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Advection diffusion equation models in near-surface geophysical and environmental sciences

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ABSTRACT

Basic near-surface geological and environmental processes such as groundwater flow, contaminants transport in aquifers, heat transport, air pollution etc. concern transport of mass in the near-surface and environmental media. Mathematical models are constructed using conservation laws such as mass/heat conservation and supplemented by constitutive relations such as Fick's laws for concentration distribution and Fourier law for heat conduction. Combing both equations, an advection-diffusion equation is formulated for constructing the spatio-temporal distribution of the mass and heat fields in air, water and subsurface environments. We present first derivation of advection-diffusion model equation and necessary initial and boundary conditions for a well-posed problem and summarize methods which are used to construct solutions. We then present few examples of such models for solute transport in the groundwater, flow in sloping aquifer, thermal distribution in subsurface for use inferring climatic signals from borehole geothermal data, steady and transient air quality and river water quality distributions. Environmental forensics requires to find the sources of pollution from observations. This is typical inverse problem, non well-posed problem, and can be solved by least squares theory. Lastly a brief discussion is presented about fractional advection diffusion theory which is now being used to understand anomalous dispersion of pollutants in the environment.

INTRODUCTION

Observations of processes taking on the earth's interior and environment are made from satellites to atomic microscopes. These observations span a vast space – time scales of processes ranging from atmospheric general circulation to electron transport on enzymes in the near surface regions. There are hierarchies of processes, processes linked across the scales both upwards and downwards. A great challenge for geophysical and environmental scientists is to develop hierarchy of models to explain working of earth's interior and its environment at this vast space – time scales. The models also help in making forecasts and do experimentation, being less costly than actual experiments.

An important class of processes in the geophysical and environment sciences consists of mass and heat transport processes. A large part of environmental modeling concerns the transport of pollutants in the environmental media. The transport takes place by advection and diffusion processes. Chemical reactions modify these fields. The advection – diffusion equation (ADE) models have been highly useful in describing and predicting these fields. In this paper, we first describe the origin of advection – diffusion equation for chemical transport along with the necessary initial and boundary conditions. An advection – diffusion equation model can be written for heat and mass transport in the near earth's surface. We then indicate various methods of solving this equation. Finally several applications involving transport of pollutants in subsurface, water and air environment have been presented. Basics of environmental forensics are also presented.

ADVECTION – DIFFUSION EQUATIONS

Governing equation of chemical concentration

The heat / mass fields described by $C(\underset{\sim}{r},t)$ where $(\underset{\sim}{r},t)$ refers to spatial and time coordinates, follows the following mass / energy conservation law :

$$\frac{\partial C}{\partial t} + \nabla.(VC) = -\nabla.Q + G(\underset{\sim}{r},t) \qquad (1)$$

where V is the velocity, Q the flux and G, the source term. For incompressible media, the velocity field satisfies

$$\nabla.V = 0 \qquad (2)$$

Using equation (2), the second term of left hand side is reduced as

$$\nabla.(CV) = V.\nabla C \tag{3}$$

For obtaining the governing equation for C, another equation relating Q with C, called the constitutive relationship, is needed. For mass flux, this is provided by Fick's law. For heat flux, that is provided by Fourier's law of heat conduction. We thus have

$$Q = -D\nabla C \tag{4}$$

Here D is the diffusivity of mass transport. Substituting eqn. (4) and eqn. (3) into eqn. (1), we get advection- diffusion equation as

$$\frac{\partial C}{\partial t} + V.\nabla C = \nabla.(D\nabla C) + G(\underline{r},t) \tag{5}$$

As the transport processes take place in a finite domain and are initiated at a particular time, for deriving the space – time characteristics of mass (heat) field, we need the initial and boundary conditions.

Initial condition

The initial condition prescribes the spatial distribution of chemical field at time t = 0:

$$C(r,t=0) = C_0(r) \tag{6}$$

As only the first derivative with respect to time occurs in eqn. (5), such specification as in eqn. (6) is sufficient to provide unique solution to the advection-diffusion equation.

Boundary conditions

For the boundary conditions at $\underline{r} = \underline{r}_s$, any of the following three types of conditions namely, Dirichlet, Neumann or mixed conditions can be prescribed depending on the physical conditions of the cases:

$$\begin{gathered} C(\underline{r}_s,t) = f(\underline{r}_s,t) \\ \text{or} \\ \nabla C(\underline{r}_s,t) = f(\underline{r}_s,t) \\ \text{or} \\ a\, C(\underline{r}_s,t) + b\nabla C(\underline{r}_s,t) = f(\underline{r}_s,t) \end{gathered} \tag{7}$$

Equation (5) together with the initial condition (6) and boundaries conditions (7) completes the derivation of advection – diffusion equation along with the specification of the associated initial and boundary conditions.

Governing equation for mean field

Advection – diffusion equation also arises when the velocity is taken as a random function in an advection equation and the equation for the mean field is derived using eddy diffusivity concepts. The advection equation is given as:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(VC) = 0 \tag{8}$$

Substituting the following decomposition of concentration and velocity fields

$$C = \overline{C} + C' \tag{9}$$

$$V = \overline{V} + V' \tag{10}$$

(– denotes mean field, and ' denotes small perturbation with its mean as zero) in Eq(8) and taking the mean of the resulting equation, we get

$$\frac{\partial \overline{C}}{\partial t} + V\frac{\partial \overline{C}}{\partial x} + \frac{\partial \langle V'C' \rangle}{\partial x} = 0 \tag{11}$$

Using the following approximation:

$$\langle V'C' \rangle = -D_e \frac{\partial \overline{C}}{\partial x} \tag{12}$$

where D_e is eddy diffusivity, we get the advection – diffusion equation for the mean field as

$$\frac{\partial \overline{C}}{\partial t} + \overline{V}.\nabla\overline{C} = \nabla.(D_e\nabla\overline{C}) + G(\underline{r},t) \tag{13}$$

Thus for random velocity fields, the equation for mean concentration is an advection- diffusion equation with eddy diffusivity.

Reduction of ADE as Diffusion equation

Advection – Diffusion Equation in one dimension can be reduced to diffusion equation by substituting (Ozisik 1993)

$$C = W\exp\left[\frac{V}{2D}x - \frac{V^2}{4D}t\right] \tag{14}$$

as

$$\frac{\partial W}{\partial t}=D\frac{\partial^2 W}{\partial x^2}+G\exp\left\{-\left[\frac{V}{2D}x-\frac{V^2}{4D}t\right]\right\} \qquad (15)$$

This helps to use interesting solutions of diffusion equation for advection-diffusion equation.

Peclet number

The solution of ADE depends upon a non-dimensional number called Peclet Number, P_e. It is defined as

$$P_e = (VL/D) \qquad (16)$$

Here L is the length scale. For purely diffusive transport, $P_e=0$. For values of $P_e < 1$, diffusion dominates and for $P_e > 1$, advection dominates as the transport processes.

METHOD OF SOLUTION

Well – posed criteria for the solution of advection-diffusion equation:

Hadamard (1902) has proposed the following three criteria for the well-poseness of a mathematical model equation:

i. A solution should exist
ii. The solution should be unique and
iii. The solution should depends continuously on the given data

Forward solution of diffusion equation is well posed in the above sense. But backward integration of the equation is not wel-posed. A small change in the condition at t = 0, will lead to large change in the solution for negative times. Such backward ill-posed problems can be modified as well-posed problems using method of regularization proposed by Tikhonov and Arsenin (1977).

Analytical methods

Before advent of cheap and faster computing machines, analytical methods have been used to solve these equations. The solutions are written in terms of trigonometric, polynomial and special functions. Transform methods have been highly useful. As advection – diffusion equation is a partial differential equations (PDE) with first order in time, the Laplace transform is used to transform PDE to second order ordinary differential equations (ODE) of a space variable for one – dimensional problem. For one/two/three - dimensional problems if boundary shape and conditions are simple, the transformed advection – diffusion equation can be written in terms of ordinary differential equations using the method of separation of variables. Each ordinary differential equation for a particular space variable can then be solved in terms of elementary or special functions. Fourier, Hankel and several other transform pairs are also available to solve the boundary value problem for each ordinary differential equation. Solutions ultimately consist of infinite series, which need to be computed making truncation errors as small as possible. If parameters are large or small, perturbations methods can be used to derive approximate expressions for the solution. A large class of solutions of various problems is given in Carslaw and Jaeger (1959), Bird et al (1960), Pollubariniva- Kochina (1962), Crank (1975) and Ozisik (1993). Analytical solution is helpful in understanding geophysical environmental processes. Effects of variations of various parameters can be easily assessed.

Numerical methods:

Numerical methods are now finding increasing applications for realistic media properties and geometries. Even the numerical results from analytical solutions also require numerical techniques of function calculations and series summations. In numerical methods, the differential equation is reduced to a system of algebraic equations. Two main classes of numerical methods have been proposed: Finite difference method and finite element method. In the finite difference method, the difference forms of the derivatives are substituted in the equations. These difference forms are obtained by using the functional values at the grids spanning the media using Taylor's series expansion. The linear ordinary differential equation is reduced to a system of linear algebraic equations. The solution is obtained by solving this system of equations. Several efficient algorithms are available to obtain direct or iterative solution of these equations. The linear partial differential equations are also reduced to solving a set of linear equations. In the finite element method

(Reddy and Gartling, 1994), the media is subdivided into elements and the variations of field functions inside the elements are written in terms of function values at nodes of these elements. Such interpolating basis functions are substituted in the variational form of ordinary differential equation/ partial differential equation. By minimizing the errors of approximation, a system of algebraic equations for nodal values is obtained. Solution of this system of equations is used in constructing the solution of the problem.

By confronting the solution with data the unknown parameters in the model can be estimated. In general least squares theory is used for this purpose. A part of the available data can be used for parameter estimation and the remaining data can be used for validation. Environmental forecasting can be done by such validated model.

Cellular automata

Recently cellular automata methods are also used to simulate transport phenomena. Here, in addition to discretisation of space and time variables, the dependent variables such as chemical concentration / temperature are also discretized in finite number of levels. Earlier the dependent variables needed infinite number of points, but now these require only finite number of values. Recently such methods have been used to describe a vast range of physical, chemical and biological phenomena (Wolfram, 2002).

SOLUTE TRANSPORT IN AQUIFERS

The solute concentration, C in porous media is governed by

$$\frac{\partial(C\phi)}{\partial t} - V\nabla C = \nabla.(D(C\phi)) + G \tag{17}$$

Here, G represents the source / sinks term and ϕ represents porosity of the solid matrix. If the solute is adsorbed on the pore surface, then

$$G = -\frac{\partial}{\partial t}(\rho S) \tag{18}$$

where ρ is the density of the solid matrix and S is the adsorbed solute on the pore surface. S is related to concentration C in a simple case, as

$$S = K_d \tag{19}$$

where K_d is the equilibrium distribution coefficient.

Thus

$$G = -K_d\,\rho\frac{\partial C}{\partial t} \tag{20}$$

Substituting eqn. (20) in eqn. (17) we get, in one dimension,

$$D\frac{\partial^2 C'}{\partial X^2} - \bar{V}\frac{\partial C}{\partial X} = \phi\frac{\partial C}{\partial t} + K_d\rho\frac{\partial C}{\partial t} = \left(1 + \frac{K_d\rho}{\phi}\right)\frac{\partial C}{\partial t} = R\frac{\partial C}{\partial t} \tag{21}$$

where $V = V/\phi$, the seepage velocity and $R = (1 + K_d\,\rho/\phi)$ the retardation factor. For the following initial and boundary conditions:

$$C(x,0) = 0 \tag{22i}$$

$$C(0,t) = C_0$$
$$C(\infty,t) = 0 \tag{22ii}$$

The solution of eqn (21) can be obtained by applying Laplace Transformation (Carslaw and Jaeger, 1959; Ogata, 1970). The Laplace transformation of the eqn (21), using the initial condition (22i), gives

$$D\frac{d^2\bar{C}}{dx^2} - \bar{V}\frac{d\bar{C}}{dx} - R\,p\,\bar{C} = 0 \tag{23}$$

where

$$\bar{C} = \int_0^\infty \exp(-pt)C(x,t)dt \tag{24}$$

The solution of eqn(23) satisfying the transformed boundary conditions given by eqn (22ii) gives

$$\bar{C} = C_0 / \exp(-Vx/2D)\,\exp(-x\sqrt{(V^2/4D^2 + pR/D)})/p \tag{25}$$

Taking inverse Laplace transformation of eqn (25), the following expression for C is obtained:

$$\frac{C(X,t)}{C_0} = \exp(\alpha)\left[\exp(-\alpha)erfc(\beta^-) + \exp(\alpha)erfc(\beta^+)\right] \tag{26}$$

where

$$\alpha = V\,x/2D \tag{27}$$

and $$\beta^{\pm} = (x + Vt/R)/(4Dt/R)^{1/2} \tag{28}$$

The solution of eqn (26) is written in terms of complementary error function (erfc(x)) given by

$$erfc(x) = \frac{2}{\pi}\int_x^\infty e^{y^{-2}}\,dy \tag{29}$$

Approximate form of equation (29) is given by

$$erfx(x) \approx \frac{e^{x^2}}{\sqrt{\pi}\,x}\left[1+\sum_{n=1}^{\infty}(-1)^n \frac{1.3.5....(2n-1)}{\left(2x^2\right)^n}\right] \tag{30}$$

Equation (26) can be used to plot C vs x for various times or C vs t for various values of x with various values of parameters V, K and D. These results can be compared with the experimental results. A large number of analytical models have been presented by Lee (1999).

GROUND WATER MOTION IN POROUS MEDIA

Porous media models are constructed by combining mass conservation law given by

$$\frac{\partial}{\partial t}(q\rho)+\nabla.(\phi q)=0 \tag{31}$$

and the Darcy's law as

$$q = -K \nabla \psi \tag{32}$$

where ϕ, ρ, q, K and ψ are porosity, density, Darcy's specific discharge, hydraulic conductivity and piezometric head respectively. The equation for the unconfined aquifer is obtained by integrating eqn (31) over the depth of the aquifer (Bear, 1979). In terms of h, the height of water table, the governing equation is given by

$$S\frac{\partial h}{\partial t}=\overline{\nabla}.\left(Kh\overline{\nabla}h\right)+N \tag{33}$$

where S and N are the storage coefficient and recharge.

Equation of groundwater height on a sloping aquifer in one dimension is given by

$$S\frac{\partial h}{\partial t}=K\left[\frac{d}{dx}\left(h\frac{\partial h}{\partial x}\right)-\alpha\frac{\partial h}{\partial x}\right]+N(t) \tag{34}$$

where α is the slope. Eqn (34) is a nonlinear equation whose exact solution is not available. However, this can be linearized using the following transformation:

$$y = h^2 \tag{35}$$

$$\frac{\partial^2 y}{\partial x^2}-2a\frac{\partial y}{\partial x}+\frac{2N(t)}{K}=\frac{1}{\kappa}\frac{\partial y}{\partial t} \tag{36}$$

Here

$$a=\frac{\alpha}{2D},\quad \kappa=\frac{KD}{S}$$

and D is the mean depth of saturation. The boundary conditions, the case where the aquifer is connected to streams on both sides are

$$y(0,t) = 0$$
$$y(L,t) = 0 \tag{37}$$

The initial condition is taken as

$$y(x,0) = 0 \tag{38}$$

By the separation of variables technique, the partial differential equation (36) for y leads to two ordinary differential equations for X and T by substituting $y = X(x)T(t)$

$$\frac{d^2X}{dx^2}-2a\frac{dX}{dx}+\lambda X=0 \tag{39}$$

$$\frac{dT}{dt}=-\lambda\kappa T \tag{40}$$

The boundary conditions for X are

$$X(0) = 0 = X(L) \tag{41}$$

The solution for the boundary value problem after applying eqns. (40) and (41) is

$$\phi_n(x)=\sqrt{\frac{2}{L}}\,\exp(ax)\sin\left(\frac{n\pi x}{L}\right) \tag{42}$$

The solution of eqn. (36) then becomes

$$y(x,t)=\sum_{n=0}^{\infty}\phi_n(x)T_n(t) \tag{43}$$

Substituting y into equation (36) and integrating it after multiplying with $exp(-2ax)\phi_n(x)$ and using orthogonal property, we get

$$\frac{dT_n}{dt}+\kappa\lambda_n T_n=g_n(t) \tag{44}$$

where

$$g_n(t) = \kappa \int_0^t \frac{2N(t)}{K} \exp(-2ax)\phi_n(x)\,dx \tag{45}$$

$$T_n(0) = \int_0^L y(x,0)\exp(-2ax)\phi_n(x)\,dx \tag{46}$$

Substituting the expressions for $T_n\ (0)$ and $g_n\ (t)$ the solution of the problem is

$$T_n(t) = \sqrt{\frac{2}{L}}\,\frac{2\kappa n\pi \exp(-\lambda_n \kappa t)}{KL}\left[1-(-1)^n \exp(-aL)\right]\int_0^t N(t')\exp(\lambda_n \kappa t')\,dt' \tag{47}$$

For given expression for the recharge function, $N(t)$ the expression for $T_n\ (t)$ can be obtained and substituting it in eqn(43), we get the expression for y $(=h^2)$. For the details of the derivations and the numerical results of water table fluctuations Singh et al (1991) can be referred.

TEMPERATURE DISTRIBUTION IN NEAR SUBSURFACE

The temperatures in the subsurface have memory of climate change and also how groundwater recharge or discharge has been changing. Thus borehole temperature data can be used to infer both climate change and groundwater velocities. The governing equation for the distribution of temperature T in subsurface is obtained by using the conservation law of energy as

$$(\rho C)_s \frac{\partial T}{\partial t} + (\rho C)_f \nabla\{VT\} = \nabla.Q \tag{48}$$

where ρ, C and A are density, heat capacity and radiogenic heat source. Subscript *s* and *f* refer to solid and groundwater properties. *V* is groundwater velocity, positive for recharge and negative for discharge. And the constitutive relationship between Q and gradient of temperature is given by Fourier law of heat conduction as

$$Q = -K \nabla T \tag{49}$$

Combing equations (48) and (49), we get, for using eqn(2),

$$(\rho C)_s \frac{\partial T}{\partial t} + (\rho C)_f \nabla\{VT\} = \nabla.(K\nabla T) \tag{50}$$

This equation can describe the effects of the fluid flow through the subsurface media on the temperature distribution in the subsurface.

The governing equation of temperature T in one dimension (Z – depth) is written as

$$\left(\frac{1}{\kappa}\right)\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial Z^2} - \frac{U}{\kappa}\frac{\partial T}{\partial Z} \tag{51}$$

Here κ is heat diffusivity. U denotes $(\rho C)_f V/(\rho C)_s$. The boundary conditions at Z = 0 is

$$T = T_0 + aZ \qquad at\ t=0 \qquad for\ all\ \ Z>0 \tag{52}$$

$$K\frac{dT}{dZ} = H\left(T - T_A - bt\right) \qquad at\ Z=0\ for\ all\ t>0 \tag{53}$$

in which T_0 is the initial surface temperature and *H* denotes a constant, representing coupling between atmosphere and surface meterological interactions. Eqn (53) includes the effects of the surface air temperature variation. Initially surface temperature is T_0 and increase with depth by a gradient. The surface air temperature, T_A varies with time as $T_A + bt$, *b* is a constant. The solution of eqn(51) can be obtained by taking Laplace transformation with respect to time and then solving the spatial ordinary differential equation. The expressions for constants of the solutions are obtained by applying the boundary conditions. Solution in (Z,t) are obtained by inverse Laplace transformation. There are tables available to obtain the inverse Laplace transforms. Solution for a linearly varying air surface temperature and constant value of ground water flux is given by Kumar et al (2012). The analytical solution is

$$\begin{aligned}
T(Z,t) = {} & \left(T_0 + aZ - aUt\right) + \frac{1}{2K_1}\left\{K_1\left(T_0 - T_A\right) - a + \frac{aU+b}{\kappa K_1}\right\} \\
& \left\{\begin{bmatrix}\left(\dfrac{2K_1\kappa - U}{K_1\kappa - U}\right)\exp\left(K_1 Z - K_1 t\left(U - \kappa K_1\right)\right) erfc\left(\dfrac{Z + \left(2K_1\kappa - U\right)t}{2\sqrt{\kappa t}}\right) \\ - erfc\left(\dfrac{Z - Ut}{2\sqrt{\kappa t}}\right) - \dfrac{\kappa K_1}{\kappa K_1 - U}\exp\left(\dfrac{UZ}{\kappa}\right) erfc\left(\dfrac{Z+Ut}{2\sqrt{\kappa t}}\right)\end{bmatrix}\right\} \\
& + \frac{aU+b}{2U}\left\{(Z+Ut)\exp\left(\frac{UZ}{\kappa}\right) erfc\left(\frac{Z+Ut}{2\sqrt{\kappa t}}\right) - (Z-Ut)\, erfc\left(\frac{Z=Ut}{2\sqrt{\kappa t}}\right)\right\} \\
& - \frac{(aU+b)\sqrt{t}}{K_1\sqrt{\kappa}}\left\{\begin{bmatrix}\exp\left(\dfrac{UZ}{\kappa}\right)\left[\dfrac{1}{}\exp\left(-\left(\dfrac{Z+Ut}{2\sqrt{\kappa t}}\right)^{1/2}\right) - \dfrac{Z+Ut}{2\sqrt{\kappa t}}\, erfc\left(\dfrac{Z+Ut}{2\sqrt{\kappa t}}\right)\right] \\ + \exp\left(-\left(\dfrac{Z-Ut}{2\sqrt{\kappa t}}\right)^{1/2}\right) - \dfrac{Z-Ut}{2\sqrt{\kappa t}}\, erfc\left(\dfrac{Z-Ut}{2\sqrt{\kappa t}}\right)\end{bmatrix}\right\}
\end{aligned} \tag{54}$$

Kumar et al (2012) have used this solution to discuss quantitatively the effect of transient air surface temperatures and ground water flux on the surface subsurface temperatures. The observed borehole temperature data can interpreted to find out both climate as well as ground water flux.

In finding above analytical solution, a simple form of surface air temperature was assumed. However for complicated time variations of air surface temperature, it would not be possible to get analytical expressions while inverting solution in Laplace domain. In such cases inverse Laplace transforms can be obtained by numerical methods (Stehfest, 1970). Further in the above case, whole half – space was undergoing groundwater recharge/discharge with changing air temperature. However one can limit the depth extent of model by prescribing either basal temperature or basal heat flux or a combination of both. For such problems one can use method of eigen-functions for the solutions, avoiding the need to obtain inverse Laplace transforms of complex functions.

AIR QUALITY- 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)

$$u\frac{\partial C}{\partial x}=K\left(\frac{\partial^2 C}{\partial y^2}+\frac{\partial^2 C}{\partial z^2}\right) \tag{55}$$

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

$$C(0,y,z) = Q\delta(x)\delta(y)\delta(z-H) \tag{56}$$

The boundary conditions for the model equations are:

$$C(x,\pm\infty,z) = 0 \tag{57}$$

$$C(x,y,\infty) = 0 \tag{58}$$

$$K\frac{\partial C}{\partial z}(x,y,0) = 0 \tag{59}$$

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

$$C(x,y,z)=\frac{Q}{4\pi Kx}e^{-\frac{y^2u}{4Kx}}\left[e^{-\left(\frac{u(z-H)}{4Kx}\right)^2}+e^{-\left(\frac{u(z+H)}{4Kx}\right)^2}\right] \tag{60}$$

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:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=K\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}+\frac{\partial^2 C}{\partial z^2}\right) \tag{61}$$

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

$$C(x,y,z,0) = 0 \tag{62}$$

The boundary condition in x-coordinate is

$$C(\pm\infty,y,z) = 0 \tag{63}$$

All other boundary conditions remain the same as in steady state case. The solution is given as (Kathirgamanathan et al, 2003a)

$$C(x,y,z,t)=\int_0^t\frac{Q(\tau)}{(2\pi K)^{3/2}(t-\tau)^{3/2}}\exp\left(\frac{(x-u(t-\tau))^2-y^2}{4K(t-\tau)}\right)\left[\exp\left(-\frac{(z-H)^2}{4K(t-\tau)}\right)+\exp\left(-\frac{(z+H)^2}{4K(t-\tau)}\right)\right]d\tau \tag{64}$$

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

RIVER QUALITY: ADVECTION-DIFFUSION MODEL

The concentration of pollutant in a river is governed by an advection diffusion equation in steady state in one horizontal dimension as

$$D \frac{d^2C}{dx^2} - u \frac{dC}{dx} - kC = 0 \tag{65}$$

Here D, u and k are respectively dispersion coefficient, velocity of river and decay rate of pollutants. If the steady source pollutant is Q at x=0, then the solution of this equation can be written a

$$C_1(x \geq 0) = A \exp(-m_1 x) \tag{66}$$

$$C_2(x \leq 0) = B \exp(m_2 x) \tag{67}$$

Here, A and B are constants and m_1 and m_2 are:

$$m_{1,2} = \frac{u}{2D}\left[1 \pm \sqrt{1 + 4kv / D^2}\right] \tag{68}$$

A and B can be obtained by using the following two conditions:

$$C_1(0) = C_2(0) \tag{69}$$

$$\int_{-\infty}^{\infty} C(x) dx = Q \tag{70}$$

The first condition gives

$$A = B \tag{71}$$

And the second condition gives

$$A = \frac{kQ}{u\sqrt{1 + 4ku / D^2}} \tag{72}$$

Thus we have

$$C_1(x \geq 0) = \frac{kQ}{u\sqrt{1 + 4ku / D^2}} \exp\left[-\frac{ux}{2D}\left[1 + \sqrt{1 + 4kv / D^2}\right]\right] \tag{73}$$

$$C_1(x \leq 0) = \frac{kQ}{u\sqrt{1 + 4ku / D^2}} \exp\left[\frac{ux}{2D}\left[1 - \sqrt{1 + 4kv / D^2}\right]\right] \tag{74}$$

Thus the steady state distribution can be determined for given values of source, velocity, and diffusion coefficient and decay rate.

In case the source, $Q(t)$ is time dependent, then the governing eqn (65) is given by

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} - kC \tag{75}$$

The following condition is needed to solve this equation:

$$C(x,0) = C_0 \tag{76}$$

$$C(0,t) = C_s \tag{77}$$

$$C(\pm\infty,t) = 0 \tag{78}$$

The analytical solution of the distribution of concentration of pollutants is given by Socolofsky and Jirka (2005) as:

$$C(x,t) = C_0 + \frac{(C_S - C_O)}{2}\left[erfc\left(\frac{x - ut}{\sqrt{4D}}\right) + \exp\left(-\frac{ux}{D}\right) erfc\left(\frac{x + ut}{\sqrt{4D}}\right)\right] \tag{79}$$

These solutions for steady state and transient cases have been used extensively in the literature in predicting changes in the water quality in the rivers. For more general case of time dependent variations of the concentration in vertical and both horizontal directions and also in estimating the three dimensional distribution of the velocity field of rivers for use in concentration equation, numerical methods are applied for solving fluid flow Navier-Stokes equation. For fuller description of the river water quality, interactions of river water with atmosphere and river bed sediments need to be included. Temperature variation in the river and its underlying sediments also have signature past changes in the river dynamics and water quality. The advection diffusion equation for temperature can be solved following the same approach as for water quality.

ENVIRONMENTAL FORENSICS

Industrial waste is being released surreptitiously into the environment. The regulators are required to decipher noncompliance by industries. The changes on the environmental quality are governed by ADE and these models can be used to trace backward from the observed effects. Such problems are non well-posed. Regularization method (Tichonov and Arsenin 1977)has been used to modify the problem as well posed by imposing smoothness of the solutions.

Such inverse problems have been extensively studies in recent times (Tarantola 1987).

For source of concentration of contaminants at x= 0 as $C_{in}(t)$, the concentration at a point x and time T for 1D media ($0 \le x \le \infty$) is given by, solving corresponding ADE equation (Eq.75 with $k=0$) for concentration decaying to zero as x goes to infinity (Jury and Roth, 1990; Skaggs and Kabala ,1994):

$$C(x,T) = \int_0^T C_{in} K(x,T-t)dt \tag{80}$$

where

$$K(x,T-t) = x\exp\{-(x-V(T-t)^2)[4D(T-t)]\}/2\{D(T-t)^3\}^{1/2} \tag{81}$$

The above formula can be discretised as

$$\mathrm{d} = \mathrm{K\ m} \tag{82}$$

where column vector d consists of values of concentration at various locations (x_i), column vector m consists of unknown concentration at x=0, unknown parameters, and at times (t_j) and K is matrix given as

$$K_{i,j} = K(x_i, T-t_j)\Delta t \tag{83}$$

Estimate of m denoted by $\hat{m}$, can be made by using theory of generalized inverse and singular value decomposition. The least squares solution of above problem in case of over determined system is given by (Aster et al, 2012):

$$\hat{m} = (K^T K)^{-1} K^T d \tag{84}$$

Estimates of m can be done efficiently using singular value decomposition of matrix K (Press et al 1992) as

$$\underset{nxm}{K} = \underset{nxm}{U} \quad \underset{mxm}{\Lambda} \quad \underset{mxm}{V^T} \tag{85}$$

Here U and V are orthogonal matrices and Λ are made of eignevalues. The solution for m is then

$$\hat{m} = \mathrm{V}\ \Lambda^{-1}\ U^T\ d \tag{86}$$

The model resolution and the information density used in the model estimate can also be appraised by calculating respectively following matrices:

$$R_m = VV^T \tag{87}$$

$$R_d = UU^T \tag{88}$$

For well resolved model and also full utilization of data in arriving at model, these matrices should be closest to identity matrix. These matrices which based on physics and geometry of the media under investigation are used for experimental design purposes.

Skaggs and Kalaba (1994, 1995) and Neupauer et al (2000) have analyzed the problem of reconstructing the history of release of groundwater contaminants in great detail. Kathirgamanathan et al (2003a) have reconstructed the transient release of air pollutants from a given location of source from observations of their time distribution at another location. When location of source is unknown, multiple observational locations, at least three (Kathirgamanathan et al, 2003b) are used to reconstruct both the location of the source and also the release pattern of the pollutants.

FRACTIONAL ADVECTION-DIFFUSION EQUATION

In several cases of advection and diffusion of pollutants in the subsurface porous media, significant differences are noticed between the solutions of relevant ADE and the observed data. The mean square displacement of pollutant is no longer proportional to time, t, rather it show time dependence as t^{α}, α, a positive number. The exponent α takes values less than one or greater than one. In the first it is called subdiffusion and in the later case it is called super diffusion. To account for this anomalous behavior, the ADE models have been extended by considering fractional derivatives both in time and space. The advection diffusion equation assumes the following forms

$$\frac{\partial C}{\partial t} = -V\frac{\partial C}{\partial X} + D\frac{\partial^{\alpha} C}{\partial X^{\alpha}} \tag{89}$$

$$\frac{\partial^{\beta} C}{\partial t^{\beta}} = -V\frac{\partial C}{\partial X} + D\frac{\partial^2 C}{\partial X^2} \tag{90}$$

The analytical solutions for infinite domains can be obtained by using Laplace and Fourier transformations. However it is very difficult to get analytical solution to these equations as applied in the field. In those cases numerical solution have been applied. Recently there have been extensive applications of this fractional advection diffusion equation approach to model mass transport in the porous media and other disciplines (Benson et al, 2000, Benson et al 2012, Magin 2006, Vazquez, 2011).

CONCLUDING REMARKS

Processes like diffusion, advection, reaction, storage, sources and sinks take place in the near-surface and environmental media, such as air, water and soil. ADE models describe a large part of environmental problems where quantification of the evolution of physical and chemical fields is required. In using these models we need to know the values of parameters and also knowledge of initial and boundary condition besides that of sources of fields. A large class of problems have been solved and used in various areas of science and engineering. These solutions can be used to interpret geophysical and environmental data. Newer theoretical developments in numerical analysis and inverse theories are also finding application in environmental sciences. The scope of the geophysical and environmental diffusion problems is also being extended to random and fractal media. We have presented a small part of the extensive literature on advection diffusion equation based models in the area of geophysical and environmental modeling and many more challenging problems remain for development of theory and applications.

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