This equation says that the rate of increase of the chemical in any domain D is equal to the flow of chemicals across the boundary. If diffusion is not ignored then (3.1) is replaced by a more complicated partial differential equation.

$$\frac{\partial c}{\partial x} + \nabla.(\vec{u}c) = \sum_{i,j=1}^{3} \frac{\partial}{\partial x_i}\left(k_{ij}\, \frac{\partial c}{\partial x_i}\right), \tag{3.3}$$

where k_{ij} is a positive definite matrix, called the diffusion matrix.

In either case (3.1) or (3.2), we are given the concentration c at an initial time, say at $t = 0$;

$$c(x_1, x_2, x_3, 0) = c_0(x_1, x_2, x_3) \tag{3.4}$$

and our task is to compute the concentration $c(x_1, x_2, x_3, t)$ at subsequent times.

3.2. One dimensional advection equation:

Firstly, we consider the one dimensional situation where there is advection but no diffusion. Suppose at time $t = 0$ the density of the fumes has a distribution given by profile $c_0(x)$. This profile moves to the right with the constant wind velocity U, giving rise to the moving profile for the concentration

$$c(x, t) = c_0(x - Ut). \tag{3.2.1}$$

Differentiating partially, using the chain rule, we get

$$\frac{\partial c}{\partial x}(x, t) = c_0'(x - Ut), \frac{\partial c}{\partial t}(x, t) = c_0'(x - Ut).(-U). \tag{3.2.2}$$

Thus giving us the "advection equation"

$$\frac{\partial c}{\partial t}(x, t) + \frac{\partial (Uc)}{\partial x}(x, t) = 0 \tag{3.2.3}$$

With "initial" condition $c(x, 0) = c_0(x)$.In the particular situation described here, we knew the solution of the partial differential equation in advance. In a more complicated situation, such as when the "wind velocity" U is not a constant, this will not be the case.

Looking at the form with the concentration profile (3.2.1) we see that the noxious fumes will arrive at "your" house in the same concentration as they left the factory: very high! Luckily all is not lost! As we have hinted earlier, there is another process at work: diffusion. This is the reason that even without the presence of wind, foul smelling odors usually disappear after a time.

Now, we ignore diffusion and assume that the wind velocity is only in the horizontal direction. For simplicity we also assume that the direction of the wind is fixed. Say, in the x-direction. Then $\vec{u} = (U, 0,0)$ and the transport equation reduces to

$$\frac{\partial c}{\partial t} + \frac{\partial (Uc)}{\partial x} = 0; \tag{3.2.4}$$

This is called the advection equation. We also assume that initially c depends only on x, i.e.,

$$c(x,0) = c_0(x), \qquad -\infty < x < \infty. \tag{3.2.5}$$

The velocity $U = U(x)$ is a function of x. To solve (3.2.4), (3.2.5), we rewrite (3.2.5) in the form

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = f \qquad (f = -U_x c) \tag{3.2.6}$$

And assume that $U(x)$ is continuously differentiable $(U_x = dU/dx)$. Consider the differential equation

$$\left\{\frac{dx}{dt} = U(x), t > 0 \; and \; x(0) = x_0, \; t = 0 \right\} \tag{3.2.7}$$

And denote its solution $x(t)$ by $(t; x_0)$. Geometrically, $x(t; x_0)$ determines a unique curve γ_{x_0} passing through the point $(x_0, 0)$.we can show that $x(t; x_0)$ is actually differentiable in the parameter x_0 and the derivative

$$z(t) \equiv \frac{\partial x\,(t; x_0)}{\partial x_0} \tag{3.2.8}$$

Satisfies

$$\frac{dz}{dt} = U_x\big(x(t; x_0)\big)\mathrm{z}, \quad \mathrm{z}(0) = 1. \tag{3.2.9}$$

We now examine the function

$$c(x(t; x_0), t), \tag{3.2.10}$$

as a function of the variable t. We find that

$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{\partial x}{\partial t} = \frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = f = -U_x\big(x(t; x_0)\big)\mathrm{c}, \tag{3.2.11}$$

or

$$\frac{\partial}{\partial t}\; logc == -U_x\big(x(t; x_0)\big). \tag{3.2.12}$$

It follows that

$$c(x(t; x_0), t) = c_0(x_0)\; exp\left\{-\int_0^t U_x\big(x(s; x_0)\big)\mathrm{ds}\right\}. \tag{3.2.13}$$

Solution of (3.2.4) with (3.2.5) is given by the formula (3.2.13).

4. GAUSSIAN PLUME MODEL

The variation of concentration of air pollutants, *C*, from an elevated source in presence of wind, in steady state, is described by the following partial differential equation (Stockie, 2011) [26]

$$u\frac{\partial C}{\partial x} = K\left(\frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{4.1}$$

where u is wind speed and *K*, the diffusion coefficient. Here, wind direction is in *x*-direction which is horizontal, *y* is horizontal and perpendicular to *x*, and *z*-direction is vertical increasing upwards. The source of pollutant having strength as *Q* is located at coordinates: (0,0,*H*). This source is represented in terms of Delta function as [22]

$$C(0, y, z) \;=\; Q\delta(x)\delta(y)\delta(z - H) \tag{4.2}$$

The boundary conditions for the model equations are:

$$C(x, \pm\infty, z) \;=\; 0 \tag{4.3}$$

$$C(x, y, \infty) \;=\; 0 \tag{4.4}$$

$$K\,\frac{\partial C}{\partial z}\;(x, y, 0) \;=\; 0 \tag{4.5}$$

These conditions respectively assume that concentration, C decays to zero as x tends to ∞, y tends to $\pm\infty$ and flux is zero at the earth's surface. We have all necessary boundary conditions for the air quality equation. This equation can be solved by the method of separation of variables. Stockie (2011) has given a detailed analysis of mathematics of this solution. The solution for concentration $C(x, y, z)$, called Gaussian plume solution, is given as

$$C(x, y, z) = \frac{Q}{4\pi K x}\, e^{-\frac{y^2 u}{4Kx}}\left[e^{-\left(\frac{u(z-h)}{4Kx}\right)^2} + e^{-\left(\frac{u(z+h)}{4Kx}\right)^2}\right] \tag{4.6}$$

This equation is made of simple exponential functions. Each exponential function is Gaussian type, like e^{-p^2}having value as one at $p = 0$ and decaying to zero as p tends to infinity. This solution can be used to build solution for various sources located at various locations as the air quality equation given above is linear and principle of superposition can be used. Stockie (2011) has presented several numerical results. This model can be used both for physical understanding and also regulations.

For transient release of the air pollutants, the model equation for concentration $C(x, y, z, t)$ is given as:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = K\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{4.7}$$

We now have Q as a function of time, non-zero for $t \geq 0$. We also need initial condition for concentration, which can be taken as

$$C(x, y, z, 0) \;=\; 0 \tag{4.8}$$

The boundary condition in *x*-coordinate is

$$C(\pm\infty, y, z) \;=\; 0 \tag{4.9}$$

All other boundary conditions remain the same as in steady state case. The solution is given as [11]

$$C(x, y, z, t) = \int_0^l \frac{Q(\tau)}{(2\pi K)^{\frac{3}{2}}} \exp\left(\frac{\left(x-u(t-\tau)\right)^2 - y^2}{4K(t-\tau)}\right)\left[\exp\left(-\frac{(z-H)^2}{4K(t-\tau)}\right) + \exp\left(-\frac{(z+H)^2}{4K(t-\tau)}\right)\right] d\tau \tag{4.10}$$

This solution can be used to find the distribution of air pollutants for given location and time history of the sources.

5. CONCLUSIONS

Analytical solutions of the one dimensional advection equation have been provided. We also described Gaussian plume model for the variation of concentration of air pollutants, *C*, from an elevated source in presence of wind, in steady state. This solution can be used to find the distribution of air pollutants for given location and time history of the sources.

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