



Prediction of Water Pollution Concentration Transport Using Finite Difference Methods

by

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LIST OF SYMBOLS

r	Courant number, dt / dx
D	Diffusion rate of water
u	Velocity rate of water
dt	Time step size
dx	Spatial step size

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LIST OF ABBREVIATION

1D	One Dimensional
2D	Two Dimensional
3D	Three Dimensional
FTCS	Forward Time Centered Space
CAN	Crank Nicolson
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method
ADE	Advection Diffusion Equation
WHO	World Health Organization
UNEP	United Nations Environment Programme
DO	Dissolved Oxygen
BOD	Biological Oxygen Demand
IBVP	Initial Boundary Value Problem
erfc	Error Function

Ramalan Pengedaran Kepekatan Pencemaran Air Menggunakan Kaedah Perbezaan Terhingga

ABSTRAK

Air adalah satu komponen yang penting bagi bumi. Manusia dan organisma hidupan tidak hanya menuntut kepada kuantiti air tetapi juga kualitinya. Aktiviti-aktiviti manusia pada masa kini adalah penyebab berlakunya pencemaran air. Pencemaran tersebut memberi kesan yang buruk kepada fizikal dan ciri-ciri kandungan air. Ianya adalah tidak praktikal untuk memantau semua aspek pengaliran air dan agihan pengedaran. Jadi, bagi membantu manusia untuk mengakses kawasan yang telah tercemar, ramalan kepekatan pencemaran air perlu dimodelkan. Kajian ini membentangkan satu persamaan penyerapan lintang dalam satu dimensi bagi meramalkan pengedaran kepekatan pencemaran air. Untuk menyelesaikan persamaan penyerapan lintang, proses pendiskretan telah dijalankan dengan menggunakan kaedah masa hadapan ruang pusat tersurat dan kaedah tersirat Crank Nicolson. Satu masalah agihan kepekatan pencemaran air telah digunakan dalam mengesahsahkan kaedah masa hadapan ruang pusat tersurat dan kaedah Crank Nicolson tersirat. Selepas proses pengesahsahan, algoritma berangka telah dibangunkan dalam perisian MATLAB untuk menyelesaikan persamaan penyerapan lintang dalam satu dimensi bagi kepekatan pencemaran air. Bagi tujuan simulasi, syarat-syarat awal dan sempadan, langkah ruang dan langkah masa serta persamaan penyerapan lintang dalam bentuk beza terhingga telah dikodkan. Keputusan berangka bagi persamaan penyerapan lintang dalam satu dimensi telah berjaya meramalkan pengedaran kepekatan pencemaran air dengan memanipulasi parameter halaju dan penyerapan. Oleh itu, kedua-dua pemboleh ubah ini memberi kesan terhadap kelajuan pengedaran dan kepekatan pencemaran pada jarak yang tertentu apabila berlakunya pencemaran air.

Prediction of Water Pollution Concentration Transport Using Finite Difference Methods

ABSTRACT

Water is an important component of the earth. Human being and living organisms are not only demand for the quantity of water but also the quality of the water. Human activities nowadays is one of the causes of the water pollution. The pollution give bad effect to the physical and characteristic of water contents. It is not practical to monitor all aspects of water flow and transport distribution. So, in order to help people to access the polluted area, prediction of water pollution concentration must be modelled. This study proposed a one dimensional advection diffusion equation for predicting the water pollution concentration transport. In order to solve the advection diffusion equation, the discretization process has been conducted using the explicit forward-time central-space method and implicit Crank Nicolson method. A problem in water pollution concentration distribution has been used in validating the explicit forward-time central-space method and the implicit Crank Nicolson method. After the validation process, the numerical algorithms have been developed in MATLAB software in order to solve one dimensional advection diffusion equation for water pollution concentration. For the purpose of the simulation, the initial and boundary conditions, the spatial steps and time steps as well as the advection diffusion equation in finite difference form have been encoded. The numerical results of one dimensional advection diffusion equation had successfully predicted the transportation of water pollution concentration by manipulating the velocity and diffusion parameters. Therefore, these two parameters give effect towards the speed of the pollutant transport and concentration of pollutant travel at certain distance when the pollution happen.

CHAPTER 1

INTRODUCTION

1.1 Overview

Water is an important component of the earth. It covered two thirds of the earth's surface. Almost all earth's population, especially human being depend on freshwater to continue their growth. By changing years, people are not only demand for the quantity of the water but also the quality of the water. Many aspects of social lifes depend on the economic availability and acceptable quantity of water. Therefore, water quality has became an issue increasing by years (Bartram and Ballance, 1997).

Water pollution can be defined in many ways. The pollution happened when there exist modification or changes in the physical, chemical and biological characteristics of water which gives bad effects on living things. Surface water and ground water are the two types of water resources which affected by pollution. Surface water such as rivers, lakes and oceans are the most useful sources to the human being and wildlife habitats (Jackson, 2003). Most water pollutions are caused by human activities. Human activities can give bad effects on the quality of water environment. As stated by the World Health Organization (WHO) and United Nations Environment Programme (UNEP), some examples of the activities which can cause water pollution are chemical fertilizers and chemical release by smokestacks. Farmers fertilized the fields and the chemical from the fertilizer used are washed by rain and moves to the surface water nearby. Pollution also happen when chemical release by the smokestacks enter the atmosphere and they fall back to the earth as rain and entering the rivers, ocean or lake (Bartram and Ballance, 1997).

Water pollution gives bad impacts especially to the human health because water is the most important resources for human to use in daily life. Besides, water pollution also affects the animals live in the water when poisoned through pollutant. Furthermore, this pollution will resulted in a lot of cost to treat and recover the polluted water contents (Jackson, 2003).

Gane (2000) stated that there are two techniques which can be applied to water transport problem, which are experimental and numerical modelling. Numerical modelling is considered to be more portable than experimental model. This is because, the parameters can be simply adjusted which make it easier to handle in industrial side. There are many numerical methods to solve the mathematical equations in order to deal with the water pollution problem. The mathematical models introduced can contribute to save the cost of human effort and material for a large number of chemical experiments to some degree. Moreover, it is inaccessible for on-site experiments in some cases due to environmental pollution issues (Wang, Li, Jia, Qi and Ding, 2013).

Advection diffusion equation (ADE) is one of the most important partial differential equations that have been used in transport of pollutants. An appropriate numerical method can give an accurate information on the concentration of pollution at different times and at different location efficiently and quickly (Ahsan, 2012). Therefore, many researchers have studied the numerical methods to solve the ADE in predicting the water pollution problem. One of the method to predict water pollution concentration is finite difference method (FDM). According to Magnus, Igboekwe and Achi (2011), FDM has been used to solve the flow equations in order to obtain the flow rate and flow direction of water pollution concentration. In this study, FDM will be used for solving 1D ADE because of its ability to predict the concentration of pollutant as stated by Landage (2014).

1.2 Problem Statement

The water pollution either on surface or in ground is a crucial problem. In most pollution transport investigations it is not practical to monitor all aspects of the water flow and transport distributions. The estimation of pollutant transport has been done before by field experiment but it is costly, time consuming and sometimes it is impossible to conduct due to inaccessibility to the wide area or lose of tracking of pollution sources. The 1D advection diffusion equation (ADE) will be used in order to clarify how to predict the water pollution concentration transport. A lot of previous works used the explicit method to solve this problem but the result is less accuracy when compare with the exact solution. So, the implicit Crank Nicolson (CAN) method will be used for solving the 1D ADE because CAN is the best method in the finite difference method in predicting the water pollution concentration transport. Later, by applying the numerical method, the simulation of water pollution concentration transport will be implemented and the pollution distribution can be estimated to the human work in this field.

1.3 Objectives of the Study

The main objective of this study is to predict the water pollution concentration transport. In order to achieve the main objective, the following sub-objectives will be carried out:

- (a) To discretize 1D ADE using FTCS and implicit Crank Nicolson method.
- (b) To develop a computer algorithm and procedure for solving 1D ADE using MATLAB.

- (c) To verify the accuracy of the selected finite difference method in predicting water pollution concentration transport.

1.4 Scopes of the Study

In this study, the work focused on solving the linear 1D ADE using the explicit forward-time central-space method and the implicit Crank Nicolson method. The discretization domain is set about 100 meters distance in the positive x direction in the grid. Then, the discretization of ADE and the value set up for time, t and direction, x will be compiled in MATLAB to provide the approximate solution and estimating the water pollution concentration when several velocity and diffusion rate is applied.

1.5 Significant of the Study

It is important to predict the water pollution concentration transport. For the situation where the water pollution happens, the numerical modelling of water pollution concentration transport will be developed. A realistic mathematical model using 1D ADE has developed in order to interpret and enhance the understanding of the factors of water pollution transport through mathematical behaviour. Hence, through this research, the model can be used by the working industries as a tool to look into the distribution of pollutants in a certain area by the calculation of the given water velocity and diffusion rate in the channel. So, by this numerical modelling of the prediction of water pollution

concentration transport, it reduces the risk of being exposed to dangers while at the sea, lake, river and others.

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CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter reviews the existing researches on water pollution concentration and the numerical methods used in solving the advection diffusion equation (ADE). Section 2.2 discussed about the water pollution problem and issues. Section 2.3 and section 2.4 talk about the existing equations and numerical methods for estimating water pollution concentration.

2.2 Water Pollution Problem

Water quality problem is the current issue caused by the human activity. River is the one of the areas that supplies the water to human and other living beings. Water pollution can be controlled and monitored through the information systems based on pollution levels in time and space.

The earliest water quality model is the Streeter-Phelps model developed by Streeter and Phelps (1925). This model is to predict dissolved oxygen (DO) and biological oxygen demand (BOD) concentrations in the Ohio River, USA. However, Streeter-Phelps model did not consider other water pollution problem such as dispersion pollution, DO consumption by living organisms in the water bodies and others.

Water pollution is originated from a point source or a non-point source. Therefore, pollution source identification models have been investigated by several researchers. Water pollution incidents by accident or illegal case such as in Tuojing River, Songhua River and Colorado River (Zhang & Xin, 2016). Boano, Revelli and Ridolfi (2005) developed the combination of 1D water quality model with the geostatistical method to analyse the amount of pollutants where the position of the pollution source location come from.

Marusic (2013) has studied the dispersion of the pollutant in the river type of aquatic system such as Tur, Lapus, Aries and Cavnic. All these rivers were polluted by human activities. A dispersion model has been developed in order to predict the evolution of pollutant in aquatic and impact assessment to the environment. The Prut River one of the polluted water resources have been investigated by Marusic (2013). The chemical composition that polluted the Prut River consists of copper, iron, nitrate, and oil. Some of them were spread and transport in this river to determine the pollutant dispersion. From the obtained result, it has been found that after 10 hours, the value of pollutant concentration decreased significantly.

Besides that, the Murray Burn River is one of the river that was polluted by the water infiltration from the soil. Hence, the development of model for the evaluation of velocity and dispersion coefficient have been investigated by Ani (2010). The mathematical model was implemented to analyse an instantaneous pollutant release in Murray Burn River.

2.3 Mathematical Equation

In order to assess water quality impacts, it is necessary to have a good understanding of environmental processes. The physical, biological and chemical processes can be presented in mathematical equation. The transport pattern in natural water content depends on the combinations action between water flow and diffusion. Therefore, in the development of water quality model, it is needed to consider the effects of both advection and diffusion (Ahsan, 2012).

Gane (2000) has studied the prediction of the pollutant movement in a body of water. The research investigated on 1D, 2D and 3D of advection diffusion equation. The one-dimensional advection diffusion equation is given as in equation (2.1),

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D_x \frac{\partial^2 c}{\partial x^2} \quad (2.1)$$

where u is velocity in the direction of x and D_x is the diffusion coefficient. The equation is based on the fundamental principle of conservation of mass. The mass flow rate has two components which are advection and diffusion. Advection is the physical process where the pollutant is carried downstream with the stream flow velocity. The diffusion is the combination of the pollutant in the flow on a molecular scale or turbulent eddies at the macroscopic scale. The sum of the net mass flows rate in each direction which mean will form the three-dimensional ADE as shown in equation (2.2),

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} \quad (2.2)$$

where u , v and w are velocities in the directions of x , y and z directions respectively. The parameters D_x , D_y and D_z are the diffusion coefficients. The pollution concentration is defined as c .

Gane (2000) has investigated and developed the numerical method to solve one dimensional advection diffusion equation. The research focused on the prediction of the quality of the water in rivers by using 1D ADE only. This is because, Gane (2000) mentioned that the accuracy of the results give the similar readings with the 2D and 3D ADE. Furthermore, the 1D required less effort in order to obtain the results. The water pollution model can be simplified by reducing the model to one dimensional because in some cases, the multidimensional advection diffusion equation is negligibly small.

The 1D ADE was proposed by Ani (2010) in solving the pollutants transport in the river which include pollutant sources and sinks along the transport. The author has estimated the velocity and dispersion coefficient values in predicting the pollutant concentrations transport in streams.

In addition, the simple mathematical model to estimate the water river pollution has been studied by Azad (2015). The one-dimensional advection diffusion equation is used in estimating the contaminant concentration levels in a river. Moreover, the ADE is used in this research because it reflects the physical phenomena where involved diffusion process of the particles move with certain velocity. Previously, Rahaman, Andallah and Begum (2014) presented the water model by estimation of the extent of water pollution at different times and different points. The authors used the 1D ADE and an initial boundary value problem (IBVP) in estimation of water pollution concentrations.

2.4 Existing Methods for Water Pollution Prediction

The last three decades, there are many numerical methods used in the investigations of water quality modelled by advection diffusion equation (Ahsan, 2012). Numerical models are important engineering tools when considering the estimation of pollution transport in a water bodies (Gane, 2000).

In fact, there are many researchers involved in solving the water pollution model equation by using several analytical solutions. This analytical solutions have been studied by Ogata and Banks (1961), Harleman and Rumer (1963), Marshall, Holmes and Rose (1996) and Marino (1974). In the same way, many researchers have solved the water pollution model equation by several numerical methods in their studies. Presently, most of the researchers show interest to the numerical solution of ADE rather than using analytical solutions to be implemented in the research problem (Kaya and Gharehbaghi, 2014).

The spline method is one of the method which can be used for solving the ADE which describe the transport of pollution. There are several types of spline methods such as quasi-Langarian cubic spline which is obtained by Pepper, Kern and Long (1979) and Okamoto, Sakai, Matsumoto, Horiuchi and Kobayashi (1998). Ahmad and Kothiyari (2001) solved the ADE using cubic spline interpolation method for the advection term while the diffusion term is solved using the Crank Nicolson scheme technique. Thongmoon and Mckibbin (2006) proved that the results obtained from cubic spline method is less accurate then finite difference method. This is because, the error estimations of forward-time central-space (FTCS) and Crank Nicolson methods are less than cubic spline method.

Besides that, Gray and Pinder (1976) analysed the combination of Eulerian and Langarian methods that are used for solving advection term and diffusion term separately since these methods are simple and easy to be implemented to the models. The advection term is solved by using Eulerian method while diffusion term is treated by semi-Langarian scheme which is one of the Langarian methods. However, these methods are less stable and less accurate. Besides, semi-Langarian scheme has poor mass conservation properties as stated by Chen, Naseri-Neshat and Ho (1981) and Li and Yu (1994).

Finite element method (FEM) has evolved significantly over the last few years. Sheu and Chen (2002) solved the contaminant concentration problem by using FEM for solving advection-dispersion equation in one-dimensional. However, Magnus et.al (2011) stated that the FEM needs more computation time which is difficult to apply the FEM in larger seas area. Thus, Magnus et.al (2011) suggested to used FDM in predicting the future direction flow and particles location by solving the governing flow equation. Even though FDM is not widely explored method but it becomes more useful with the advent of high speed computers.

Agusto and Bamigbola (2007) have studied the numerical treatment of the water pollution problem. In this research, the authors used various mathematical models for solving water pollution problem. All the mathematical models have been studied by using finite difference methods. Rahaman et al. (2014) and Azad (2015) have presented the numerical methods in their research studies. Both authors solve their water pollution problem by using finite difference method for solving ADE equation. The authors only used the explicit FTCS and FTBS method for solving the equation. Unfortunately, these two methods is less accuracy when compare with the exact solution (Thongmoon et.al,2006).

The hydrodynamics or water quality equations can be solved by using different numerical scheme techniques such as explicit and implicit numerical schemes. The first equation of the 1D ADE provided by Horgarth et.al (1990) is the first and second order diffusion equation, which is linear as reported by Hoffman and Chiang (2000). Many researchers have used finite difference approximation either in explicit or implicit forms (Hoffman & Chiang, 2000). However, the equation in this study is approximated in explicit FTCS and implicit Crank Nicolson form, which are the most stable numerical schemes in FDM stated by Horgarth et al. (1990). The explicit method is the simplest method in FDM and has three basic operators in its discretization part which are forward, backward and central approximation operator. The time derivative is discretized using forward difference approximation because it is conditionally stable compared to backward difference (Ahsan, 2012).

Manteghian and Mohammadi (2011) used FDM for solving 1D ADE with constant coefficients by changing the values of temporal parameter, ϕ and spatial weighted parameter, θ . The researcher obtained the solutions by comparing the explicit and implicit scheme techniques. Then, the results clarified that the Crank Nicolson method has a very good agreement with analytical results. Implicit Crank-Nicolson method is also a stable numerical schemes among six implicit finite difference methods used to solve ADE studied by Horgarth et al. (1990). In this study, author analysed the theoretical order of accuracy of first, second and third order. Hence, the order of accuracy affect the errors with changes in time and space. The two parameters r , the Courant number and p , the diffusion number in the numerical method were investigated by changing the value of Δt and fixing the value of Δx . The results show that the value of

$$r \text{ is stable when } r = \frac{\Delta t}{\Delta x^2} \leq 0.5 .$$

Based on the previous studies, the finite difference method is the suitable method in this study for solving 1D ADE. In order to predict water pollution concentration transport, the Crank Nicolson method will be used because this method never have been used in previous work.

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