

Numerical Treatment of the Mathematical Models for Water Pollution

¹F.B. Agosto and ²O.M. Bamigbola

¹Department of Mathematical Sciences, Federal University of Technology Akura, Nigeria

²Department of Mathematics, University of Ilorin, Nigeria

Abstract: To evaluate the environmental impact of pollution, mathematical models play a major role in predicting the pollution level in the regions under consideration. This study examines the various mathematical models involving water pollutant. We also give the implicit central difference scheme in space and a forward difference method in time for the evaluation of the generalized transport equation.

Key words: Pollution, numerical treatment, mathematical models, water, regions

INTRODUCTION

“Pure water is the best of gifts that man to man can bring Spectator, July 30, 1920. Water, comprising over 70% of the earth surface, is undoubtedly the most precious natural resource that exists on our planet. Without the seemingly invaluable compound comprised of hydrogen and oxygen, life on earth would be non-existent. It is essential for everything on our planet to grow and prosper David and Brad (1991).

It is easy to dispose of waste by dumping it into a river or lake. In large or small amounts, dumped intentionally or accidentally, it may be carried away by the current, but will never disappear. It will reappear downstream, sometimes in changed form, or just diluted. Freshwater bodies have a great ability to break down some waste materials, but not in the quantities discarded by today society. This overload that results, called pollution, eventually puts the ecosystem out of balance (The Green Lane™).

Sometimes nature itself can produce these imbalances. In some cases, the natural composition of the water makes it unfit for certain uses: e.g., water flowing in the highly saline terrain of the prairies or gushing from highly mineralized springs in some parts of the country cannot sustain fish populations.

But most often our waterways are being polluted by municipal, agricultural and industrial wastes, including many toxic synthetic chemicals which cannot be broken down at all by natural processes. Even in tiny amounts, some of these substances can cause serious harm.

Many causes of pollution including sewage and fertilizers contain nutrients such as nitrates and phosphates. In excess levels, nutrients over stimulate the growth of aquatic plants and algae.

Excessive growth of these types of organisms consequently clogs our waterways, use up dissolved oxygen as they decompose, and block light to deeper waters. This, in turn, proves very harmful to aquatic organisms as it affects the respiration ability of fish and other invertebrates that reside in water.

Pollution is also caused when silt and other suspended solids, such as soil, washoff plowed fields, construction and logging sites, urban areas, eroded river banks when it rains. Under natural conditions, lakes, rivers and other water bodies undergo Eutrophication, an aging process that slowly fills in the water body with sediment and organic matter. When these sediments enter various bodies of water, fish respiration becomes impaired, plant productivity and water depth become reduced and aquatic organisms and their environments become suffocated. Pollution in the form of organic material enters waterways in many different forms as sewage, leaves and grass clippings, or as runoff from livestock feedlots and pastures. When natural bacteria and protozoan in the water break down this organic material, they begin to use up the oxygen dissolved in the water. Many types of fish and bottom-dwelling animals cannot survive when levels of dissolved oxygen drop below two to five parts per million. When this occurs, it kills aquatic organisms in large numbers which leads to disruptions in the food chain.

Pathogens are another type of pollution that prove very harmful. They can cause many illnesses that range from typhoid and dysentery to minor respiratory and skin diseases. Pathogens include such organisms as bacteria, viruses and protozoan. These pollutants enter waterways through untreated sewage, storm drains, septic tanks, runoff from farms and particularly boats that dump sewage. Though microscopic, these pollutants have a tremendous effect evidenced by their ability to cause sicknesses.

Oxygen is required to support aquatic life and maintain water quality, it is the most important dissolved gas in water. Water in equilibrium with air at 25°C contains 8.3 mg L⁻¹ of dissolved O₂. Although water molecules contain an oxygen atom, this oxygen is not what is needed by aquatic organisms living in natural waters. A small amount of oxygen, up to ten molecules of oxygen per million of water, is actually dissolved in water. Fish and zooplankton breath dissolved oxygen and without sufficient oxygen mortality will occur.

Dissolved Oxygen (DO) concentrations are affected by a number of factors. Higher DO is produced by turbulent actions such as waves, which mix air and water. Lower water temperatures also allows for retention of higher DO concentrations. Low DO levels tend to occur more often in warmer, slow moving waters. In general, low DO levels occur during the warmest summer months and particularly during low flow periods. Water depth is also a factor. In deep slow moving waters DO concentrations may be high near the surface due to wind action and plant photosynthesis, but may be entirely depleted (anoxic) at the bottom.

Oxygen consuming wastes include decomposing organic matter or chemicals that reduce DO in the water. Raw domestic wastewater contains high concentrations of oxygen consuming wastes that need to be removed before it can be discharged into a waterway. Maintaining a sufficient level of DO in water is critical to most forms of aquatic life.

Microorganisms such as bacteria are responsible for decomposing organic waste. When organic matter such as dead plants, leaves, grass clippings, manure, sewage, or even food waste is present in a water supply, the bacteria will begin the process of breaking down this waste. When this happens, much of the available dissolved oxygen is consumed by aerobic bacteria, robbing other aquatic organisms of the oxygen they need to live.

Biological Oxygen Demand (BOD) is an indicator for the concentration of biodegradable organic matter present in a sample of water. It can be used to infer the general quality of the water and its degree of pollution. BOD measures the rate of uptake of oxygen by micro-organisms in the sample of water at a fixed temperature and over a given period of time.

Dissolved Organic Matter (DOM) is widely present in aquatic subsurface environments. It contains many biochemically identifiable classes of compounds such as sugars or amino acids, as well as fractions that are more coarsely classified, such as humics.

To evaluate the environmental impact of pollution, mathematical models play a major role in predicting the

pollution level in the regions under consideration (Theim, 1906; Brebbia, 1976; Canale, 1976; Kremmer and Nixon, 1978; Nihoul, 1975; Rich, 1973; Thomann, 1972; Ames, 1988; Gambolati *et al.*, 1990).

In the subsurface, colloidal/bacterial particles are generated and/or mobilized by various mechanisms. The presence of colloids can affect the transport behavior of organic contaminants in soils and groundwater due to sorption on the surface of colloids/bacteria (McCarthy and Zachara, 1989; Ryan and Elimelech, 1996; Choi and Corapcioglu, 1997). In riverbank filtration, the mobile colloidal particles can increase the mobility of contaminants and change the degree of sorption and microbial degradation.

Several researchers have reported that organic compounds have strong affinity to DOM. Hassett and Anderson (1979) have reported that hydrophobic organic compounds such as PCBs were bound to DOM in water. Carter and Suffet *et al.* (1982) have examined the sorption of DDT to DOM. Chiou *et al.* (1986) have shown that the sorption of hydrophobic organic compounds onto DOM increased their aqueous solubility. Magee *et al.* (1991) have reported that hydrophobic compounds moved faster in the presence of DOM. In riverbank filtration, DOM can facilitate the contaminant transport as the mobile carrier. In addition, it can be utilized as a food source for bacteria.

In riverbank filtration, contaminant transport can be affected by the presence of bacteria. Lindqvist and Enfield (1992) have reported that the transport of DDT and hexachlorobenzene could be facilitated in groundwater owing to their attachment on bacteria. Jenkins and Lion (1993) have demonstrated that highly mobile bacteria could increase the mobility of organic contaminants such as PAHs. In addition, bacteria can reduce the contaminant concentration by microbial transformation.

Kim and Corapcioglu (2002) gave a model to simulate contaminant transport in riverbank filtration in the presence of DOM and bacteria. The model equations are solved numerically with a fully implicit finite difference method.

This study considers the various mathematical models which can be used to stimulate the dispersion of pollutants in aquatic media: In this study we discuss the numerical solution, via the central finite difference method, to the 2-space dimensional transport model.

CONTAMINANT TRANSPORT MODELS

Describing contaminant transport requires the solution of the equation for saturated water transport and the convection-dispersion-reaction equation for contaminant transport through porous media. For the

saturated zone of the subsurface, contaminant transport is assumed to be isothermal and a heat balance equation is not required. Microscopic contaminant transport model equations are developed using a small representative element of volume in the subsurface.

Water transport: If only isothermal contaminant transport in the saturated zone of the subsurface is considered, the general physical law equation for saturated water transport through a representative small volumetric element in the porous structure of the subsurface is given as:

$$S_t \frac{\partial h}{\partial t} + W(x,t) = \nabla \cdot (K_{sat} \nabla \cdot h) \quad (1)$$

Where S_t is the storage coefficient of the aquifer, dimensionless, h is hydraulic head, cm, $W(x,t)$ is the volume flux per unit area source term (positive for out flow and negative for in flow) $cm \text{ hr}^{-1}$, ∇ is the del operator defined as $(\partial / \partial x^{-1})$, cm^{-1} , \bullet denotes the dot product of vectors and tensors, K_{sat} is the hydraulic conductivity tensor, related to fluid velocity, V , by Darcy's law, $cm \text{ hr}^{-1}$.

Contaminant transport: The general physical-chemical law, convective-dispersive-reaction contaminant transport equation for this same element of volume for a single chemical is given as:

$$\frac{\partial}{\partial t} (C + \frac{\rho B}{\epsilon} C) = \nabla \cdot (D \cdot \nabla C) - V \cdot \nabla C - \Lambda C^\omega - \frac{S_s Q}{\epsilon V_{ol}} \quad (2)$$

Where S is contaminant concentration sorbed to soil or other solid surfaces, $g \text{ cm}^{-3}$, C is contaminant concentration, $g \text{ cm}^{-3}$, B is bulk density, $g \text{ cm}^{-3}$, ω is porosity, dimensionless, D is the hydrodynamic dispersion tensor, $cm^2 \text{ hr}^{-1}$, V is the fluid velocity vector in a porous media calculated from Darcy's law, $cm \text{ hr}^{-1}$, Λ is the reaction rate coefficient of order ω for transformation of the contaminant by either chemical or biological processes, $(cm^3 \text{ g})^{-1} \text{ hr}$, S_s is contaminant concentration in the source or sink fluid, $g \text{ cm}^{-3}$, Q is volumetric flow rate, $cm^3 \text{ hr}$, V_{ol} is the volume of the volumetric element used in developing this model, cm^3 .

For equilibrium sorption approximated by a linear Freundlich isotherm, the amount sorbed to solid components of the subsurface is approximated as

$$S = K\omega C,$$

Where $K\omega$ is the equilibrium sorption coefficient, $cm^3 \text{ g}^{-1}$. As used here, $K\omega$ is an overall or composite equilibrium

sorption coefficient and is a function of sorption to all solid components, e.g., silica, clay minerals and organic matter. Substituting for S and assuming that all biological and chemical transformations are first order reaction processes, gives

$$R_f \frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) - V \cdot \nabla C - \Lambda C - \frac{S_s Q}{\epsilon V_{ol}} \quad (3)$$

Where the retardation factor, R_f (dimensionless), for equilibrium sorption is defined as

$$R_f = 1 + \frac{\rho B K\omega}{\epsilon} \quad (4)$$

If sorption is not an equilibrium process, it can be described by an interphase mass transfer process as

$$S = KC^\omega \quad (5)$$

Where K is an overall mass transfer coefficient with units of $(cm^3 \text{ g}^{-1})$ and ω is the order of the mass transfer reaction of the chemical with the solid surfaces of the porous media. With this modification, the retardation factor is given as:

$$R_f = 1 + \left[\frac{\rho B K\omega}{\epsilon} KC^{\omega-1} \right] \quad (6)$$

Equation 2 is valid for a single chemical contaminant that is present in the aqueous phase in dilute concentrations. For most chemical contaminants, single chemical models are appropriate because the solubility of the chemical in the aqueous phase is very low. Thus, changes in time and space of contaminant concentrations are substantial. The first two terms on the right-hand side of Eq. 2 are associated with the transport dynamics of flow in porous media, namely hydrodynamic dispersion and convective transport. The last term accounts for first-order chemical and biological reaction rate processes that transform or convert contaminants into other chemicals in the subsurface. For dilute solutions, the assumption that reaction rate processes can be represented as first-order processes is reasonable because only the concentration of the contaminant changes substantially during degradation or transformation. For example, with hydrolysis reactions the water concentration remains virtually unchanged, a pseudo first-order degradation mechanism. For the element of volume in the saturated zone of the subsurface, a general form of the concentration profile for contaminant transport in the subsurface is given as a function of these transport parameters and subsurface characteristics as:

$$C(x, y, z, t) = F(D, K_{sat}, \nabla, K, \epsilon, \rho, B) \quad (7)$$

However, some subsurface contaminant transport problems occur in conduit-type flow aquifers that do not behave like flow-through porous media. For these aquifers and flow regimes, equiv-alent hydraulic characteristics must then be defined and used in Eq. 7 to describe the contaminant concentration profile.

Bacteria transport: Wastewater contain a great variety of pathogenic bacterias and viruses. In what follows, we consider a mixture of N reacting species with partial densities $d_i, i=1, \dots, N$. Let d be the density of the mixture and Y_i the mass fracture of species i . We have

$$d = \sum_{i=1}^N d_i, Y_i = d_i/d, i=1, \dots, N.$$

If v_i denotes the velocity of species i , the macroscopic velocity is defined by

$$v = \sum_{i=1}^N Y_i v_i$$

The difference between v and v_i can be decomposed in the migration velocity and the diffusion velocity, the former representing, for instance, sedimentation:

$$v - v_i = \sigma_i + V_i.$$

According to Onsager 's law (Bermudez, 1993) we can write

$$d_i V_i = -\beta_i \nabla_{di}, i=1, \dots, N$$

The mass conservation equation is:

$$\frac{\partial d_i}{\partial t} + \nabla \cdot (d_i v) + \nabla \cdot (d_i \sigma_i) - \beta \nabla_{adi} = R_i + S_i \quad (8)$$

Where β_i is the diffusivity term, while R_i and S_i represent the biochemical reaction term and the external sources, respectively.

After discharge, concentration of bacterias or viruses decrease very quickly due to unfavorable conditions like lack of nutrients, low temperature, sun rays, etc. Death rate is frequently modeled as a first order reaction (Bermudez, 1993). This means that the R_i term in Eq. 8 is given by

$$R_i = -k_i C$$

Where k_i is a kinetic constant.

Actually, biologists prefer to speak of the $T_{90,i}$, which is the time after which concentration decreases 90 %. This parameter is related to k_i by

$$T_{90,i} = \frac{\log 10}{k_i}$$

On the other hand, assuming pointwise wastewater discharges, as those from outfalls, the term S_i in Eq. (8) is given by

$$S_i = \sum_{j=1}^N q_j r_i^j \delta(P_j)$$

Equation 8 becomes

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - K_i C + \sum_{j=1}^N q_j r_i^j \delta(P_j) \quad (9)$$

Where j is the number of the discharge, q_j is the flow rate, r_i^j is the partial density of species i for the j -th discharge, $\delta(P_j)$ denotes the Dirac measure at the discharge point P_j

Biological oxygen demand bod/Dissolved Oxygen (DO):

Oxygen plays a major role in all kinds of life. In particular, it is used by bacteria to decompose the organic matter. If the oxygen demand is not satisfied, plankton and other higher forms of animal life disappear. However, decomposition of organic matter goes on by anaerobic processes which do not use oxygen but produce sulfur of hydrogen and methane both having a nauseous smell. The organic matter can be measured in terms of the need of oxygen to decompose it, the so-called Biological Oxygen Demand (BOD). If the pollution level is not too high this need can be satisfied by the Dissolved Oxygen (DO).

If the quantity of organic matter increases beyond a maximum value the dissolved oxygen is not enough to decompose it leading to modifications in the ecosystem. To avoid this phenomena some physico-chemical and/or biological treatments prior to discharge have to be made.

In what follows, we recall a classical model given by Streeter and Phelps for the evolution of BOD and DO:

$$\left. \begin{aligned} \frac{\partial \rho_1}{\partial t} + u \cdot \Delta_{\rho_1} - \beta_1 \nabla_1 \rho_1 &= K_1 \rho_1 + \frac{1}{h} \sum_j^N q_j r_1^j \delta(P_j) \\ \frac{\partial \rho_2}{\partial t} + u \cdot \nabla_{\rho_2} - \beta_2 \nabla_2 \rho_2 &= K_1 \rho_1 + \frac{1}{h} K_2 (d_s - \rho_2) \\ -\frac{1}{h} \rho_1 M + \frac{1}{h} \frac{1}{ha + bI_B + cI_B^2} M + \frac{1}{h} F & \end{aligned} \right\} \quad (10)$$

Where ρ_1 is the concentration of the Biochemical Demand of Oxygen (BOD), ρ_2 is the concentration of the Dissolved Oxygen (DO), j is the number of the discharge, q_j is the flow rate, r'_i is the partial density of species i for the j -th discharge, $\delta(P_j)$ denotes the Dirac measure at the discharge point P_j , k_1 is a kinetic parameter (function of temperature), k_2 is the interface transfer rate for oxygen, β_1 and β_2 are dispersion coefficients, d is the saturation density of oxygen in water depending on temperature, I_B is the intensity of sunlight on the bottom, M is the surface population density of algae, r_p is a coefficient for respiration of algae, F represents other external sources of oxygen.

Dissolved Organic Matter (DOM)

Bacteria transport in presence of DOM: The movement of bacteria in soils and groundwater is mainly controlled by the advective-dispersive transport. The mass balance equation for the aqueous-phase bacteria can be described as

$$\frac{\partial(\theta C_b)}{\partial t} = -\frac{\partial}{\partial x} \left[-D_b \frac{\partial(\theta C_b)}{\partial x} + v_o \theta C_b \right] - K_c \theta C_b + k_1 \rho_b \sigma_b + \mu \left(C_c + \frac{\rho_s K_1 C_c}{\theta} C_d \sigma_{cd} + C_b \sigma_{cbm} \right) \theta C_b - k_{dm} \theta C_b - k_o Y \theta C_d$$

Where θ is the water content ($=n \cdot \sigma_b$), n is the porosity, σ_b is the volumetric fraction of bacteria attached onto the solid matrix (volume of bacteria deposited per unit total volume of porous media), C_b is the concentration of the aqueous-phase bacteria, C_d is the concentration of DOM in the aqueous phase, D_b is the hydrodynamic dispersion coefficient for bacteria [$L^2 T^{-1}$], v_o is the pore-water velocity [LT^{-1}], σ_{cd} is the mass fraction of the contaminant sorbed to DOM (mass of contaminant sorbed to DOM per unit mass of DOM), σ_{cbm} is the mass fraction of the contaminant sorbed to the mobile bacteria (mass of contaminant sorbed to mobile bacteria per unit mass of mobile bacteria), ρ_b is the density of bacteria, K_c and K_r are the deposition and release rate coefficients of bacteria on the solid matrix [T^{-1}], respectively. K_{dm} is the decay rate coefficient for the mobile bacteria [T^{-1}], K_o is the first order decay rate coefficient for DOM [T^{-1}] and Y is the yield factor (mass of bacteria formed per unit mass of food source utilized).

Contaminant transport in presence of DOM: The mass balance equation of the contaminant dissolved in the aqueous phase can be expressed as:

$$\frac{\partial(\theta C_c)}{\partial t} + \frac{\partial(\rho_s \sigma_{cs})}{\partial t} = -\frac{\partial}{\partial x} \left[-D_c \frac{\partial(\theta C_c)}{\partial x} + v_o \theta C_c \right] - K_p \theta C_c - k_q \theta C_d \sigma_{cd} + k_3 \theta C_c - k_4 \theta C_b \sigma_{cbm} - k_c \theta C_b \sigma_{cbm} - \frac{\mu C_c}{Y} (\theta C_b + \rho_b \sigma_b) - \frac{\mu \rho_s \sigma_{cs}}{Y \theta} (\theta C_b + \rho_b \sigma_b)$$

Where C_c is the concentration of the contaminant dissolved in the aqueous phase, ρ_s is the dry bulk density of the solid matrix, σ_{cs} is the mass fraction of the contaminant sorbed onto the solid matrix (mass of contaminant sorbed per unit solid mass of porous media). D_c is the hydrodynamic dispersion coefficient of the contaminant dissolved in the aqueous phase [$L^2 T^{-1}$], k_p and k_q are the adsorption and desorption rate coefficients for the contaminant on DOM [T^{-1}], k_3 and k_4 are adsorption and desorption rate coefficients of the contaminant on bacteria [T^{-1}], respectively. $\mu = \mu_{max}/K_s$, μ_{max} is the maximum growth rate [T^{-1}] and K_s is the half-constant [ML^{-3}].

If the sorption relationship between the aqueous phase and the solid matrix is assumed to be an equilibrium-controlled process and represented by a linear isotherm, the mass fraction of the contaminant sorbed onto the solid matrix can be presented as:

$$\sigma_{cs} = K_1 C_c$$

Where K_1 is the equilibrium distribution coefficient of contaminant between the aqueous phase and the solid matrix [$L^3 M^{-1}$].

$$\frac{\partial(R_c \theta C_c)}{\partial t} = -\frac{\partial}{\partial x} \left[-D_c \frac{\partial(\theta C_c)}{\partial x} + v_w \theta C_c \right] - K_p \theta C_c - k_q \theta C_d \sigma_{cd} - 2k_3 \theta C_c - k_4 \theta C_b \sigma_{cbm} + \frac{\mu R_c}{Y} (C_b + \frac{\rho_b \sigma_b}{\theta}) \theta C_c$$

Where R_c is the contaminant retardation factor, and represented as $R_c = 1 + (\rho_s K_1)/\theta$

The one dimensional transport equation for the contaminant sorbed to DOM is:

$$\frac{\partial(C_d \theta C_d)}{\partial t} = -\frac{\partial}{\partial x} \left[-D_d \frac{\partial}{\partial x} (\theta C_d \sigma_{cd}) + v_o \theta C_d \sigma_{cd} \right] + K_p \theta C_c - k_p \theta C_c - k_q \theta C_d \theta C_d \sigma_{cd} - \frac{\mu C_b}{Y} (\theta C_d \sigma_{cd})$$

The one-dimensional transport equation for the contaminant sorbed to the mobile bacteria is:

$$\frac{\partial(\theta C_b \sigma_{cbm})}{\partial t} = -\frac{\partial}{\partial x} \left[-D_b \frac{\partial}{\partial x} (\theta C_b \sigma_{cbm}) + v_o \theta C_b \sigma_{cbm} \right] + K_3 \theta C_c - k_4 \theta C_b \sigma_{cbm} - k_c \theta C_b \sigma_{cbm} - \frac{\mu C_b}{Y} (\theta C_d \sigma_{cbm})$$

$$\begin{aligned} \frac{\partial}{\partial t} C(x,t) + q \frac{\partial}{\partial x} C(x,t) - D \frac{\partial^2}{\partial x^2} C(x,t) + kC(x,t) &= 0 \text{ in } Q \\ C(x,0) &= C_0 \text{ in } \Omega \\ \frac{\partial}{\partial n} C(x,t) &= 0 \text{ on } \Sigma \end{aligned} \tag{12}$$

NUMERICAL SOLUTION

2-Dimensional transport equation: The 2-D transport equation can be generalized as:

$$\begin{aligned} \frac{\partial}{\partial t} C(x,y,t) &= -\frac{\partial(uC(x,y,t))}{\partial x} + D \frac{\partial^2}{\partial x^2} C(x,y,t) - \\ \frac{\partial(vC(x,y,t))}{\partial y} &D \frac{\partial^2}{\partial y^2} C(x,y,t) + R(C) + S(C) \end{aligned} \tag{11}$$

Where C is concentration of solute (bacteria or contaminant), u and v are the fluid velocity (which may be obtained from either the Navier-Stokes equation or the shallow water equation), D is the diffusivity term, while R and S represent the biochemical reaction term and the external sources, respectively.

The boundary and initial conditions needed to solve Eq. 11 are:

$$C(x,y,0) = C_0 \text{ and } \frac{\partial C}{\partial x} \Big|_{x=0,L} = 0 = 0, \frac{\partial C}{\partial y} \Big|_{y=0,L} = 0$$

The mass transport Eq. 11 can be solved by using the classical Crank-Nicolson. Finite difference scheme which is an implicit central difference scheme in space and a forward difference method in time. The stability of the methods is controlled by the dispersion and advection Curreant number, defined as

$$C_{adv} = \frac{v\Delta t}{\Delta L} \text{ and } C_{disp} = \frac{D\Delta t}{\Delta L^2}$$

The finite difference representation (see Andrea Bagnera) of Eq. 11 is for any point i, j, (a generic point (x,y) on the grid at any time t) is:

$$\begin{aligned} \frac{C_{ij}^{t+1} - C_{ij}^t}{\Delta t} + u \frac{C_{i+1,j}^{t+1} - C_{i-1,j}^{t+1}}{2\Delta x} v_{ij}^{t+1} \\ \frac{C_{ij}^{t+1} - C_{ij}^t}{2\Delta y} = D \frac{C_{i+1,j}^{t+1} - 2C_{ij}^{t+1} + C_{i-1,j}^{t+1}}{\Delta x^2} \\ + D \frac{C_{ij}^{t+1} - 2C_{ij}^{t+1} + C_{ij-1}^{t+1}}{\Delta y^2} + R(C)_{ij}^{t+1} S(C)_{ij}^{t+1} \end{aligned}$$

1-Dimensional transport equation: The 1-D transport equation can be generalized as:

Where R(C) in (11) is $-kC(x,t)$ and assuming there are no source term, i.e., $S(C) = 0$. If the velocity u(x,t) is taken as a constant i.e. q, thus we have (12)

The mass transport Eq. 12 can be solved by using the Crank-Nicolson finite difference scheme. The finite difference representation of Eq. 12 is for any point i, (ageneric point (x) on the grid) at any time t) is:

$$\begin{aligned} \frac{C_i^{j+1} - C_i^j}{\Delta t} + \frac{q}{2} \left\{ \frac{C_{i+1}^{j+1} - C_{i+1}^j}{2\Delta x} + \frac{C_i^j - C_i^{j+1}}{2\Delta x} \right\} - \\ \frac{D}{2} \left\{ \frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{\Delta x^2} + \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta x^2} \right\} + KC_i^{j+1} = 0 \end{aligned} \tag{13}$$

Thus we have

$$\begin{aligned} -\gamma C_{i-1}^{j+1} + (2 - \delta + 2\gamma - 2k) C_i^{j+1} + (\delta - \gamma) C_{i+1}^{j+1} \\ = \gamma C_{i-1}^j + (2 + \delta - 2\gamma) C_i^j + (\gamma - \delta) C_{i+1}^j \end{aligned} \tag{14}$$

Where

$$\delta = \frac{q\Delta t}{2\Delta x}, \quad \gamma = \frac{d\Delta t}{\Delta x^2}$$

The boundary and initial conditions needed to solve Eq. 12 are:

$$C(x,0) = C_0 \text{ and } \frac{\partial C}{\partial x} = g(t)$$

The boundary conditions (Schilling and Harris, 2000) can be stated in general as:

$$(1 - u_1) C(0,t) - u_1 C_x(0,t) = g_1(t) \tag{15}$$

$$(1 - u_2) C(a,t) - u_2 C_x(a,t) = g_2(t) \tag{16}$$

If $u_1 = 0$ we have the Dirichlet boundary condition on the lower boundary of the domain Ω which we have taken to be regular in order to be able to apply the finite difference method of numerical approach to the solution. Otherwise we would need to propose another numerical method that will handle the nature of the domain, such as

the finite element method. If on the other hand we have $u_2 = 0$ we have the Neumann boundary condition on the upper boundary of the domain.

In order to evaluate (14) at $i = 1$ and $i = n$, the boundary values C_0^j and C_{n+1}^j are needed. To develop expressions for these values, we can use a two-point forward difference for the derivative in (15) and a two-point backward difference for the derivative in (16). This converts the boundary condition constraints into the following difference equations.

$$(1-u_1)C_0^j + u_1\left(\frac{C_1^j - C_0^j}{\Delta x}\right) = g_1(t_j) \tag{17}$$

$$(1-u_2)C_{n+1}^j + u_2\left(\frac{C_{n+1}^j - C_n^j}{\Delta x}\right) = g_2(t_j) \tag{18}$$

Solving (3.6) for the boundary values yields

$$C_0^j = \frac{g_1(t_j)\Delta x + u_1 C_1^j}{u_1 + (1-u_1)\Delta x} \tag{19}$$

$$C_{n+1}^j = \frac{g_2(t_j)\Delta x + u_2 C_n^j}{u_2 + (1-u_2)\Delta x} \tag{20}$$

The Crank-Nicolson equations can be expressed in vector form by letting $C^j = [C_1^j, C_2^j, \dots, C_n^j]^T$ denote the solution at time t_j for $0 \leq j \leq m$. Suppose both boundary conditions are Neumann, which means $u_1 = 1, u_2 = 1$ in (16). For the case $n = 5$, this results in the following implicit linear algebraic systems.

$$\begin{bmatrix} (2-\delta+2\gamma+2k) & (\delta-\gamma) & 0 & 0 & 0 \\ -\gamma & (2-\delta+2\gamma+2k) & (\delta-\gamma) & 0 & 0 \\ 0 & -\gamma & (2-\delta+2\gamma+2k) & (\delta-\gamma) & 0 \\ 0 & 0 & -\gamma & (2-\delta+2\gamma+2k) & (\delta-\gamma) \\ 0 & 0 & 0 & -\gamma & (2-\delta+2\gamma+2k) \end{bmatrix} C^{j+1} = \begin{bmatrix} (2+\delta-2\gamma) & (\gamma-\delta) & 0 & 0 & 0 \\ \gamma & (2+\delta-2\gamma) & (\gamma-\delta) & 0 & 0 \\ 0 & \gamma & (2+\delta-2\gamma) & (\gamma-\delta) & 0 \\ 0 & 0 & \gamma & (2+\delta-2\gamma) & (\gamma-\delta) \\ 0 & 0 & 0 & \gamma & (2+\delta-2\gamma) \end{bmatrix} C^j + \begin{bmatrix} \gamma(C_0^{j+1} + C_0^j) \\ 0 \\ 0 \\ 0 \\ (\delta-\gamma)(C_{n+1}^{j+1} + C_{n+1}^j) \end{bmatrix}$$

The stability of the methods is controlled by the dispersion and advection Courant number, defined as

$$C_{adv} = \frac{v\Delta t}{\Delta x} \text{ and } C_{disp} = \frac{D\Delta t}{\Delta x^2}$$

RESULTS

We solve the contaminant transport model by implementing the Crank-Nicolson numerical scheme, while varying the different parameter values. We observe in general, a decrease in contaminant concentration. In Fig. 1, the profile for varying the decay rate, we observe that with a higher decay rate, the concentration of contaminant decreases faster than with a lower decay rate. In Fig. 2, the profile for varying contaminant velocity, we observe that the contaminant concentration with a higher velocity decreases at a higher rate than that with a lower velocity. In Fig. 3, the profile for varying the diffusive term, we saw that when the rate of diffusion is high, the concentration of contaminant decreases faster.

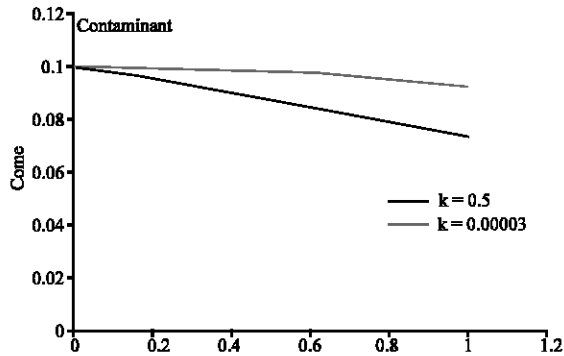


Fig. 1: Varying the value for the rate of decay k

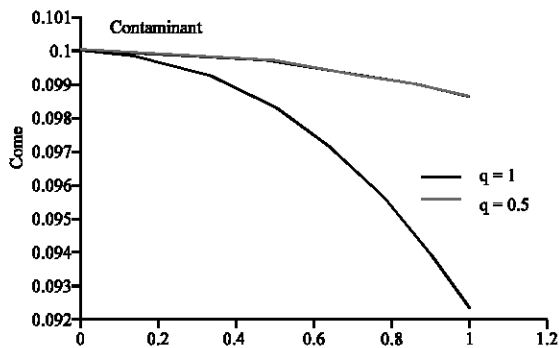


Fig. 2: Varying the value for the velocity term q

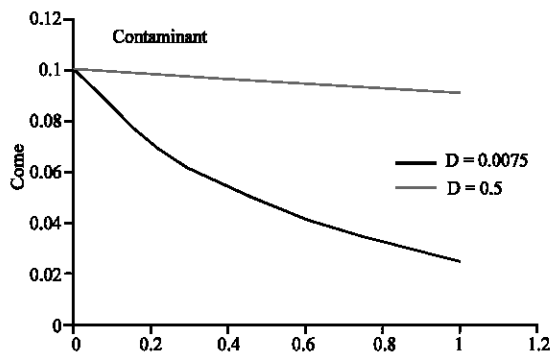


Fig. 3: Varying the value for the dispersive term D

CONCLUSION

In this study we have discussed the various models involving water pollutant transport equation. We have also given the implicit central difference scheme in space and a forward difference method in time for the evaluation of the generalized transport equation. And have given profiles for different parameter values.

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