NUMERICAL COMPUTATIONS FOR WATER-QUALITY MODELS USING UNCONDITIONAL STABLE EXPLICIT FINITE DIFFERENCE SCHEMES

PAWARISA SAMALERK

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENT FOR THE
DEGREE OF DOCTOR OF PHILOSOPHY IN DEPARTMENT OF APPLIED
MATHEMATICS
FACULTY OF SCIENCE
KING MONGKUT'S INSTITUTE OF TECHNOLOGY LADKRABANG
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หัวข้อวิทยานิพนธ์	การคำนวณเชิงตัวเลขของตัวแบบคุณภาพน้ำโดยใช้วิธีผลต่างอันตะชัดแจ้งที่เสถียรโดยไร้เงื่อนไข
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บทคัดย่อ

ตัวแบบเชิงคณิตศาสตร์ สามารถใช้ในการอธิบายในหลายปัญหาของการเคลื่อนที่และการแพร่ของสารละลาย เช่น มลพิษของน้ำ และสารแขวนลอยในแม่น้ำหรือคลอง ถ้าความเข้มข้นของสารก่อมลพิษ ณ จุดปล่อยที่มีการไหลไม่คงที่ เทคนิควิธีการเชิงตัวเลขที่แตกต่างกันหลายแบบได้ถูกนำมาใช้ในงานวิจัยนี้ โดยได้นำเสนอการจำลองเชิงตัวเลขเพื่อสร้างแบบจำลองคุณภาพของน้ำแบบหนึ่งมิติในต้นน้ำลำธาร สมการเริ่มต้นที่ใช้คือสมการการพา การแพร่ ปฏิกริยา แบบหนึ่งมิติ ภายใต้เงื่อนไขฟังก์ชันขอบการไหลไม่คงที่ การประมาณค่าความเข้มข้นของสารก่อมลพิษ ได้มาโดยใช้เทคนิควิธีผลต่างอันตะของโซเยฟอย่างไร้เงื่อนไข ในเทคนิคนี้ขนาดของช่วงเวลาการคำนวณที่มีขนาดของกริดใหญ่ หรือเล็กนั้น สามารถเลือกนำมาใช้ในการคำณวนได้อย่างอิสระตามที่ต้องการ ในสภาวะฟังก์ชันเงื่อนไขเริ่มต้นขอบที่เกิดจากความเข้มข้นของสารก่อมลพิษ ณ จุดปล่อยของการไหลไม่คงที่จะถูกกำหนดให้ใช้เทคนิคการประมาณค่าในช่วงกำลังสอง การหาผลเฉลยโดยการประมาณค่าของแบบจำลองจะได้รับการตรวจสอบว่าสอดคล้องกับผลเฉลยโดยการเปรียบเทียบกับที่คำนวณได้ การเพิ่มอัตราการสลายตัวของมวลมีผลต่อระดับความเข้มข้นสูงสุด เทคนิควิธีการเชิงตัวเลขของเรานี้ได้นำเสนอวิธีการหาผลเฉลยที่สามารถนำไปประยุกต์กับปัญหาจริงทางธรรมชาติได้อย่างแท้จริงและเชื่อถือได้

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Abstract

Mathematical models can be used to describe the behaviour of dissolved matter transport as a pollutant suspended in a river or canal If the pollutant concentration at the discharged point is not uniform, then several numerical techniques are needed. In this research, the numerical simulation to the one-dimensional water-quality model in a stream is proposed. The governing equation is a one-dimensional advection-diffusion-reaction equation with non-uniform boundary condition functions. The approximated pollutant concentrations are obtained by unconditionally Saulyev finite difference technique. The time step and grid size are free as computational requirement. The numerical experiments show reasonable approximations. The initial-boundary condition functions due to non-uniform pollutant concentrations at the discharge point are defined by the quadratic interpolation technique. The approximated solutions to the model are verified by a comparison with the analytical solution. Increasing the mass decay rate affects the maximum concentration level. Our proposed numerical techniques give dependable and accurate solutions to these kinds of several natural phenomenas applications.

Keywords: Advection-diffusion–reaction equation, Saulyev scheme, Quadratic interpolation, Water-Quality model, Unconditionally stable.

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Chapter 1

Introduction

1.1 The water pollution problem

Water pollution is a big problem in the world. Water everywhere is being affected by a water pollution global issue that everyone should all be paying attention to. Any water in the world without digging is surface water. This can include rivers, lakes, ponds, streams, and the oceans. Water pollution refers to water that's dirty or full of things, and substance into water that is a part of that water. These substances are not always pollutants. If the substances present in water are not dangerous or toxic to human beings is called contaminants. There are a lot of cities around the world that face terrible problems with water pollution. The most common sources of water pollution are three types, the first is Organic pollutants that animal waste products and some type of bacteria or parasite present in water. The second is Inorganic pollutants that made up of man-made chemicals or other substances, and the third is Radioactive pollutants that places near nuclear power plants and certain types of factories are at the greatest risk. the biggest water pollution countries have got 7 countries. There are United States, India, Japan, Indonesia, Germany, and Brazil, respectively. Especially, the Yangtze River in China, seriously polluted in others, and it can't sustain fish or animal life well anymore. The river is contaminated with industrial runoff and wastewater from nearby factories. The Chinese government has a list of water quality standards surface water are held to fairly high standards to check water quality. The Yangtze River in China flow into MeKong river, this river flow through our hometown. The water quality in our destination city is at Khemmarat, Ubonrachatanee, Thailand as shown in Fig. 1.1. People live near this river are most affected by pollution water sources worldwide. We believe that the result of upstream Hydropower Dams in Laos (Xayaburi & Don Sahong Dams) and probably upstream point sources of pollution, such as: mining, agro-chemicals runoff and sewage from Laos/Thailand/Myanmar as shown in Fig. 1.4. The researcher lives near Bang Bua Canal is about 9 km in area of Don Muang, BangKhen, and Laksi as shown in Fig. 1.2-1.3. There are 12 communities are most affected by the problem of waste and sewage in the canal. The most water pollution in Thailand to seem Ta Nang canal as shown in Fig.1.5. We always think about how to overcome water pollution problem. We wish could find a way to help out around the world and improve the quality of water for our fellow human beings. Thus, how can water pollution be reduced, improved, or stopped altogether. We propose the Mathematics model for measurement quality water.

Figure 1.1 Mekong river and Bangko canal (separate from Mekong river) in Khemrat Ubonratchatanee, Thailand

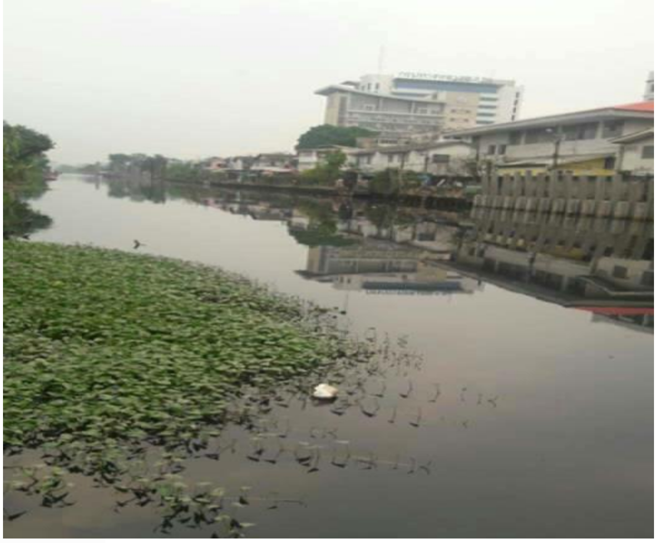


Figure 1.2 Bangbua canal, Chatuchak Bangkok, Thailand

Figure 1.3 Water pollution experiment at Bangbua canal, Chatuchak, Thailand

Figure 1.4 Pollution in the Mekong in Can Tho, Vietnam

From : https://www.mekongeye.com/2017/09/24/how-environmental-pollution-is-ruining-the-mekong-delta/

Figure 1.5 Pollution in Ta Nang canal, Bangkrabi Bangkok, Thailand

Models are used to express the characteristics of reality which are considered important and to neglect those which seem secondary. These simplifications, good models allow obtaining an easily understandable, mathematically calculable image of the natural phenomenas. A model is formulated with the aid of mathematical relation, that is a mathematical model. A model is a set of rules, or formulas, which try to represent the behavior of a given phenomenon. Several classes of mathematical models three classes appear: Models which come from laws of physics, this is the case for gravitation laws, Max well equations (wave). Navier – Stokes equations (fluid dynamics), and so on; Model which come from empirical laws, such as air resistance for a movement. Model which come from statistical laws, for instance that fit a line between several points and assume the response to be linear. There are three reasons why we build mathematical models. It gives a better understanding of the phenomenon, which leads to a more precise tuning of the parameters; It warns you get off limits for instance, an empirical knowledge usually is not enough to answer the questions. It allows you to find the values of the parameters, which lead to a given result, so building a mathematical model usually means better control upon the phenomenon, which, in turns, mean more precision, cheaper results and better quality output. Those are the reasons to use Mathematical Model and how different from the fieldwork.

Figure 1.6 The gutter for put ink in to the water flow

From : http://www.phunnara.com/gutter.php

Figure 1.7 Diffusion phenomenon form in water

From : https://www.printerbase.co.uk/news/which-printer-uses-the-least-ink/

Figure 1.8 Dispersion phenomenon form in water

From : https://vn.sputniknews.com/politics/201801104613866-my-giai-mat-ke-hoach-tan-cong-hat-nhan-lien-co/

Figure 1.9 Advection-Diffusion or dispersion phenomenon form in water

From : https://www.shutterstock.com/video/clip-11195045-stock-footage-blue-ink-reacting-in-water-creative-slow-motion-on-a-white-background.html

Figure 1.10 Advection- Diffusion or dispersion phenomenon form in polluted-rivers

From : https://www.globalcitizen.org/en/content/indias-polluted-rivers-now-legally-humans/

We consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one-dimensional advection-diffusion – reaction equation (ADRE).

Figure 1.11 Mekong river in Khemmarat Ubon ratchathani, Thailand
From : https://earth.google.com/

Figure 1.12 Bangbua canal in Chatuchak Bangkok, Thailand
From : https://earth.google.com/

The simple explicit schemes have the advantages of simplicity in coding and time effectiveness in computing without losing more accuracy and these schemes are preceding for several model applications. To identify the best one these simple schemes, comparative studies of these are necessary.

The object of this research is to propose a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes. The proposed numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. The examples are calculated for three values 0, 0.5 and 1, respectively. In the numeric solution of ADRE by using finite differences, either the small values of a Courant number is used for oscillation free results. We apply the method to three problems. The results of the model show that the calculated results are reasonable approximations.

The proposed Saulyev finite difference scheme with quadratic interpolated initial-boundary conditions technique uses are unconditionally stable methods. It is the large or small of time step and/or grid size can be employed in the techniques. The numerical experiment shows that the calculated results are reasonable approximations. The revision shows good agreement solutions. Increasing the mass decaying rate affects the maximum concentration level. The interpolation results must be crude mesh as field data. The numerical results can be fine mesh or crude mesh. The compare of analysis and interpolation technique is show in Figure 4.5-4.10. The numerical techniques are proposed for the interpolation technique gives the results closest to the analytical solution. The accuracy of the Lagrange interpolation technique is used to predict their initial and boundary conditions as needed. The proposed interpolation technique is suitable to be used in the natural phenomenas problem due to it easily to computer coding and the straight forwardness of the computer implementation. According to field water quality data need to implement to be a function of the boundary conditions. The computed results are verified by the numerical accuracy. The proposed technique gives reliable solutions to these processes.

1.2 Literature review

The water quality must be protected and maintained for several uses, the principal ones being domestic water supply, energy production, industry, agriculture, fish and wildlife. Mathematical modeling of the water pollution measurement and control in the water area has been examined. In [1], a simulation process showing that water pollution levels can be reduced to an agreed standard at the lowest cost is proposed.

In [2], mathematical modeling of the transport salinity, pollutants and suspended matter in shallow water that involves the numerical solution of an advection-diffusion equation is proposed. A novel technique of finite difference methods is proposed. In [3], they also propose a mathematical modelling of the transport salinity, pollutants and suspended matter in shallow water that involves the numerical solution of an advection-diffusion equation in the technique of flux-corrected scheme of finite difference methods. It is available for the solution of the depth-integrated form of the advection-diffusion equation. In [4] and [5], the advection and diffusion term are solved by two different numerical methods.

In [6], they use a weighted discretization method with the modified equivalent partial differential equation for solving one-dimensional advection-diffusion equation. In [7], the central difference approximation gives overestimation that is negative concentration in the neighboring cell due to a large advection flux. In [8], they propose a numerical dispersion by introducing an up-stream interpolation method, namely QUICK (Quadratic Upstream Interpolation Convective Kinematics) for one-dimensional unsteady flow. In [9], the parabolic partial differential equations with nonstandard initial condition, featured in the mathematical modeling of many phenomena are proposed. The Saulyev's explicit schemes are an economical implement to use. These unconditionally explicit schemes are very simple to program and compute. The new explicit schemes developed are very efficient and they need less CPU time than the implicit methods. The explicit finite difference schemes are very easy to implement for similar higher dimensional problems. In [10], a user friendly and a flexible solution algorithm are proposed for the numerical solution of the one-dimensional advection-diffusion equation (ADE), explicit spreadsheet simulation (ESS) technique is used instead of computer code. In the numeric solution of ADE by using finite differences, either the small values of a Courant number such as 0.05-0.10 is used for oscillation free results or an artificial diffusion is used in order to reduce oscillation. In order to provide for small Courant numbers, it is necessary to choose a small time step and /or grid size; however, this increases the computer time. While the proposed ADEESS solution technique uses an unconditional stable Saulyev scheme, it gives highly accurate results even for the values of the Courant numbers as high as 2-3. By varying only the values of the temporal weighted parameter θ namely, 0, 0.5 and 1, respectively, the problems are solved. The model results for the value of $\theta = 0$ appear to be in good agreement with the analytical solutions.

In [11], a better finite difference scheme to solve the dynamic one-dimensional advection-dispersion-reaction equations (ADRE) is focused, and the effect of non-uniform water flows in a stream is considered. There are two mathematical models used to simulate pollution due to sewage effluent. First model is a hydrodynamic model for numerical techniques. The Crank-Nicolson method is used to approximate the solution. Second model is an advection-dispersion-reaction model; the explicit schemes is introduced. The revised explicit schemes are modified from two computation techniques of uniform flow stream problems, forward time central space (FTCS) and Saulyev schemes for dispersion model. A comparison of both schemes regarding stability aspect is provided so as to illustrate their applicability to the real-world problem.

The dispersion model provides the pollutant concentration field. In [12], a modified MacCormack method is subsequently employed in the dispersion model. The proposed method is a simply remarkable alteration to the MacCormack method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicate that proposed modified MacCormack scheme does improve the prediction accuracy compared to that the tradition MacCormack method. They propose the simple revision to the MacCormank and Saulyev schemes that improve their accuracy for high Peclet number problems, which are named the Saulyev$_c$ and MacCormack$_c$ schemes respectively, greatly improved the prediction accuracy over the original ones [13]. They propose a new scheme that guarantees the positivity of the solutions for arbitrary step sizes. In [14], they develop a numerical technique to approximate the solution of an advection-diffusion-reaction equation in one spatial dimension with constant velocity and diffusion. In [16], the Preissmann four-point partial-node implicit scheme is used to solve a one-dimensional hydrodynamic and water quality model. In [17], a nondimensional form of a two-dimensional hydrodynamic model with generalized boundary condition and initial conditions for describing the elevation of water wave in an open uniform reservoir is proposed. The separation of variables method with mathematical induction is employed to find an analytical solution to the model. In [18], the traditional Crank-Nicolson method is also used in the hydrodynamic model. At each step, the flow velocity fields calculated from the hydrodynamic model are the inputs into the water-quality model. A new fourth-order scheme and a Saulyev scheme are simultaneously employed in the water-quality model. In [19], the hydrodynamics model coupled with water quality is established by MIKE21FM software to simulate the current situation of Erhai Lake. The water quality is also simulated by the two-dimensional hydrodynamics and water quality coupled model. The simple explicit schemes have the advantages of simplicity in computing without losing more accuracy and these schemes are precedent for several model applications. To identify the best one these simple schemes, comparative studies of these are necessary.

The collected field data is not suitable to input in a mathematical model. The data is varied by time. The time-dependent distribution of discharged pollutant concentration and water flow velocity are required. It is complicated work if we input them into a computer implementation while a given function has simpler operation.

The object of this research is to propose an interpolation technique to all of collected field data such as water pollutant concentration at released polluted water point and the water flow velocity along the considered water stream. The revision shows good agreement solutions. The proposed technique is suitable to be used in several real-world problems due to it easily to program and the straight forwardness of the implementation. According to field water-quality data, the data will be implemented to be a function of the boundary condition. The Lagrange interpolation technique is used to synthesis their boundary conditions as required. A simple advection-diffusion-reaction numerical simulation is proposed by using the Saulyev scheme. The proposed numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. We apply the method to two problems with different data for obtaining the right and left boundary conditions. The results of the model are show that the calculated results are reliable approximations. The computed results are verified by the numerical accuracy. The proposed technique gives reliable solutions to these processes.

1.3 Goal and Objectives of The Study

1.3.1 To propose a simple numerical simulation by using the Saulyev's explicit schemes for a one-dimensional advection-diffusion-reaction equation in an opened Uniform Flow Stream.

1.3.2 To propose numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques.

1.3.3 According to collected water – quality data need to implement to be a function of the boundary condition. We propose a Lagrange interpolation technique due to non-uniform pollutant concentrations at the discharge point are defined by the quadratic interpolation technique.

1.3.4 To propose numerical simulation to a one-dimensional water-quality model in a non-uniform flow stream using an iterative explicit finite difference technique.

1.4 Scope of The Study

1.4.1 The finite difference scheme is applied to a one-dimensional advection-diffusion-reaction equation in a river or canal by using the traditional Saulyev's schemes.

1.4.2 The propose numerical technique uses an unconditionally stable method.

1.4.3 To apply the model to the problem with different derivative right boundary and left boundary conditions technique, Lagrange interpolation, and Quadratic interpolation technique.

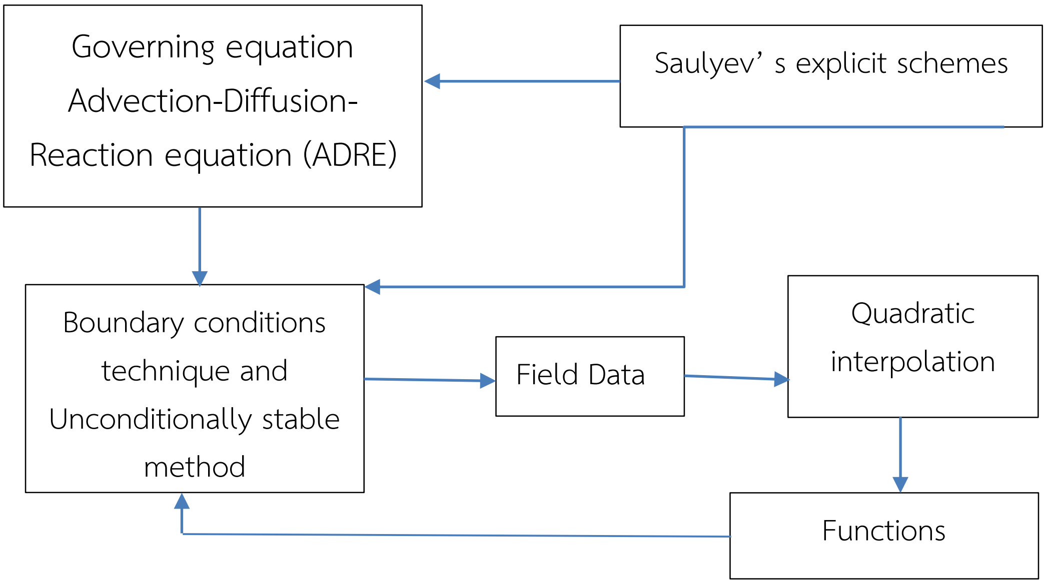


Figure 1.13 Flowchart of water quality measurement model

1.5 Process of The Study

The thesis explains the mathematical modeling of water pollution measurement and water quality. The one-dimensional advection-diffusion-reaction equation is a mathematical model describing the transport and diffusion problems such as pollutants and suspended matter in a river or canal. If the velocity field is non-uniform the model cannot be theoretically manipulated, therefore numerical techniques are required. The proposed numerical technique uses an unconditionally stable method.

The first part will study the basic knowledge about the water pollution and mathematical model for water quality measurement by defining the domain of problem in thesis and domain of study case.

The second part will study the numerical method for solving the one-dimensional advection-diffusion equation and the one-dimensional advection-diffusion-reaction equation.

The third part is the computation of the one-dimensional advection-diffusion equation by using the unconditionally stable Saulyev method.

The forth part is the computation of the one-dimentional advection-diffusion equation by using the Saulyev schemes and an unconditionally stable method. We employ the forward, backward and central difference methods to the conditions boundary.

Finally, we use their proposed interpolation technique to all of field collected data such as water pollutant concentration at released point and the water flow velocity along the considered water area.

1.6 Benefits of The Study

My purpose is the numerical simulation techniques are the modified model of water pollution and application to a stream water assessment problem. The proposed numerical techniques are unconditionally stable methods. It is the large or small of time step and/or grid size can be employed in the techniques. The numerical experiments can show that the calculated results are reasonable approximations. The revision shows good agreement solutions. The proposed technique is suitable to be used in the renatural phenomenas problem due to it easily to program and the straight forwardness of the implementation**.** According to field water-quality data, the data will be implemented to be a function of the boundary condition. The Lagrange interpolation technique is used to synthesis their boundary conditions as required. The computed results are verified by the numerical accuracy. The proposed technique gives reliable solutions to these processes.

Chapter 2

Basic Concepts and Preliminaries

Water Quality Modeling and Prediction are used to simulate pollutant concentration in a river and canal. The first part of the section, characteristics of surface waters, water quality monitoring, water quality modeling and Prediction, governing equations for a one - dimensional advection-diffusion equation (ADE). In the second part of the section, numerical Technique, and Iterative Method for the Initial and Boundary Conditions.

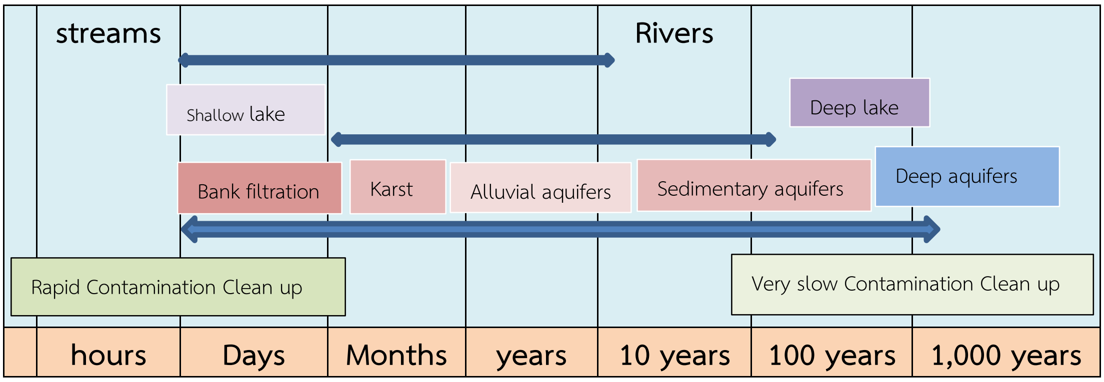
The importance attached to quality will depend on the actual and planned use or uses of the water (e.g. water that is to be used for drinking should not contain any chemicals or microorganisms that could be hazardous to health). Since there is a wide range of natural water qualities, there is no universal standard against which a set of analyses can be compared. If the natural, pre-polluted quality of a water body is unknown, it may be possible to establish some reference values by surveys and monitoring of unpolluted water in which natural conditions are similar to those of the water body being studied.

2.1 Characteristics of surface waters

2.1.1 Hydrological characteristics

Continental water bodies are of various types including flowing water, lakes, reservoirs and ground waters. All are inter-connected by the hydrological cycle with many intermediate water bodies, both natural and artificial. Wetlands, such as floodplains, marshes and alluvial aquifers, have characteristics that are hydrologically intermediate between those of rivers, lakes and groundwaters. Wetlands and marshes are of special biological importance.

Table 2.1 Typical water residence times in inland water bodies [20].



Note: Actual residence times may vary. Residence times in karstic aquifers may vary from days to thousands of years, depending on extent and recharge. Some karstic aquifers of the Arabian peninsula have water more than 10,000 years old. It is essential that all available hydrological data are included in a water quality assessment because water quality is profoundly affected by the hydrology of a water body. The minimum information required is the seasonal variation in river discharge, the thermal and mixing regimes of lakes, and the recharge regime and underground flow pattern of groundwaters. The common ranges of water residence time for various types of water body are shown in Figure 2.1. The theoretical residence time for a lake is the total volume of the lake divided by the total outflow rate ($V / \Sigma Q$). Residence time is an important concept for water pollution studies because it is associated with the time taken for recovery from a pollution incident. For example, a short residence time (as in a river) aids recovery of the aquatic system from a pollution input by rapid dispersion and transport of waterborne pollutants. Long residence times, such as occur in deep lakes and aquifers, often result in very slow recovery from a pollution input because transport of waterborne pollutants away from the source can take years or even decades. Pollutants stored in sediments take a long time to be removed from the aquatic system, even when the water residence time of the water body is short. River flow is unidirectional, often with good lateral and vertical mixing, but may vary widely with meteorological and climatic conditions and drainage pattern. Still surface waters, such as deep lakes and reservoirs, are characterised by alternating periods of stratification and vertical mixing. In addition, water currents may be multi-directional and are much slower than in rivers. Moreover, wind has an important effect on the movement of the upper layers of lake and reservoir water. The residence time of water in lakes is often more than six months and may be as much as several hundred years. By contrast, residence times in reservoirs are usually less than one year.

2.1.2 The Rivers

An understanding of the discharge regime of a river is extremely important to the interpretation of water quality measurements, especially those including suspended sediment or intended to determine the flux of sediment or contaminants. The discharge of a river is related to the nature of its catchment, particularly the geological, geographical and climatological influences.

Tropical rivers

The regime of a tropical river is largely determined by the annual cycle of wet and dry seasons. Some regimes, and some of the climatic and geographical conditions that affect regimes, are as follows:

Equatorial rivers with one flow peak, resulting from heavy annual precipitation (1,750-2,500 mm) in areas with no marked dry season.

Equatorial rivers with two flow peaks, produced by precipitation totaling more than 200 mm monthly and well over 1,750 mm annually. Equatorial forest predominates in the catchment area.

Rivers in the moist savannah of tropical wet and dry lowlands exhibit pronounced seasonal effects of rainfall patterns. In these areas, the dry season persists for at least three months.

In some areas of the tropical wet and dry highlands, the length of the dry season varies significantly. River basins in such areas are covered by woodland and relatively moist savannah.

In the relatively drier regions of the tropical wet and dry highlands, river basins are located in the marginal parts of the dry climate zones. Precipitation rarely exceeds 500-700 mm annually, which is typical of semi-desert regions, and vegetation in the river basins is predominantly dry savannah.

In areas where the dry season is prolonged, ecologists may divide the associated vegetation into wooded steppe and grass steppe. River regimes, however, do not differ between the two types of region, and flow is likely to be intermittent.

In desert regions, where annual rainfall is less than 200 mm, river basins are covered with sand, desert grass or shrubs, and rivers are of the wadi type. The drainage network is poor and where it is traceable, it is likely to have developed before the area reached its present stage of aridity.

Many of the rivers of tropical mountain regions have drainage basins of very limited size. The great rivers of the tropics do not fall exclusively into any of these categories, because their drainage basins extend over many regions of differing climate and vegetation. The regime of the Congo (Zaire) River, for example, is largely a combination of regimes of the equatorial wet region and the tropical highland climate. Mean monthly flow is highest in April (76,000 m^3 s^{-1}) and lowest in July (32,000 m^3s^{-1}). The Niger has its headwaters in a wet zone near the ocean, but then flows into a semi-arid region where it is subject to evaporation losses. Lower still in its course, the river flows into wet and dry tropical lowland. The Zambezi river basin is located largely in wet and dry tropical highland and semi-arid regions, while the Nile exhibits the most complex regime of all African rivers, extending over many widely different climatic zones. The Amazon has a complex flow regime because of the different precipitation patterns of its main tributaries. Flow begins to increase in November, reaches a peak in June and then falls to a minimum at the end of October. The Orinoco, although draining a similar area to the Amazon, reaches peak flow a month later than the Amazon but also has minimum flow in October.

Most of the large rivers of Asia that flow generally southward have their sources in the mountains and flow through varied climatic conditions before discharging to the sea. Peak flows generally occur when run-off from melting snow is supplemented by monsoon rains. The Ganges and Irrawaddy receive snow-melt from the Himalayas and southern Tibet respectively from April to June, and the flow rate is just beginning to decline when the July monsoon begins. Flooding can occur from July to October. The Mekong is somewhat similar. It has its beginnings at an altitude of about 4,900 m in China's Tanglha Range. Snow-melt is later here, so peak flows do not occur until August/September in the upper reaches of the river and October in the lower reaches. Minimum flow in the Mekong occurs from November to May.

In western Asia, the Indus has some of its source tributaries in the Hindu Kush mountains, while the Tigris and Euphrates rise in the mountains of Turkey and Armenia respectively. Monsoon rains cause the Indus to flood between July and September. The Tigris and Euphrates are affected by seasonal rains that overlap with snow-melt run-off and cause flooding from March to June. The floods on the Euphrates inundate low-lying areas to form permanent lakes that have no outlets. Water loss from these lakes is mainly by evaporation, although some of the water is withdrawn for irrigation. Data on erosion in all of the world's river basins are far from complete. In general, however, erosion can be said to vary according to the following influences:

1. Amount and pattern of rainfall and resultant river regime,
2. Slope of the land,
3. Extent of destruction of vegetation,
4. Regeneration of vegetation, and
5. Soil type and resistance to the effects of temperature changes [20].

2.2 Water quality monitoring

Water is necessary for the survival of living beings, whether human or animal. When there is growth from industrial development of the community, water, naturally, is unable to make modifications to restore itself. Water pollution in water resources occurs and causes an impact on the ecosystem, including the use of water as well. Therefore, to determine the water status in the current situation, it is important to monitor the water quality. When the facts, will lead the way in solving and preventing water quality caused by pollution. Monitoring water quality, includes the process of exploring and water quality monitoring. Determining the water samples are generally defined by 3 main points [21]:

1. The reference points include the upstream or points that are not affected by any pollution source.

2. The checking change points in water quality during the utilization or affected by the pollution of water resources.
3. The checkpoint downstream estuaries or before the end when the water is drained into the water.

The parameters used to monitor water quality parameters need to be defined in the audit. The parameters that are important or indicate the water quality such as color, temperature, pH, conductivity, dissolved oxygen and biochemical oxygen demand (BOD) should be selected.

2.2.1 Biochemical oxygen demand (BOD)

In the analysis of water quality, one of the important factors that is indicative of the quality of water is the quantity of dissolved oxygen (DO), but with the wastewater the quantity of oxygen that the microorganisms used in the decomposition of organic matter biochemical oxygen demand (BOD), must be taken into account as the BOD is very useful to apply the water treatment system and water quality control.

BOD is the amount of oxygen that microorganisms use to decompose organic substances achieved by the difference of the amount of dissolved oxygen or dissolved oxygen (DO) before and after incubation in a closed container. BOD will be an indication of contamination of water used to make and can be used as input for the treatment of water.

2.2.2 The importance of the BOD

1. Used to control the contamination of water sources to determine how much organic matter should be removed so the oxygen arrives at the required level.
2. Check the quality of wastewater.
3. The design of wastewater treatment.
4. Evaluate the ability of water to get rid of the dirt by natural sources.

2.2.3 Calculation of BOD

Determination of the BOD, the most common is called Dilution BOD, which is the standard method of EPA.

1. Water samples were analyzed and then adjust the temperature of about 20 degrees Celsius.
2. Fill the air with oxygen saturation (about 5 - 10 minutes).
3. Fill the sample water into the BOD bottle fully for at least 3 bottles. Be careful not to have an air bubbles in the bottle, then close stopper tightly,

and then finds the DO for one bottle, and incubated 2 bottles at 20 ° C for 5 days.

4. After 5 days, then take a water sample that was incubated for dissolved oxygen is left.
5. Calculation BOD = D1 - D2

   D1 = Dissolved oxygen measured in days. (mg/l)

   D2 = Dissolved oxygen was measured on day 5 (mg/l).

Water is a little dirty, when BOD is less than 7 mg/l

Wastewater, when BOD is more than 7 mg/l

Wastewater treatment is the removal or destruction of contaminants in the waste water to the required standard which does not cause pollution to the environment. Wastewater from different sources have different properties, so there are many ways for water treatment process.

2.2.4 Reaeration in open-channel flow

Reaeration, the physical absorption of oxygen from the atmosphere, is the primary process by which a stream replaces oxygen consumed in the biodegradation of organic wastes. The reaeration process in a stream is characterized by its surface reaeration coefficient. Hence, knowledge of the reaeration coefficient permits determination of the quantity of waste that can be discharged into a stream without causing serious depletion of the dissolved-oxygen content of the stream. The three basic methods for measuring the reaeration coefficient are the dissolved-oxygen balance, disturbed-equilibrium, and tracer procedures. The dissolved-oxygen balance method consists of measuring the various sources and sinks of dissolved oxygen and determining by difference the amount of reaeration needed to balance the equation. The disturbedequilibrium method consists of artificially producing dissolvedoxygen deficits by adding sodium sulfite to the stream and subsequently measuring upstream and downstream concentrations of dissolved oxygen at two different concentration levels. The tracer method consists of using an inert radioactive gas as a tracer for oxygen and correlating the rate of desorption of the tracer gas with the rate of absorption of oxygen. Various theoretical models of the oxygen-absorption process exist; however, these models are generally not suited for prediction of the reaeration coefficient in streams because the model parameters have not been adequately related to bulkflow hydraulic variables. Semiempirical and empirical equations developed from experimental data adequately predict reaeration coefficients for streams of the type on which the equations were based, but large errors may occur when the equations are applied to other types of streams or to conditions outside the range of variables considered in the original correlation. INTRODUCTION Rivers and streams are used for the disposal of municipal and industrial wastes, and Hull (1963) suggested that this use is one of the most important factors contributing to the general health and welfare of the people of the United States. Discharge of wastes into a stream, however, does not simply dilute the wastes. Each stream and river has a natural capacity for oxidizing biodegradable wastes, thus purifying the waters. This purification capacity is dependent upon many factors, including the water discharge, the depth of flow, the velocity of flow, and the various sources and sinks of dissolved oxygen along the stream. The natural purification capacity of a stream therefore will vary as the hydraulic conditions in the stream change with time. Although the flow in a specific stream may have varied greatly from day to day and from year to year, the total annual runoff for the United States as a whole showed only a small, apparently cyclic, variation with time for the years 1895 to 1955 (Leopold and Langbein, 1960). On the other hand, the population and the number of industrial facilities have increased tremendously, and this growth has placed an ever increasing burden on the rivers and streams of the United States. In many instances, the purification capacities of streams and rivers have been exceeded. The fact that municipal and industrial wastes are discharged into a stream does not necessarily mean that the stream is polluted, because the stream does have the capacity for self-purification. The definition of pollution has received considerable attention. The Colorado Supreme Court in 1934 (Gindler, 1967, p. 5) defined pollution as follows: For the purpose of this case, the word "pollution" means an impairment, with attendant injury, to the use of water that the plaintiffs are entitled to make. Unless the introduction of extraneous matter so unfavorably affects such use, the condition is short of pollution. In reality, the thing forbidden is injury. The quantity introduced is immaterial. Other definitions were discussed by Haney (1966), and he proposed (p. 110) that "pollution is the impairment of water quality, with resultant significant interference with beneficial water use." Apparently, from these definitions, the determination of when pollution exists depends both on the intended use of the stream and on some water quality parameter that will insure that the water is of a quality adequate for the intended purpose. Of the various indicators of water quality (such as the coliform bacteria count, the hydrogen ion concentration, and the concentrations of phosphates, nitrates, synthetic organics, and industrial chemicals), the one most often used as a measure of pollution by biodegradable organic wastes is DO (dissolved oxygen) concentration (Wolman, REAERATION IN OPEN-CHANNEL FLOW 1960). This report uses DO concentration as the principal measure of water quality. Thus the condition of a stream is determined from a DO balance which includes all the sources and sinks of DO along the reach of interest. The various types of DO balances for streams and rivers that have appeared in the literature are discussed in the following paragraphs [22].

Table 2.2 Typical values of the first-order decay rate, k , and the temperature correction factor, θ, for some constituents [23].

Constituent	**Rate constant**		**Units**
Total coliform bacteria (freshwater)	1.0-5.5	-a	l/day
Total coliform bacteria (sediments)	0.14-0.21	-a	l/day
Total coliform bacteria (seawater)	0.7-3.0	-a	l/day
fecal coliform bacteria (seawater)	37-110	-a	l/day
BOD (no treatment)	0.3-0.4	-a	l/day
BOD (activated sludge treatment)	0.05-0.1	-a	l/day
carbofuran	0.03	-b	l/day
DDT	0.0-0.007	-b	l/day
PCB	0.0-0.007	-b	l/day
Pentachlorophenol	0.0-33.6	-b	l/day
Constituent	θ		Units
coliform bacteria (freshwater)	1.07	-b	-----
coliform bacteria (saltwater)	1.10	-b	-----
BOD	1.04	-a	-----
a-Thomann and Mueller (1987)	b- Schnoor(1996)		

Table 2.3 Some equations for defining the reaeraction rate constant, k_r (1/day) [23].

units

Watwer and wind velocity (m / day)   water deep (m)

k_r = Mass transport coefficient for reacration(m/day) / (water depth)

= $5.026\ (\text{water velocity})^{0.969} / (\text{water depth})^{1.673}$ (Churchill,1962)

= $3.95\ (\text{water velocity})^{0.5} / (\text{water depth})^{1.5}$ (O'Connor and Dabbien,1958)

= $3.95\ (\text{water velocity})^{0.5} / (\text{water depth})^{1.5}$

= $5.344\ (\text{water velocity})^{0.670} / (\text{water depth})^{1.85}$ (Owens, Edwards, Gibb, 1964 ,1962)

= $5.13\ (\text{water velocity}) / (\text{water depth})^{1.333}$ Langbien, Durum,1967)

= $\{0.065\ (\text{wind velocity})^2 + 3.86[(\text{water velocity})/(\text{water depth})]^{0.5}\}/(\text{water depth})$
(van Pagee 1978, Deivigne 1980)

Table 2.4 Typical values of parameters used in the dissolved oxygen models. [23].

Parameter	value		units
k_r , slow, deep rivers	0.1-0.4	-a	l/day
k_r , typical conditions	0.4-1.5	-a	l/day
k_r , swift, deep rivers	1.5-4.0	-a	l/day
k_r , swift, shallow rivers	4.0-10.0	-a	l/day
k_{CBOD} , untreated discharges	0.35 (0.20-0.50)	-b	l/day
k_{CBOD} , primary treatment	0.20 (0.10-0.30)	-b	l/day
k_{CBOD} , activateed sludge	0.075 (0.05-0.10)	-b	l/day
θ_{CBOD}	1.04	-a	----
	1.047	-a	----
	1.04 (1.02-1.09)	-c	----
θ_r	1.024 (1.005-1.030)	-c	----

Sediment oxygen demand*	value		units
Municipal sludge(outfall vicinity)	4 (2-10)	-cd	$gO_2/m^2/day$
Municipal sewage sludge	1.5 (1-2)	-cd	$gO_2/m^2/day$
Sandy bottom	0.5 (0.2-10)	-cd	$gO_2/m^2/day$
Mineral soils	0.07 (0.05-0.1)	-cd	$gO_2/m^2/day$
Natural to low pollution	0.1-10.00	-a	$gO_2/m^2/day$
Moderate to heavy pollution	5-10	-a	$gO_2/m^2/day$

a-Schnoor(1996) c-Thomann and Mueller (1987)

b-Chapra (1997) d-Bowie et al.(1985)

*value has to be divided by the water height(m)

2.3 Water Quality Modeling and Prediction

Water quality management is a critical component of overall integrated water resources management. Most users of water depend on adequate levels of water quality. When these levels are not met, water users must then either pay for water treatment or incur increased risks of using lower quality water. As populations and economies grow, more wastewater pollutants are generated. Many of these are discharged into surface and ground water bodies. Increasingly the major efforts and costs involved in water management are aimed at water quality protection and management. Conflicts among various users of water are increasingly over issues involving water quality. Natural water bodies are able to serve many uses. One of them is the transport and assimilation of many waterborne wastes. As natural water bodies transport and assimilate wastes, their quality changes. If the quality of water drops to the extent that other uses are adversely impacted, the assimilative capacities of those water bodies have been exceeded with respect to those impacted uses. Water management measures are actions taken to ensure that the total pollutant loads discharged into receiving water bodies do not exceed the waste assimilative capacity of those water bodies and that the quality meets the quality standards set for those waters. What uses depend on water quality? Almost all one can identify. As everyone knows, all living organisms require water of sufficient quantity and quality to survive. Different aquatic species can tolerate different levels of pollutant concentrations that impact water quality. In much of the developed world it is no longer ‘‘safe’’ to drink natural surface or ground waters. Treatment is usually required before these waters are safe for humans to drink. Treatment is not a practical option for improving the quality of water found in nature yet this is the water that impacts the health of fish and shellfish and other organisms in natural aquatic ecosystems. Hence the focus in practice is on the use of wastewater treatment facilities to improve the quality of effluents being discharged into natural water bodies. Standards specifying minimum acceptable levels of quality are commonly set for most ambient waters. Various uses may have their own quality requirements as well. Irrigation water must not be too saline nor contain toxic substances that can be absorbed by the plants or destroy the microorganisms in the soil. Water quality standards for industry can be very demanding, depending on course of the requirements of particular industrial processes. Domestic wasteloads can contain high concentrations of bacteria, viruses, and other organisms that impact human health. High organic loadings can reduce dissolved oxygen (DO) to levels that can kill parts of the aquatic ecosystem and cause obnoxious odors. Nutrient loadings from both urban and agricultural land runoffs can cause excessive algae growth that in turn may degrade the water aesthetically, inhibit boating and swimming, and upon death cause low DO levels. Toxic heavy metals and other micropollutants can accumulate in the bodies of aquatic organisms, including fish, making them unfit for human consumption even if they themselves survive. Pollutant discharges originate from point to non-point sources. A common approach to controlling point source discharges, such as from stormwater outfalls, municipal wastewater treatment plants or industries, is to impose standards specifying maximum allowable pollutant loads or concentrations in their effluents. This is often done in ways that are not economically efficient or even environmentally effective. Effluent standards typically do not take into account the particular assimilative capacities of the receiving water body. Nevertheless, they are relatively easy to monitor and control. Non-point sources such as agricultural runoff or atmospheric deposition are not as easily controlled and hence it is difficult to apply effluent standards to non-point source pollutants. Pollutant loadings from non-point sources can be much higher than point source loadings. Management of non-point water quality impacts requires a more ambient-focused water quality management program. The goal of an ambient water quality management program is to establish appropriate standards for water quality in water bodies receiving pollutant loads and then to ensure that these standards are met. Realistic standard setting takes into account the basin's hydrologic, ecological, and land use conditions, the potential uses of the receiving water bodies, and the institutional capacity to set and enforce water quality standards. Ambient-based water quality prediction and management involves considerable uncertainty. No one can predict what pollutant loadings will be in the future, especially from area-wide non-point sources. In addition to uncertainties inherent in measuring water quality, there are uncertainties in models used to predict the effectiveness of actions taken to meet water quality standards. The models available to help managers predict water quality impacts are relatively simple compared to the complexities of actual water systems. If water quality models are being used to inform those setting standards and permissible waste loadings, these limitations and uncertainties should be understood and addressed.

2.3.1 Models of Water Quality Processes

Water quality models can be applied to many different types of water systems including streams, rivers, lakes, reservoirs, estuaries, coastal waters, and oceans. The models describe the main water quality processes and typically require the hydrologic and constituent inputs (the water flows or volumes and the pollutant loadings). These models include terms for dispersive and/or advective transport depending on the hydrologic and hydrodynamic characteristics of the water body, and terms for the biological, chemical and physical reactions among constituents. Adjective transport dominates in flowing rivers. Dispersion is the predominant transport phenomenon in estuaries subject to tidal action. Lake water quality prediction is complicated by the influence of random wind directions and velocities that often affect surface mixing, currents, and stratification. For this and other reasons, obtaining reliable lake quality predictions is often more difficult than for streams, rivers, and estuaries. In coastal waters and oceans, larges scale flow patterns and tides are the most important transport mechanisms.

As with water quantity modeling, the development and application of water quality models is both a science as well as an art. Each model reflects the creativity of its developer, the particular water quality management problems and issues being addressed, the available data for model parameter calibration and verification, and the time available for modeling and associated uncertainty and other analyses.
The fact that most, if not all, water quality models cannot accurately predict what actually happens does not necessarily detract from their value. Even relatively simple models can help managers understand the real-world prototype and estimate at least the relative if not actual change in water quality associated with given changes in the inputs resulting from water and land management policies or practices.

2.3.2 Mass Transport by Advection and Dispersion

Taking the asymptotic limit $\Delta t \to 0$ and $\Delta x \to 0$, the advection–diffusion equation for one dimension results

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(vC) \tag{2.1}$$

By adding terms for transport in the *y* and *z*-direction a three-dimensional model is obtained. Taking the asymptotic limit again will lead to a three-dimensional advection– diffusion equation. Here dispersion is much more important than advective transport and the concentration profile approaches a symmetric distribution, as shown in Figure.2.1 about the point of discharge at $x = 0$.

Water quality management models are often used to assess the effect of pollutant loadings on ambient waters and to compare the results with specific water quality standards. The above steady state equations can be used to construct such a model for estimating the wastewater removal efficiencies required at each wastewater discharge site that will result in an ambient stream quality that meets the standards along a stream or river [23].

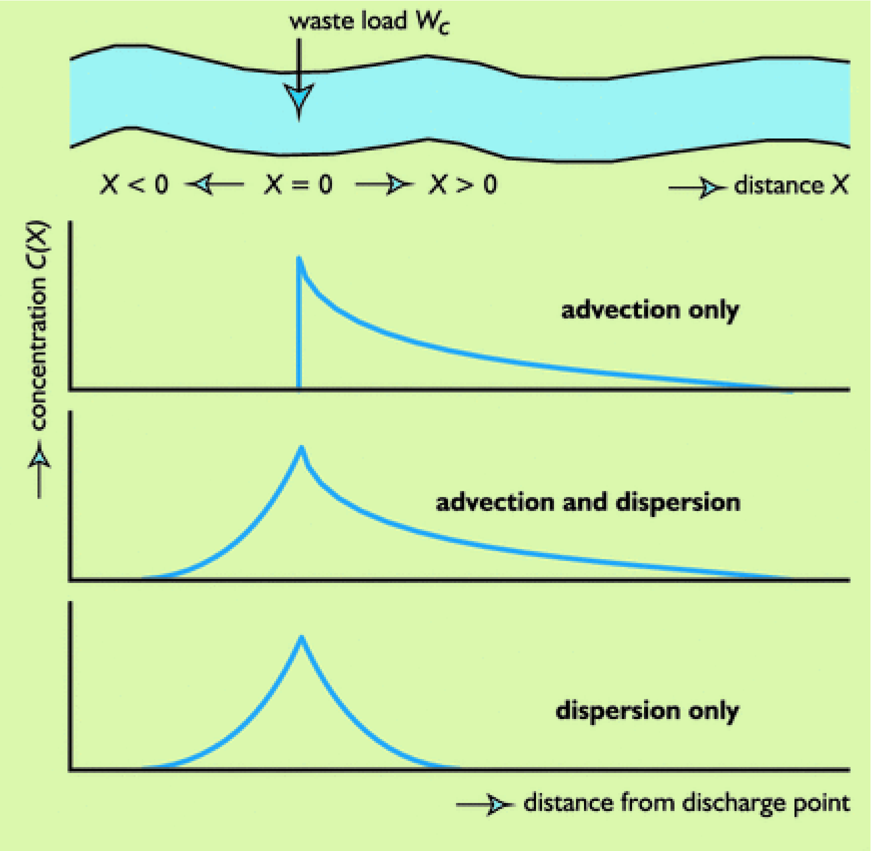


Figure 2.1 Constituent concentration distributions along a river or estuary resulting from a constant discharge of that constituent at a single point source in that river or estuary [23]

2.4 One-dimensional advection-diffusion equation (ADE)

We consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one - dimensional advection-diffusion equation (ADRE)

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}=D\frac{\partial^2 c}{\partial x^2},\ \ 0<x<L, 0<t\leq T, \tag{2.2}$$

with initial conditions

$$c(x,0)=f(x),\ \ \ 0\leq x\leq L, \tag{2.3}$$

and boundary conditions

$$c(0,\mathrm{t})=g(t),\ \ \ 0\leq t\leq T, \tag{2.4}$$

$$\left.\frac{\partial c}{\partial x}\right|_{x=L} = h(\mathrm{t}), \quad 0 \le t \le T, \tag{2.5}$$

where x is the longitudinal distance along the stream, t is time, T is the last time, $f(x), g(t)$ and $h(x)$ are known functions, while $c(x,t)$ is the concentration averaged in depth at the point x and at time t, the function c is unknown, $u(x,t)$ is the velocity of the water in the x direction for all $x \in [0,1]$ at time t, D is the dispersion coefficient and K is the mass decay rate. We will consider the model with the following conditions, that $u(x,t)$ and D are positive constant values. The initial conditions $c(x,0) = f(x)$ at $t = 0$ for all $x > 0$. The boundary conditions are $c(0,\mathrm{t}) = g(t)$ at $x = 0$ and $\partial c / \partial x = 0$ at $x = 1$.

2.5 Saulyev medthod for one-dimentional advection-diffusion equation (there is no reaction term)

The solution domain of the problem is covered by a mesh of grid-lines. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0,1,2,\ldots,M$ and $t_n = n\Delta t$ for all $n = 0,1,2,\ldots,N$ in which M and N are positive integers, where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid-spacing are $\Delta x = \dfrac{L}{M}$ and $\Delta t = \dfrac{T}{N}$.

Consider the following approximations of the derivative in the advection – diffusion equation which incorporate time weights θ as follows

$$\frac{\partial c}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{2.6}$$

$$u\frac{\partial c}{\partial x} = u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right], \tag{2.7}$$

$$D\frac{\partial^2 c}{\partial x^2} = D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] + D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i-1}^n - 2c_i^n + c_{i+1}^n\right], \tag{2.8}$$

where θ is the weighting factor. Substituting the Equation (2.6) – (2.8) into the Equation (1).

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right]$$

$$= D\left(\frac{\theta}{\left(\Delta x\right)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^{n} - c_i^{n}\right] + D\left(\frac{\left(1-\theta\right)}{\left(\Delta x\right)^2}\right)\left[c_{i-1}^{n} - 2c_i^{n} + c_{i+1}^{n}\right], \tag{2.9}$$

$$\frac{c_i^{n+1}}{\Delta t} - \frac{c_i^{n}}{\Delta t} + \frac{u_i^{n+1}c_i^{n+1}}{2\Delta x} - \frac{u_i^{n+1}c_{i-1}^{n+1}}{2\Delta x} + \frac{u_i^{n+1}c_{i+1}^{n}}{2\Delta x} - \frac{u_i^{n+1}c_i^{n}}{2\Delta x}$$

$$= \frac{\theta Dc_{i-1}^{n+1}}{\left(\Delta x\right)^2} - \frac{\theta Dc_i^{n+1}}{\left(\Delta x\right)^2} + \frac{\theta Dc_{i+1}^{n}}{\left(\Delta x\right)^2} - \frac{\theta Dc_i^{n}}{\left(\Delta x\right)^2} + \frac{\left(1-\theta\right)Dc_{i-1}^{n}}{\left(\Delta x\right)^2} - \frac{2\left(1-\theta\right)Dc_i^{n}}{\left(\Delta x\right)^2} + \frac{\left(1-\theta\right)Dc_{i+1}^{n}}{\left(\Delta x\right)^2}$$

$$\frac{c_i^{n+1}}{\Delta t} + \frac{u_i^{n+1}c_i^{n+1}}{2\Delta x} + \frac{\theta Dc_i^{n+1}}{\left(\Delta x\right)^2} - \frac{u_i^{n+1}c_{i-1}^{n+1}}{2\Delta x} - \frac{\theta Dc_{i-1}^{n+1}}{\left(\Delta x\right)^2} = \frac{c_i^{n}}{\Delta t} + \frac{u_i^{n+1}c_i^{n}}{2\Delta x} - \frac{\theta Dc_i^{n}}{\left(\Delta x\right)^2} - \frac{2\left(1-\theta\right)Dc_i^{n}}{\left(\Delta x\right)^2}$$

$$+ \frac{\theta Dc_{i+1}^{n}}{\left(\Delta x\right)^2} + \frac{\left(1-\theta\right)Dc_{i+1}^{n}}{\left(\Delta x\right)^2} - \frac{u_i^{n+1}c_{i+1}^{n}}{2\Delta x}, \tag{2.10}$$

$$\left(\frac{1}{\Delta t} + \frac{U_1^{n+1}}{2\Delta x} + \frac{\theta D}{\left(\Delta x\right)^2}\right)c_i^{n+1} - \left(\frac{u_i^{n+1}}{2\Delta x} + \frac{\theta D}{\left(\Delta x\right)^2}\right)c_{i-1}^{n+1}$$

$$= \left(\frac{D}{\left(\Delta x\right)^2} - \frac{\theta D}{\left(\Delta x\right)^2}\right)c_{i-1}^{n} + \left(\frac{1}{\Delta t} + \frac{u_i^{n+1}}{2\Delta x} - \frac{\theta D}{\left(\Delta x\right)^2} - \frac{2D}{\left(\Delta x\right)^2} + \frac{2\theta D}{\left(\Delta x\right)^2}\right)c_i^{n}$$

$$+ \left(\frac{\theta D}{\left(\Delta x\right)^2} + \frac{D}{\left(\Delta x\right)^2} - \frac{\theta D}{\left(\Delta x\right)^2} - \frac{U_i^{n+1}}{2\Delta x}\right)c_{i+1}^{n}, \tag{2.11}$$

$$\left(\frac{\Delta t}{\Delta t} + \frac{U_1^{n+1}\Delta t}{2\Delta x} + \frac{\theta D\Delta t}{\left(\Delta x\right)^2}\right)c_i^{n+1} - \left(\frac{u_i^{n+1}\Delta t}{2\Delta x} + \frac{\theta D\Delta t}{\left(\Delta x\right)^2}\right)c_{i-1}^{n+1}$$

$$= \left(\frac{D\Delta t}{\left(\Delta x\right)^2} - \frac{\theta D\Delta t}{\left(\Delta x\right)^2}\right)c_{i-1}^{n} + \left(\frac{\Delta t}{\Delta t} + \frac{u_i^{n+1}\Delta t}{2\Delta x} - \frac{\theta D\Delta t}{\left(\Delta x\right)^2} - \frac{2D\Delta t}{\left(\Delta x\right)^2} + \frac{2\theta D\Delta t}{\left(\Delta x\right)^2}\right)c_i^{n}$$

$$+ \left(\frac{\theta D\Delta t}{\left(\Delta x\right)^2} + \frac{D\Delta t}{\left(\Delta x\right)^2} - \frac{\theta D\Delta t}{\left(\Delta x\right)^2} - \frac{U_i^{n+1}\Delta t}{2\Delta x}\right)c_{i+1}^{n}. \tag{2.12}$$

for $1 \le i \le M-1$ and $1 \le n \le N-1$. Letting that $Cr = \dfrac{u\Delta t}{\Delta x}$ is Courant number for one dimentional case $Cr = \dfrac{u\Delta t}{\Delta x} \le c_{\max}$, where the dimentionless number is call the count number, u is the velocity (whose dimension is length/time), Δt is the time step (whose dimension is time), Δx is the length(whose dimension is length). The value of $c_{\max}$ changes with the method used to solve the discretized equation. If an explicit (time-marching) solver is used the typically $c_{\max} = 1$. Letting that $Pe = \dfrac{u\Delta x}{D}$ is Peclet number, D is the dispersion coefficient (the mass diffustion coefficient). The Peclet number is a dimentionless number relevant in the study of transport phenomena in fluid flows. It is defined to be the ratio of the rate of advection of a physical quantity. We can see that $\dfrac{Cr}{Pe} = \dfrac{U\Delta t}{\Delta x}\dfrac{D}{U\Delta x} = \dfrac{D\Delta t}{(\Delta x)^2}$. The Eq(2.12) becomes,

$$\left[1+\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]c_i^{n+1} - \left[\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1}$$

$$=\left(\frac{Cr}{Pe}-\theta\left(\frac{Cr}{Pe}\right)\right)c_{i-1}^{n} + \left[1+\frac{Cr}{2}-2\left(\frac{Cr}{Pe}\right)+\theta\left(\frac{cr}{Pe}\right)\right]c_i^n + \left[\frac{Cr}{Pe}-\frac{Cr}{2}\right]c_{i+1}^{n}. \tag{2.13}$$

Although the Equation (2.8) does not seem explicit, because c_{i-1}^{n+1} and c_i^{n+1} are on the left-hand side, a suitable use of the equation makes it explicit. Therefore, Equation (2.12) can be written in the following form

$$c_i^{n+1} = \left\{\left[\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1} + \left[\frac{Cr}{Pe}-\theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n} + \left[1+\frac{Cr}{2}-2\left(\frac{Cr}{Pe}\right)+\theta\left(\frac{cr}{Pe}\right)\right]c_i^{n}\right.$$

$$\left. + \left[\frac{Cr}{Pe}-\frac{Cr}{2}\right]c_{i+1}^{n}\right\} \Big/ \left[1+\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]. \tag{2.14}$$

This scheme is explicit. In this case, only a single value, c_i^{n+1} will be unknown. This scheme is known as Saulyev's formula and the main advantage of it is that it is unconditionally stable and explicit [10].

Chapter 3

Saulyev Explicit Scheme for a One-Dimensional Advection-Diffusion-Reaction Equation in a Uniform Flow Stream

The one-dimensional advection-diffusion-reaction equation is a mathematical model describing the transport and diffusion of pollutants and suspended matter in a river. If the flow of the river is non-uniform the model cannot be theoretically manipulated, therefore numerical special techniques are required. The objective of this research is to propose a simpler advection-diffusion-reaction technique, which is an unconditionally stable scheme of Soulyev. It is the large or small of time step and/or grid size can be employed in this techniques. Examples are calculated for three of weighted parameter θ. The case of $\theta = 0$ gives a smooth solution comparing to the another values of θ's. Increasing the mass decay rate affects the maximum concentration level. The numerical experiments have shown the expectable results.

3.1 The one-dimentional advection-diffusion-reaction equation(ADRE)

In this section, we consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one- dimensional advection-diffusion – reaction equation (ADRE),

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} - KC,\ 0 < x < L, 0 < t \le T, \tag{3.1}$$

with initial conditions,

$$c(x,0) = f(x),\quad 0 \le x \le L, \tag{3.2}$$

and boundary conditions,

$$c(0,\mathrm{t}) = g(t),\quad 0 \le t \le T, \tag{3.3}$$

$$\left.\frac{\partial c}{\partial x}\right|_{x=L} = h(\mathrm{t}),\quad 0 \le t \le T, \tag{3.4}$$

where x is the longitudinal distance along the stream, t is time, T is the stationary time, $f(x), g(t)$ and $h(x)$ are known functions, while $c(x,t)$ is the concentration averaged in depth at the point x and at time t, the function c is unknown, $u(x,t)$ is the velocity of the water in the x direction for all $x \in [0,1]$ at time t, D is the dispersion coefficient and K is the mass decay rate. We will consider the model with the following conditions, that $u(x,t)$ and D are positive constant values. The initial conditions $c(x,0) = f(x)$ at $t = 0$ for all $x > 0$. The boundary conditions are $c(0,\mathrm{t}) = g(t)$ at $x = 0$ and $\frac{\partial c}{\partial x} = 0$ at $x = 1$.

3.2 Saulyev explicit scheme for one-dimentional advection-diffusion-reaction equation

The solution domain of the problem is covered by a mesh of grid-lines. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0,1,2,...,M$ and $t_n = n\Delta t$ for all $n = 0,1,2,...,N$ in which M and N are positive integers, where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid-spacing are $\Delta x = \frac{L}{M}$ and $\Delta t = \frac{T}{N}$.

Consider the following approximations of the derivative in the advection – diffusion equation which incorporate time weights θ as follows

$$\frac{\partial c}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{3.5}$$

$$u\frac{\partial c}{\partial x} = u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right], \tag{3.6}$$

$$D\frac{\partial^2 c}{\partial x^2} = D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] + D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i-1}^n - 2c_i^n + c_{i+1}^n\right], \tag{3.7}$$

where θ is the weighting factor. Substituting the Equation (3.5) – (3.7) into the Equation (3.1).

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right]$$

$$= D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] + D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i-1}^n - 2c_i^n + c_{i+1}^n\right] - Kc_i^n,$$

$$\frac{c_i^{n+1}}{\Delta t}-\frac{c_i^n}{\Delta t}+\frac{u_i^{n+1}c_i^{n+1}}{2\Delta x}-\frac{u_i^{n+1}c_{i-1}^{n+1}}{2\Delta x}+\frac{u_i^{n+1}c_{i+1}^n}{2\Delta x}-\frac{u_i^{n+1}c_i^n}{2\Delta x}$$

$$=\frac{\theta Dc_{i-1}^{n+1}}{(\Delta x)^2}-\frac{\theta Dc_i^{n+1}}{(\Delta x)^2}+\frac{\theta Dc_{i+1}^n}{(\Delta x)^2}-\frac{\theta Dc_i^n}{(\Delta x)^2}+\frac{(1-\theta)Dc_{i-1}^n}{(\Delta x)^2}-\frac{2(1-\theta)Dc_i^n}{(\Delta x)^2}+\frac{(1-\theta)Dc_{i+1}^n}{(\Delta x)^2}-Kc_i^n,$$

$$\frac{c_i^{n+1}}{\Delta t}+\frac{u_i^{n+1}c_i^{n+1}}{2\Delta x}+\frac{\theta Dc_i^{n+1}}{(\Delta x)^2}-\frac{u_i^{n+1}c_{i-1}^{n+1}}{2\Delta x}-\frac{\theta Dc_{i-1}^{n+1}}{(\Delta x)^2}$$

$$=\frac{c_i^n}{\Delta t}+\frac{u_i^{n+1}c_i^n}{2\Delta x}-\frac{\theta Dc_i^n}{(\Delta x)^2}-\frac{2(1-\theta)Dc_i^n}{(\Delta x)^2}-Kc_i^n+\frac{\theta Dc_{i+1}^n}{(\Delta x)^2}+\frac{(1-\theta)Dc_{i+1}^n}{(\Delta x)^2}-\frac{u_i^{n+1}c_{i+1}^n}{2\Delta x},$$

$$\left(\frac{1}{\Delta t}+\frac{U_1^{n+1}}{2\Delta x}+\frac{\theta D}{(\Delta x)^2}\right)c_i^{n+1}-\left(\frac{u_i^{n+1}}{2\Delta x}+\frac{\theta D}{(\Delta x)^2}\right)c_{i-1}^{n+1}$$

$$=\left(\frac{D}{(\Delta x)^2}-\frac{\theta D}{(\Delta x)^2}\right)c_{i-1}^n+\left(\frac{1}{\Delta t}+\frac{u_i^{n+1}}{2\Delta x}-\frac{\theta D}{(\Delta x)^2}-\frac{2D}{(\Delta x)^2}+\frac{2\theta D}{(\Delta x)^2}+K\right)c_i^n$$

$$+\left(\frac{\theta D}{(\Delta x)^2}+\frac{D}{(\Delta x)^2}-\frac{\theta D}{(\Delta x)^2}-\frac{U_i^{n+1}}{2\Delta x}\right)c_{i+1}^n.$$

We multiply equation by Δt

$$\left(\frac{\Delta t}{\Delta t}+\frac{U_1^{n+1}\Delta t}{2\Delta x}+\frac{\theta D\Delta t}{(\Delta x)^2}\right)c_i^{n+1}-\left(\frac{u_i^{n+1}\Delta t}{2\Delta x}+\frac{\theta D\Delta t}{(\Delta x)^2}\right)c_{i-1}^{n+1}$$

$$=\left(\frac{D\Delta t}{(\Delta x)^2}-\frac{\theta D\Delta t}{(\Delta x)^2}\right)c_{i-1}^n+\left(\frac{\Delta t}{\Delta t}+\frac{u_i^{n+1}\Delta t}{2\Delta x}-\frac{\theta D\Delta t}{(\Delta x)^2}-\frac{2D\Delta t}{(\Delta x)^2}+\frac{2\theta D\Delta t}{(\Delta x)^2}+K\Delta t\right)c_i^n$$

$$+\left(\frac{\theta D\Delta t}{(\Delta x)^2}+\frac{D\Delta t}{(\Delta x)^2}-\frac{\theta D\Delta t}{(\Delta x)^2}-\frac{U_i^{n+1}\Delta t}{2\Delta x}\right)c_{i+1}^n.$$

$$\left[1+\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]c_i^{n+1}-\left[\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1}$$

$$=\left(\frac{Cr}{Pe}-\theta\left(\frac{Cr}{Pe}\right)\right)c_{i-1}^{n}+\left[1+\frac{Cr}{2}-2\left(\frac{Cr}{Pe}\right)+\theta\left(\frac{cr}{Pe}\right)+K\Delta t\right]c_{i}^{n}+\left[\frac{Cr}{Pe}-\frac{Cr}{2}\right]c_{i+1}^{n} \tag{3.8}$$

for $1\le i\le M-1$ and $1\le n\le N-1$, where $Cr=\frac{u\Delta t}{\Delta x}$ is Courant number and $Pe=\frac{u\Delta x}{D}$ is Pelet number, and $\frac{C_r}{Pe}=\frac{U\Delta t}{\Delta x}\frac{D}{U\Delta x}=\frac{D\Delta t}{(\Delta x)^2}$.

Although the Equation (3.8) does not seem explicit, because c_{i-1}^{n+1} and c_{i}^{n+1} are on the left-hand side, a suitable use of the equation makes it explicit. Therefore, Equation (8) can be written in the following form

$$c_{i}^{n+1}=\left\{\left[\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1}+\left[\frac{Cr}{Pe}-\theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n}+\left[1+\frac{Cr}{2}-2\left(\frac{Cr}{Pe}\right)+\theta\left(\frac{cr}{Pe}\right)+K\Delta t\right]c_{i}^{n}\right.$$

$$\left.+\left[\frac{Cr}{Pe}-\frac{Cr}{2}\right]c_{i+1}^{n}\right\}\Big/\left[1+\frac{Cr}{2}+\theta\left(\frac{Cr}{Pe}\right)\right]. \tag{3.9}$$

This scheme is explicit. In this case, only a single value, c_{i}^{n+1} will be unknown. This scheme is known as Saulyev's formula and the main advantage of it is that it is unconditionally stable and explicit [10].

3.3 Application to a stream water assessment problem

Example 3.1 Suppose that the measurement of pollutant concentration C in a non-uniform flow steam is aligned with longitudinal distance,1.0(km) total length and 1.0(m) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point is $C(0,t)=1-\sin(t)$ at $x=0$ for all $t>0$ and $C(x,0)=1-x$ at $t=0$.The approximation of pollutant concentrations c of all schemes is show in Tables 3.1.

$$\frac{\partial c}{\partial t}+(5.0)\frac{\partial c}{\partial x}=(0.01)\frac{(\partial^2 c)}{\partial^2 c}-(0.001)C, \quad 0<x<100,\ 0<t\le 25, \tag{3.10}$$

with initial conditions

$$c(x,0)=1-x,\ 0\le x\le 100 \tag{3.11}$$

with boundary conditions

$$c(0,t)=-1,\ 0<t\le 25 \tag{3.12}$$

$$c(1,t) = 1 - \sin(t),\ 0 < t \le 25 \tag{3.13}$$

where $u = 5.0\ m/s,\ D = 0.01\ m^2/\sec.$ K = 0.001.

We choose $\Delta x = 0.5,\ \Delta t = 0.1, T = 25,$ and $\theta = 0$ (explicit), where

x is the longitudinal distance along the stream,

t is time, T is the last time,

$f(x), g(t)$ and $h(x)$ are known functions,

$c(x,t)$ is the concentration averaged in depth at the point x and at time t, the function c is unknown,

$u(x,t)$ is the velocity of the water in the x direction for all $x \in [0,1]$ at time t

D is the dispersion coefficient and K is the mass decay rate.

We will consider the model with the following conditions, that $u(x,t)$ and D are positive constant values. The initial conditions $c(x,0) = f(x)$ at $t = 0$ for all $x > 0$. The boundary conditions are $c(0,\mathrm{t}) = g(t)$ at $x = 0$ and $\frac{\partial c}{\partial x} = -0.05$ at $x = 1$.

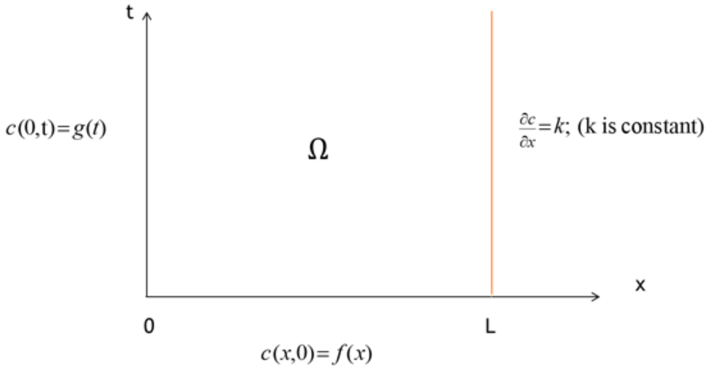


Figure 3.1 Domain diagram

We choose: $\Delta x = 0.5,\ \Delta t = 0.1, T = 25,$

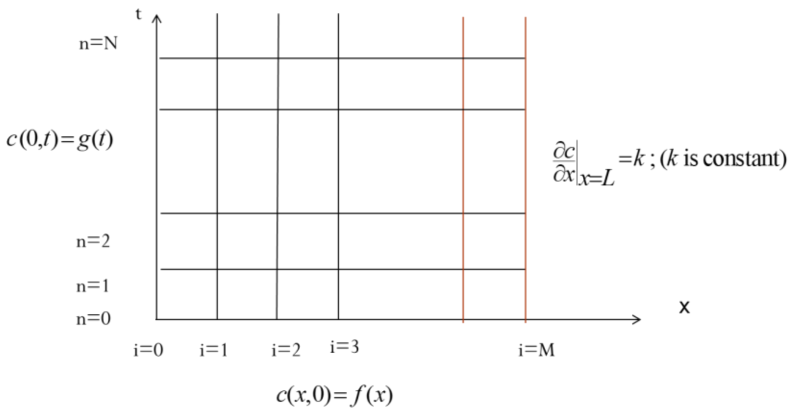


Figure 3.2 Grid spacing

Table 3.1 Pollutant Concentration $c(x,t)$ of example 1.

sec (t) \ x	0	20	40	60	80	100
0	1.0000	0.7000	0.6000	0.4000	2.2000	0.0000
5	1.9589	0.9518	0.8542	0.6532	0.4522	0.2412
10	1.5440	1.7488	0.0438	0.9088	0.7017	0.4949
15	0.3497	0.5615	0.3709	0.8501	0.9451	0.7513
20	0.0871	0.0136	1.5857	-0.0045	1.6836	0.8314
25	1.1324	0.7870	1.9610	0.6457	0.5296	2.0075

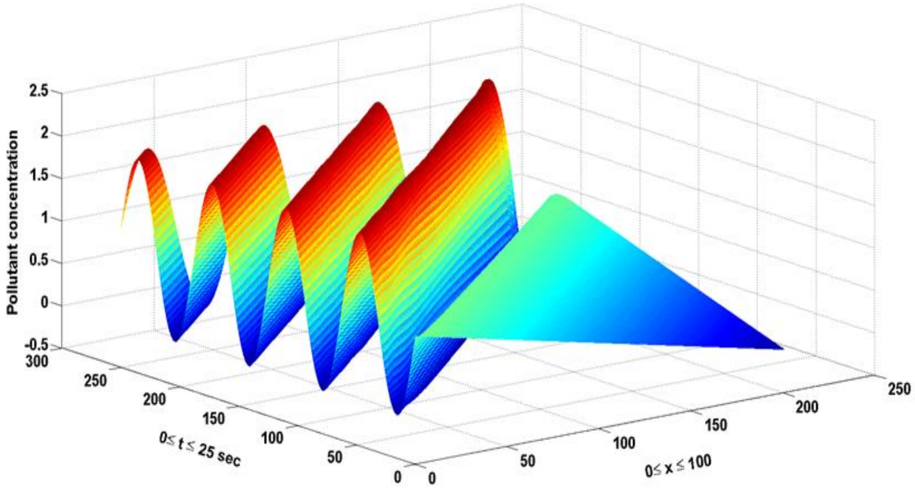


Figure 3.3 Pollutant Concentration $c(x,t)$

Example 3.2 Suppose that the measurement of pollutant concentration C in a non-uniform flow steam is aligned with longitudinal distance, 1.0 (km) total length and 1.0 (m) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharged point is $C(0,t)=2+\sin(t)$ at $x=0$ for all $t>0$. The potential pollutant concentration is described by $C(x,0)=2+x(1-x)$ at $t=0$. The approximation of pollutant concentrations C of 3 case are show in Tables 3.2, 3.3 and 3.4 repectively,

Simulation 1: There is no rate of change of pollutant concentration at $x=L$. These means that $\frac{\partial c}{\partial x}=0$, where $x=1$.

Simulation 2: If the rate of change of pollutant concentration at $x=L$ is increase. These can be assumed that $\frac{\partial c}{\partial x}=0.05$, where $x=1$.

Simulation 3: If the rate of change of pollutant concentration at $x = L$ is decrease. We can be assumed that $\frac{\partial c}{\partial x} = -0.05$, where $x = 1$.

Table 3.2 Pollutant Concentration $c(x,t)$ of Simulation 1.

sec (t) \ x	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2400	2.1600	2.0000
5	1.0411	2.8222	2.1687	2.2387	2.2588	2.1997
10	1.4560	1.7149	2.1427	2.1112	2.2332	2.2726
15	2.6503	1.0077	2.6532	2.1862	1.3591	2.2192
20	2.9129	1.7408	1.4384	3.0381	1.3591	2.2164
25	1.8676	2.8574	1.0617	2.3877	2.5125	1.0404

Table 3.3 Pollutant Concentration $c(x,t)$ of Simulation 2.

sec (t) \ x	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2500	2.1600	2.0000
5	1.0411	2.8222	2.1382	2.1985	2.2588	2.2122
10	1.4560	1.7149	2.9803	2.1546	2.2398	2.2852
15	2.6503	1.0077	2.6532	1.0615	2.0994	2.2318
20	2.9129	1.7408	1.4384	1.5235	1.3658	2.2290
25	1.8676	2.8574	1.0640	2.7136	2.5191	1.0530

Table 3.4 Pollutant Concentration $c(x,t)$ of Simulation 3.

sec (t) \ x	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2400	2.1630	2.0050
5	1.0411	2.8222	2.1382	2.2387	2.2588	2.2121
10	1.4560	1.7149	2.9803	2.1112	2.2266	2.2849
15	2.6503	1.0077	2.6532	2.1861	2.0859	2.2316
20	2.9129	1.7408	1.4384	3.0344	1.3524	2.2288
25	1.8676	2.8574	1.0594	2.3840	2.5060	1.0528

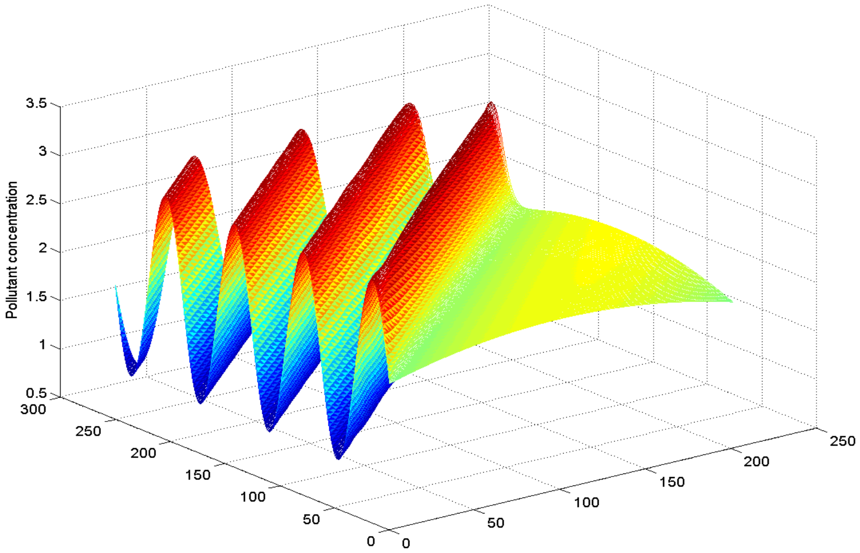


Figure 3.4 Pollutant Concentration $c(x,t)$ of Simulation 1

3.4 Discussion

The approximation of the pollutant concentrations of a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes is shown in Table 3.2, 3.3 and 3.4 and Figure 3.4. The numerical techniques are proposed for three θ values, 0, 0.5 and 1, respectively. The case of $\theta = 0$ gives a smooth solution compare to another values. Increasing the mass decaying rate affects the maximum concentration level.

Chapter 4

Numerical Simulation to a One-dimensional Water-quality Model in a Non-uniform Flow Stream using an Iterative Explicit Finite Difference Technique

The collected field data is not suitable to input in a mathematical model. The data is varied by time. The time-dependent distribution of discharged pollutant concentration and water flow velocity are required. It is complicated work if we input them into a computer implementation while a given function has simpler operation. The object of this research is to propose an interpolation technique to all of collected field data such as water pollutant concentration at released polluted water point and the water flow velocity along the considered water stream. The revision shows good agreement solutions. The proposed technique is suitable to be used in several real-world problems due to it easily to program and the straight forwardness of the implementation. According to field water-quality data, the data will be implemented to be a function of the boundary condition. The Lagrange interpolation technique is used to synthesis their boundary conditions as required. A simple advection-diffusion-reaction numerical simulation is proposed by using the Saulyev scheme. The proposed numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. We apply the method to two problems with different data for obtaining the right and left boundary conditions. The results of the model are show that the calculated results are reliable approximations.

4.1 One–dimensional water quality model

In this section, we consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one-dimensional advection-diffusion–reaction equation (ADRE),

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}=D\frac{\partial^2 c}{\partial x^2}-KC,\ 0<x<L, 0<t\le T. \tag{4.1}$$

Initial and Boundary conditions

Initial condition,

$$c(x,0)=f(x),\quad 0\le x\le L, \tag{4.2}$$

and boundary conditions,

$$c(0,\mathrm{t}) = g(\mathrm{t}), \quad 0 \le t \le T, \tag{4.3}$$

and
$$c(L,t) = h(\mathrm{t}), \quad 0 \le t \le T, \tag{4.4}$$

where x is the longitudinal distance along the stream, t is time, T is the stationary time, $f(x), g(t)$ and $h(t)$ are interpolated functions, while $c(x,t)$ is the concentration averaged in depth at the point x and at time t, $u(x,t)$ is the water flow velocity in the x-direction for all $x \in [0,L]$ at time t, D is the dispersion coefficient and K is the mass decay rate.

4.2 Saulyev method with quadratic interpolation for one-dimensional water quality model

4.2.1 Sualyev explicit scheme

The solution domain of the problem is covered by a mesh of grid-lines. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0,1,2,\ldots,M$ and $t_n = n\Delta t$ for all $n = 0,1,2,\ldots,N$ in which M and N are positive integers, where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid-spacing are $\Delta x = \dfrac{L}{M}$ and $\Delta t = \dfrac{T}{N}$.

Consider the following approximations of the derivative in the advection–diffusion equation which incorporate time weights θ as follows [10],

$$\frac{\partial c}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{4.5}$$

$$u\frac{\partial c}{\partial x} = u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right], \tag{4.6}$$

$$D\frac{\partial^2 c}{\partial x^2} = D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] + D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i+1}^n - 2c_i^n + c_{i+1}^n\right], \tag{4.7}$$

where θ is the weighting factor. Substituting Eq. (4.5) – (4.7) into Eq. (4.1), we get [10]

$$\begin{aligned}&\left[1 + \frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_i^{n+1} - \left[\frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1} \\ &= \left(\frac{Cr}{Pe} - \theta\left(\frac{Cr}{Pe}\right)\right)c_{i-1}^n + \left[1 + \frac{Cr}{2} - 2\left(\frac{Cr}{Pe}\right) + \theta\left(\frac{cr}{Pe}\right) + K\Delta t\right]c_i^n + \left[\frac{Cr}{Pe} - \frac{Cr}{2}\right]c_{i+1}^n\end{aligned} \tag{4.8}$$

for $1 \le i \le M-1$ and $1 \le n \le N-1$, where $Cr = \frac{u\Delta t}{\Delta x}$ is Courant number and $Pe = \frac{u\Delta x}{D}$ is Peclet number.

Although Eq. (4.8) does not seem explicit, because c_{i-1}^{n+1} and c_i^{n+1} are on the left-hand side, a suitable use of the equation makes it explicit. Therefore, Eq. (4.8) can be written in the following form

$$c_i^{n+1} = \frac{1}{\left[1 + \frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]} \left\{ \left[\frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right] c_{i-1}^{n+1} \right.$$

$$\left. + \left[\frac{Cr}{Pe} - \theta\left(\frac{Cr}{Pe}\right)\right] c_{i-1}^{n} + \left[1 + \frac{Cr}{2} - 2\left(\frac{Cr}{Pe}\right) + \theta\left(\frac{cr}{Pe}\right) + K\Delta t\right] c_i^n + \left[\frac{Cr}{Pe} - \frac{Cr}{2}\right] c_{i+1}^n \right\}. \tag{4.9}$$

For the advection term, we apply the scheme either $u > 0$ or $u < 0$. Thus the scheme is restricted to single-direction velocity fields, c is being transported from left to right by the flow, so the Saulyev scheme is the appropriate choice for discretizing the advective term. In Eq. (4.9), the term at time level $n+1$, c_{i-1}^{n+1} has already been computed at spatial point $i-1$ by marching in the direction of increasing i. This scheme is an explicit finite difference method. In this case, only a single value, c_i^{n+1} will be unknown. This scheme is known as Saulyev's formula and the main advantage of it is that it is unconditionally stable and explicit [10].

4.2.2 Quadratic interpolation for the initial and boundary conditions

Theorem 4.1 (Weierstrass Approximation Theorem,[15]) Suppose that f is defined and continuous on $[a,b]$. For each $\varepsilon > 0$, there exists a polynomial $P(x)$, with the property that $|f(x) - P(x)| < \varepsilon$, for all x in $[a,b]$.

The Taylor polynomials agree as closely as possible with a given function at a specific point, but they concentrate their accuracy near that point. A good interpolation polynomial needs to provide a relatively accurate approximation over an entire interval, and Taylor polynomials do not generally do this. The Taylor Polynomials are [15]

$$P_n(x) = \sum_{k=0}^{n} \frac{f^{(k)}(1)}{k!}(\mathrm{x}-1)^k = \sum_{k=0}^{n} (-1)^k (x-1)^k. \tag{4.10}$$

For the Taylor polynomials all the information used in the approximation is concentrated at the single number x_0, so these polynomials will generally give inaccurate approximations as we move away from x_0. This limits Taylor polynomial approximation to the situation in which approximations are needed only at numbers close to x_0. For ordinary computational purposes it is more efficient to use methods that include information at various points. The primary use of Taylor polynomials in numerical analysis is not for approximation purposes, but for the derivation of numerical techniques and error estimation.

The problem of determining a polynomial of degree one that passes through the (x_0, y_0) distinct points (x_0, y_0) and (x_1, y_1) is the same as approximating a function f for which $f(x_0) = y_0$ and $f(x_1) = y_1$ by means of a first- degree polynomial interpolating, or agreeing with, the values of f at the given points. Using this polynomial for approximation within the interval given by the endpoints is called polynomial interpolation. Define the functions

$$L_0(x) = \frac{x - x_1}{x_0 - x_1}, \tag{4.11}$$

$$L_1(x) = \frac{x - x_0}{x_1 - x_0}. \tag{4.12}$$

The linear Lagrange interpolating polynomial though (x_0, y_0) and (x_1, y_1) is

$$P_n(x) \quad = L_0(x) f(x_0) + L_1(x) f(x_1)$$

$$= \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1). \tag{4.13}$$

Note that

$$L_0(x_0) = 1,\ L_0(x_1) = 0,\ L_1(x_0) = 0, \text{ and } L_1(x_1) = 1.$$

which implies that

$$P(x_0) = 1 \cdot f(x_0) + 0 \cdot f(x_1) = f(x_0) = y_0 \tag{4.14}$$

and

$$P(x_1) = 0 \cdot f(x_0) + 1 \cdot f(x_1) = f(x_1) = y_1. \tag{4.15}$$

Then P is the unique polynomial of degree at most one that passes through (x_0, y_0) and (x_1, y_1). In this case we first construct, for each $k = 0, 1, ..., n,$ a function $L_{n,k}(x)$ with the property that $L_{n,k}(x_i) = 0,$ when $i \neq k$ and $L_{n,k}(x_k) = 1$. To satisfy $L_{n,k}(x_i) = 0$

for each $i \neq k$ requires that the numerator of $L_{n,k}(x)$ contain the term $(x-x_0)(x-x_1)...(x-x_{k-1})(x-x_{k+1})...(x-x_n)$.

To satisfy $L_{n,k}(x_k)=1,$ the denominator of $L_{n,k}(x)$ must be this same term but evaluated at $x=x_k$. Thus

$$L_{n,k}(x)=\frac{(x-x_0)...(x-x_{k-1})(x-x_{k+1})...(x-x_n)}{(x_k-x_0)...(x_k-x_{k-1})(x_k-x_{k+1})...(x_k-x_n)}. \tag{4.16}$$

Theorem 4.2 [15] If $x_0, x_1, ..., x_n$ are $n+1$ distinct numbers and f is a function whose values are given at these numbers, then a unique polynomial $P(x)$ of degree at most n exists with $f(x_k)=P(x_k)$ for each $k=0,1,...,n.$
This polynomial is given by

$$P(x)=f(x_0)L_{n,0}(x)+...+f(x_n)L_{n,n}(x)=\sum_{k=0}^{n} f(x_k)L_{n,k}(x), \tag{4.17}$$

where, for each $k=0,1,...,n,$

$$\begin{aligned} L_{n,k}(x) &= \frac{(x-x_0)(x-x_1)...(x-x_{k-1})(x-x_{k+1})...(x-x_n)}{(x_k-x_0)(x-x_1)...(x_k-x_{k-1})(x_k-x_{k+1})...(x_k-x_n)}, \\ &= \prod_{\substack{i=0 \\ i\neq k}}^{n} \frac{(x-x_i)}{(x_k-x_i)}. \end{aligned} \tag{4.18}$$

We will write $L_{n,k}(x)$ simply as $L_k(x)$ when there is no confusion as to its degree.

Theorem 4.3 [15] Suppose $x_0, x_1, ..., x_n$ are distinct numbers in the interval [a,b] and $f \in C^{n+1}$ [a,b]. Then, for each x in [a,b], a number $\xi(x)$ (generally unknown) between $x_0, x_1, ..., x_n,$ and hence in $(a,b),$ exists with

$$f(x)=P(x)+\frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)...(x-x_n), \tag{4.19}$$

where $P(x)$ is the interpolating polynomial given in Eq. (4.17). The error formula in Eq. (4.19) is an important theoretical result because Lagrange polynomials are used extensively numerical differentiation and integration methods.

The error in applied mathematics is the difference between a true value and an estimate, or approximation of that value. In numerical analysis, round-off error is exemplified by the difference between the true values of the irrational number. The approximation error in some data is the discrepancy between an exact value and some approximation to it. An approximation error can occur because the measurement of the data is not precise due to the instruments and approximations are used instead of the real data. In Eq. (4.18) implies that the error in linear interpolation is $|f(x)-P(x)|$, where $\tilde{f}(x)$ is the interpolating polynomial.

The interpolating the n th Lagrange interpolation polynomial are easily described one the form of $L_k(x)$ is known. It is difficult to interpolate river canal, because it is unknown functions of initial condition and boundary conditions. The interpolation of field data use Eq. (4.19) for interpolate Eq. (4.9). By using every 3 nodes $x_0, x_1, \ldots, x_n$ that are distinct numbers in the interval [a,b], by using an Iterative explicit finite difference technique to find the second Lagrange interpolation polynomial for $f(x) \approx P(x)$, where $P(x)$ is the interpolating polynomial [15].

Example 4.1: constructing the quadratic Lagrange interpolating polynomials. Construct the quadratic Lagrange interpolating polynomial $P_2(x)$ that interpolates the points (1,4), (2,1), and (5,6). We define the quadratic Lagrange interpolating polynomial, P_2 through the points (x_0, y_0) , (x_1, y_1) , and (x_2, y_2) as the following function:

$$\begin{aligned} P_2(x) &= y_0 L_0(x) + y_1 L_1(x) + y_2 L_2(x) \\ &= y_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + y_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + y_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \end{aligned} \quad (4.20)$$

Note that P_2 does in fact pass through all the points specified above since $P_2(x_0) = y_0$, $P_2(x_1) = y_1$, and $P_2(x_2) = y_2$. The quadratic Lagrange interpolating polynomial through the points (x_0, y_0), (x_1, y_1), and (x_2, y_2) where x_0, x_1, and x_3 are distinct is the polynomial $P_2(x) = y_0 L_0(x) + y_1 L_1(x) + y_2 L_2(x)$. Applying the formula given above directly and we get that

$$P_2(x) = 4\frac{(x-2)(x-5)}{(1-2)(1-5)} - 1\frac{(x-1)(x-5)}{(2-1)(2-5)} + 6\frac{(x-1)(x-2)}{(5-1)(5-2)}$$

$$P_2(x) = (x-2)(x-5) - \frac{1}{3}(x-1)(x-5) + \frac{1}{2}(x-1)(x-2)$$

The graph of $y = P_2(x)$ is given below:

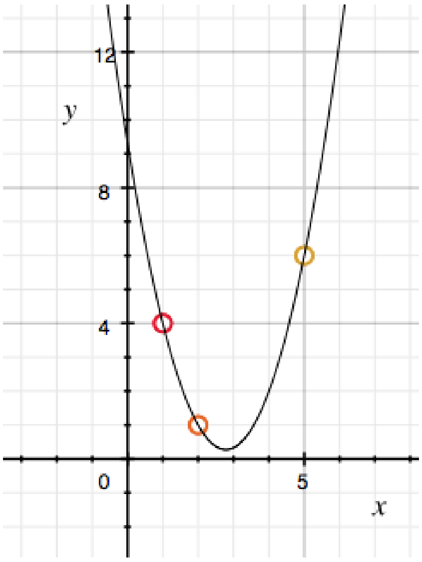


Figure 4.1 The quadratic Lagrange interpolating polynomials $P_2(x)$ that interpolates the points (1,4), (2, 1), and (5, 6)

Example 4.2 Construct the quadratic Lagrange interpolating polynomial $P_2(x)$ that interpolates the points (1,2), (3,4), and (5,6).

$$P_2(x) = 2\frac{(x-3)(x-5)}{(1-3)(1-5)} - 4\frac{(x-1)(x-5)}{(3-1)(3-5)} + 6\frac{(x-1)(x-3)}{(5-1)(5-3)}$$
$$P_2(x) = \frac{1}{4}(x-3)(x-5) - (x-1)(x-5) + \frac{3}{4}(x-1)(x-3)$$

The graph of $y = P_2(x)$ is given below:

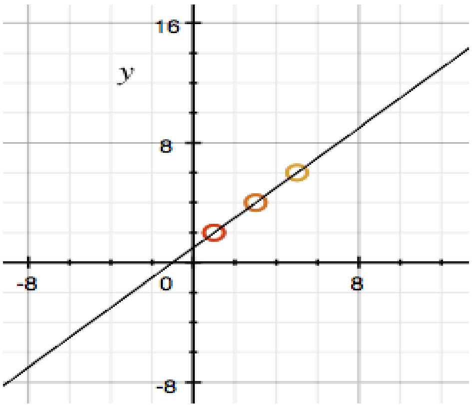


Figure 4.2 The quadratic Lagrange interpolating polynomial $P_2(x)$ that interpolates the points (1,2), (3,4), and (5,6)

Note that example 4.2 shows that P_2 need not be quadratic and may be a polynomial of lesser degree [24].

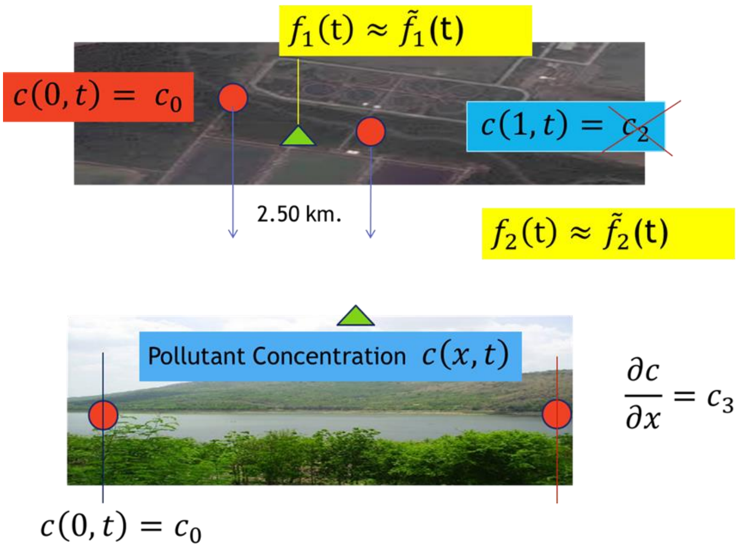


Figure 4.3 Quadratic interpolation for one-dimensional water quality model with the initial and boundary conditions

4.3 Numerical experiments

Simulation 1: Suppose that the measurement of pollutant concentration c in a non-uniform flow steam is aligned with longitudinal distance, 1.0 (km) total length and 1.0 (m) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point are $c(0,t)=g(t)$, $c(1,t)=h(t)$ at $0 \le x \le 1$ for all $t > 0$ and $c(x,0)=f(x)$ at $t=0$. The analytical solution to the one-dimensional advection-diffusion at $0 \le x \le 1$. The approximated of pollutant concentrations c is obtained by using a Saulyev finite difference technique Eq. (4.9) with the interpolated initial-boundary condition functions Eq. (4.21) - (4.23). The calculated results are appeared in Tables 4.1-4.3 and Figures 4.4.

Table 4.1 Pollutant Concentration $c(x,t)$ of the Lagrange
Interpolating at $c(x,0)=f(x)$.

x/Coefficient	a	b	c
[0.0,0.2]	0	0	0
[0.2,0.4]	0	0	0
[0.4,0.6]	0	0	0
[0.6,0.8]	0	0	0
[0.8,1.0]	0	0	0

Table 4.2 Pollutant Concentration $c(x,t)$ of the Lagrange Interpolating at $c(0,t)=g(t)$.

x/Coefficient	a	b	c
[0.0,0.2]	0.7481177	-0.07459277	0
[0.2,0.4]	-0.19923775	2.457190005	-0.388462337
[0.4,0.6]	-0.2138025	-0.73557306	0570973249
[0.6,0.8]	1.46361815	-2.266881615	0.905686948
[0.8,1.0]	0.087665	-0.16909456	0.08198636

Table 4.3 Pollutant Concentration $c(x,t)$ of the Lagrange Interpolating at $c(1,t)=h(t)$.

x/Coefficient	a	b	c
[0.0,0.2]	0	0	0
[0.2,0.4]	0	0	0
[0.4,0.6]	0	0	0
[0.6,0.8]	0.00572283	-0.00743197	0.000239896
[0.8,1.0]	0.20206455	-0.339564525	0.142341908

The approximation of the pollutant concentrations of a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes is shown in Table 4.1-4.3, and Figure 4.4. The numerical techniques are proposed for three θ values, 0, 0.5 and 1, respectively. The case of $\theta=0$ gives a smooth solution compare to another value.

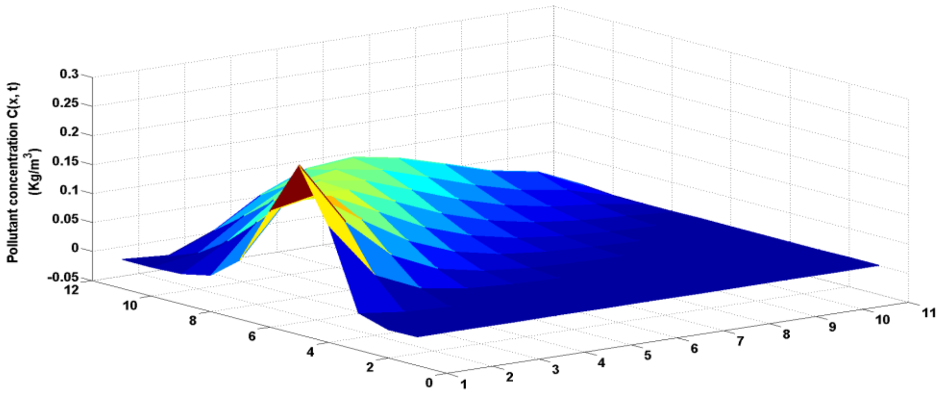


Figure 4.4 The Lagrange interpolation $c(x,t)$

Simulation 2: Suppose that the measurement of pollutant concentration c in a non-uniform flow steam is aligned with longitudinal distance, 1.0 (km) total length and 1.0 (m) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point are $c(0,t)=g(t)$, $c(1,t)=h(t)$ at $0\le x\le 1$ for all $t>0$ and $c(x,0)=f(x)$ at $t=0$. The analytical solution to the one-dimensional advection-diffusion at $0\le x\le 1$ give as [10]

$$c(x,t)=\frac{0.025}{\sqrt{0.000625+0.02t}}\exp\left[-\frac{(x+0.5-t)^2}{(0.00125+0.04t)}\right] \tag{4.21}$$

prediction of a field data at the boundary can be obtained by using a quadratic interpolated initial and boundary conditions Eq. (4.17). The interpolation is used to interpolate the right boundary condition, left boundary condition and the initial condition,

$$c(0,t)=\tilde{g}(t)\ , \tag{4.22}$$

$$c(1,t)=\tilde{h}(t)\ , \tag{4.23}$$

for all $t\in[0,1]$ and

$$c(x,0)=\tilde{f}(x) \tag{4.24}$$

at $x\in[0,1]$, where $\tilde{g}(t), \tilde{h}(t)$ and $\tilde{f}(x)$ are interpolated functions.

The approximated of pollutant concentrations c is obtained by using a Saulyev finite difference technique Eq. (4.9) with the interpolated initial-boundary condition functions Eq. (4.21) - (4.23). The calculated results are appeared in Tables 4.4-4.6 and Figures 4.5-4.10.

Table 4.4 The maximum error of approximated pollutant concentration at $x=0.25,\ 0.50,\ 0.75$, for all $t\in[0,1]$.

Δt	Δx	Cr	Pe	Maximum error		
				x=*0.25*	x=*0.50*	x=*0.75*
0.0100	0.0500	0.2000	5.0000	1.97×10^{-2}	1.99×10^{-2}	0.63×10^{-2}
0.0100	0.0250	0.4000	2.5000	5.40×10^{-3}	5.80×10^{-3}	2.00×10^{-3}
0.0100	0.0125	0.8000	1.2500	6.63×10^{-4}	7.35×10^{-4}	2.80×10^{-4}

Table 4.5 The maximum error of interpolated boundary condition functions to the analytical solution (Eq. 4.21). $E(T_g) = \max\left|g(t) - \tilde{g}(t)\right|$ and $E(T_h) = \max\left|h(t) - \tilde{h}(t)\right|$, for all $0 \le t \le 1$.

t	$E(T_g)$	$E(T_h)$
[0.0,0.2]	3.16406×10^{-10}	0.0000
[0.2,0.4]	4.4625×10^{-10}	0.0000
[0.4,0.6]	2.3796×10^{-10}	3.8500×10^{-10}
[0.6,0.8]	3.314×10^{-12}	3.3258×10^{-10}
[0.8,1.0]	2.461×10^{-12}	3.3258×10^{-10}
Maximum error	3.1640×10^{-12}	3.3258×10^{-12}

Table 4.6 The maximum error of interpolated initial condition functions to the analytical solution (Eq. 21). $E(T_f) = \max\left|f(x) - \tilde{f}(x)\right|$, for all $0 \le x \le 1$.

x	$E(T_f)$
[0.0,0.2]	2.836181×10^{-14}
[0.2,0.4]	0.0000
[0.4,0.6]	0.0000
[0.6,0.8]	0.0000
[0.8,1.0]	2.836181×10^{-14}
Maximum error	2.836181×10^{-14}

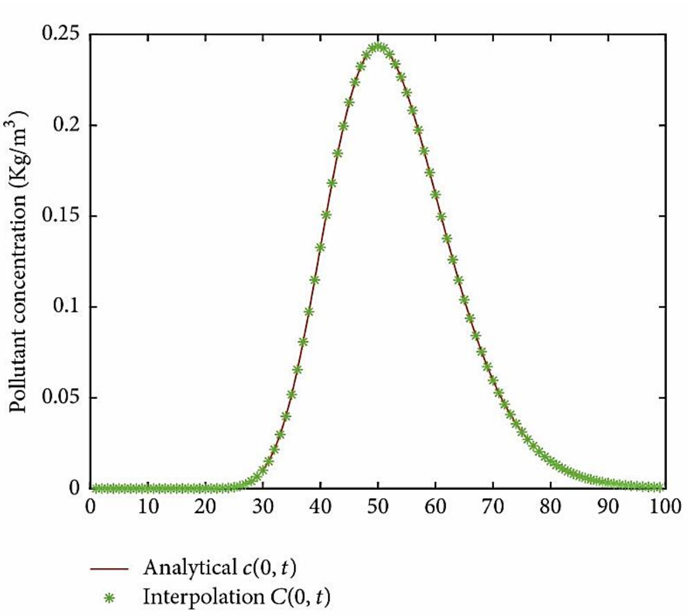


Figure 4.5 Comparison of analytical and interpolated left boundary conditions $c(0,t)$ (Δx=0.0500, Δt=0.0100, Pe=5.0)

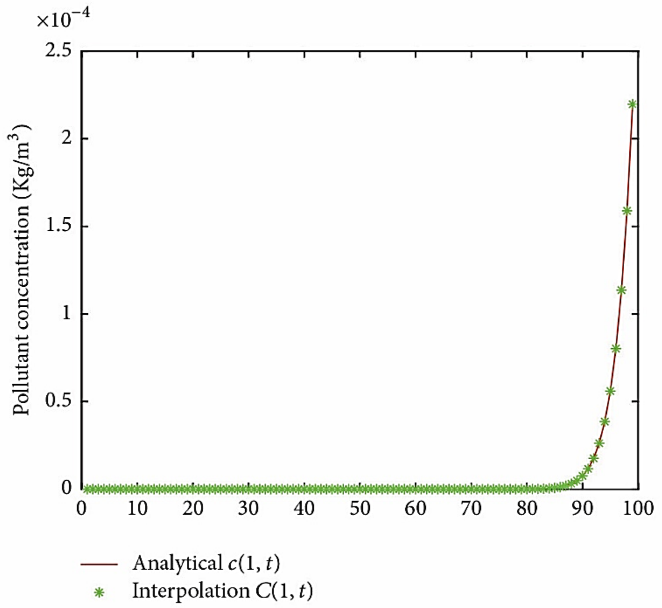


Figure 4.6 Comparison of analytical and interpolated right boundary condition $c(1,t)$ (Δx=0.0500, Δt=0.0100, Pe=5.0)

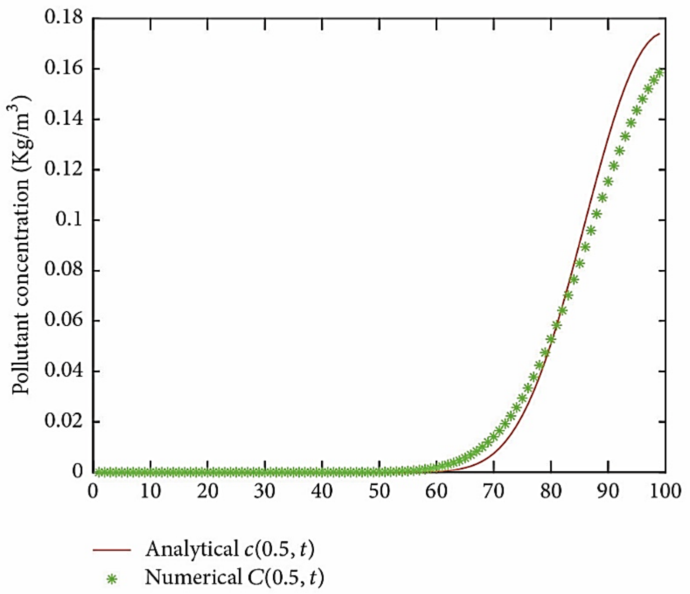


Figure 4.7 Comparison of analytical and approximated of pollutant concentrations $c(0.5,t)$ (Δx=0.0500, Δt=0.0100, Pe=5.0)

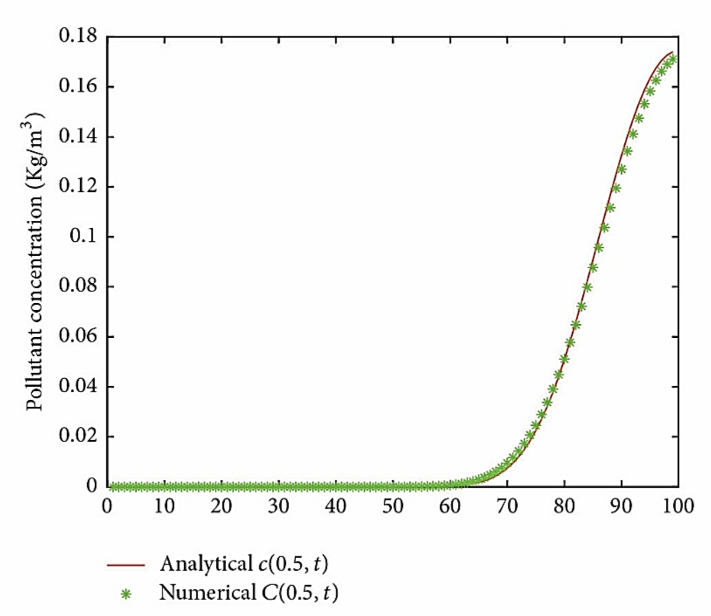


Figure 4.8 Comparison of analytical and approximated of pollutant concentrations $c(0.5,t)$ (Δx=0.0250, Δt=0.0100, Pe=2.5)

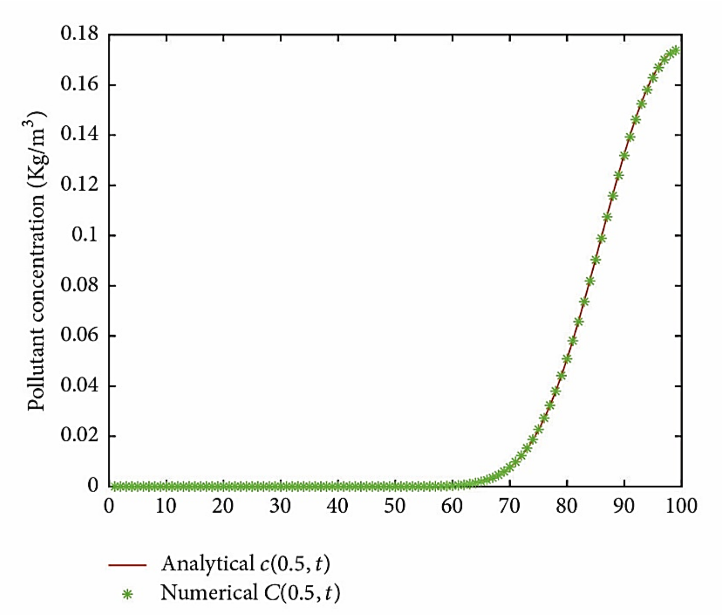


Figure 4.9 Comparison of analytical and approximated of pollutant concentrations $c(0.5,t)$ (Δx=0.0125, Δt=0.0100, Pe=1.25)

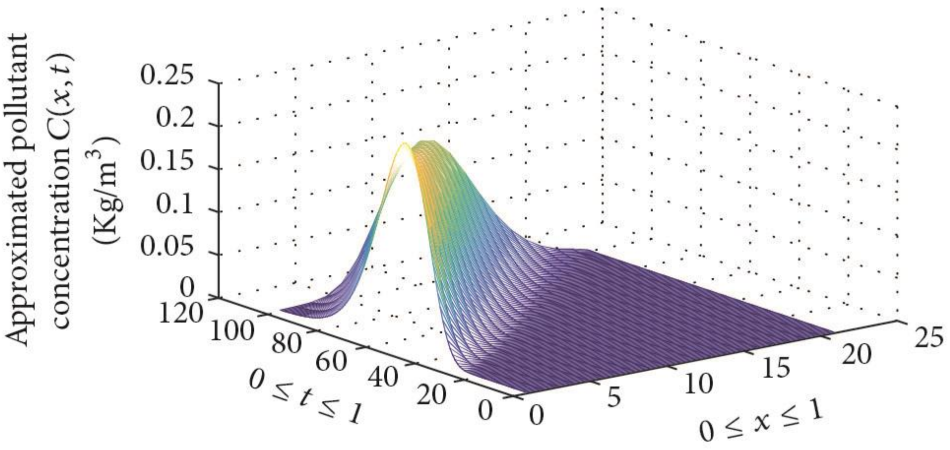


Figure 4.10 The Saulyev finite difference solution with quadratic interpolation $c(x,t)$ (Δx=0.0500, Δt=0.0100, Pe=5.0)

4.4 Discussion

First part of this research, the approximation of the pollutant concentrations of a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes is shown in Table 3.2, 3.3 and 3.4 and Figure 3.4. The numerical techniques are proposed for three θ values, 0, 0.5 and 1, respectively. The case of $\theta = 0$ gives a smooth solution compare to another values. Increasing the mass decaying rate affects the maximum concentration level.

Second part of this research, the approximation of the pollutant concentrations of a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes is shown in Table 4.5-4.7, and Figure 4.5-4.10. The numerical techniques are proposed for three θ values, 0, 0.5 and 1, respectively. The case of $\theta = 0$ gives a smooth solution compare to another values. Increasing the mass decaying rate affects the maximum concentration level. The interpolation results must be crude mesh as field data. The numerical results can be fine mesh or crude mesh. In Table 4.4 and Figures 4.6-4.10, we can see that the maximum errors of approximated pollutant concentration are reducing while the Peclet numbers are decreased. The maximum error of analytical and interpolation technique is show in Table 4.5, right boundary condition is 3.1640×10^{-8}, with left boundary condition is 3.3258×10^{-8} and initial condition is 2.836181×10^{-10}. The compare of analysis and interpolation technique is show in Figure 4.5-4.10. The numerical techniques are proposed for the interpolation technique gives the results closest to the analytical solution. The accuracy of the Lagrange interpolation technique is used to predict their initial and boundary conditions as needed.

Chapter 5

Conclusion

The proposed numerical technique used is an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. The numerical experiments show that the calculated results are reasonable approximations. The revision shows good agreement solutions. The proposed technique is suitable to be used in the natural phenomenas problem due to it easily to program and the straight forwardness of the implementation. According to field water quality, data is needed to implement of a function at the boundaries. We proposed a Lagrange interpolation technique to synthesis their boundary conditions as required. The computed results are verified by the numerical technique gives reliable solutions to the known solution of the test problem.

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Appendix

The research papers

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Research Article

Numerical Simulation of a One-Dimensional Water-Quality Model in a Stream Using a Saulyev Technique with Quadratic Interpolated Initial-Boundary Conditions

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The one-dimensional advection-diffusion-reaction equation is a mathematical model describing transport and diffusion problems such as pollutants and suspended matter in a stream or canal. If the pollutant concentration at the discharge point is not uniform, then numerical methods and data analysis techniques were introduced. In this research, a numerical simulation of the one-dimensional water-quality model in a stream is proposed. The governing equation is advection-diffusion-reaction equation with nonuniform boundary condition functions. The approximated pollutant concentrations are obtained by a Saulyev finite difference technique. The boundary condition functions due to nonuniform pollutant concentrations at the discharge point are defined by the quadratic interpolation technique. The approximated solutions to the model are verified by a comparison with the analytical solution. The proposed numerical technique worked very well to give dependable and accurate solutions to these kinds of several real-world applications.

1. Introduction

Water quality must be protected and maintained for several uses, the principal ones being domestic water supply, energy production, industry, agriculture, fish, and wildlife. Mathematical modeling of the water pollution measurement and control in the water area has been examined. In [1], a simulation process showing that water pollution levels can be reduced to an agreed standard at the lowest cost is proposed.

In [2], mathematical modeling of the transport salinity, pollutants, and suspended matter in shallow water that involves the numerical solution of an advection-diffusion equation is proposed. A novel technique of finite difference methods is proposed. In [3], the authors also proposed a mathematical modeling of the transport salinity, pollutants, and suspended matter in shallow water that involves the numerical solution of an advection-diffusion equation in the technique of flux-corrected scheme of finite difference methods. It is available for the solution of the depth-integrated form of the advection-diffusion equation. In [4, 5], the advection and diffusion terms are solved by two different numerical methods.

In [6], the authors used a weighted discretization method with the modified equivalent partial differential equation for solving the one-dimensional advection-diffusion equation. In [7], the authors introduce the central difference approximation that gives some negative concentration in the neighboring cell due to a large advection flux. In [8], the authors proposed a numerical dispersion by introducing an upstream interpolation method, namely, QUICK (Quadratic Upstream Interpolation Convective Kinematics), for one-dimensional unsteady flow. In [9], parabolic partial differential equations with a nonstandard initial condition, featured in the mathematical modeling of many phenomena, are proposed. Saulyev's explicit schemes are an economical implement to use. These unconditionally explicit schemes are very simple to program and compute. The new explicit schemes developed are very efficient and they need less CPU time than the implicit methods. The explicit finite difference schemes are very easy to implement for similar higher-dimensional problems. In [10], a user friendly and a flexible solution algorithm are proposed for the numerical solution of the one-dimensional advection-diffusion equation (ADE), and an explicit spreadsheet simulation (ESS) technique is used instead of a computer code. In the numeric solution of ADE using finite differences, either a small value of the Courant number such as 0.05–0.10 is used for oscillation-free results or an artificial diffusion is used in order to reduce oscillation. In order to provide for small Courant numbers, it is necessary to choose a small time step and/or grid size; however, this increases the computation time. While the proposed ADEESS solution technique uses an unconditional stable Saulyev scheme, it gives highly accurate results even for the values of the Courant numbers as high as 2-3. By varying only the values of the temporal weighted parameter (θ), namely, 0, 0.5, and 1, respectively, the problems are solved. The model results for the value of $\theta = 0$ appear to be in good agreement with the analytical solutions.

In [11], a better finite difference scheme to solve the dynamic one-dimensional advection-dispersion-reaction equations (ADRE) is focused upon, and the effect of nonuniform water flows in a stream is considered. There are two mathematical models used to simulate pollution due to sewage effluent. The first model is a hydrodynamic model for numerical techniques. The Crank-Nicolson method is used to approximate the solution. The second model is an advection-dispersion-reaction model; the explicit schemes are introduced. The revised explicit schemes are modified from two computation techniques of uniform flow stream problems: forward time central space (FTCS) and Saulyev schemes for the dispersion model. A comparison of both schemes regarding the stability aspect is provided so as to illustrate their applicability to the real-world problem.

The dispersion model provides the pollutant concentration field. In [12], a modified MacCormack method is subsequently employed in the dispersion model. The proposed method is a simply remarkable alteration to the MacCormack method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicate that the proposed modified MacCormack scheme does improve the prediction accuracy compared to the traditional MacCormack method. In [13], the authors proposed a simple revision to the MacCormack and Saulyev schemes that improves their accuracy for high Peclet number problems, which are named the Saulyev and MacCormack schemes, respectively, greatly improving the prediction accuracy over the original ones. They proposed a new scheme that guarantees the positivity of the solutions for arbitrary step sizes. In [14], they developed a numerical technique to approximate the solution of an advection-diffusion-reaction equation in one spatial dimension with constant velocity and diffusion. In [15], the Preissmann four-point partial-node implicit scheme is used to solve a one-dimensional hydrodynamic and water-quality model. In [16], a nondimensional form of a two-dimensional hydrodynamic model with a generalized boundary condition and initial conditions for describing the elevation of water wave in an open uniform reservoir is proposed. The separation of variables method with mathematical induction is employed to find an analytical solution to the model. In [17], the traditional Crank-Nicolson method is also used in the hydrodynamic model. At each step, the flow velocity fields calculated from the hydrodynamic model are the inputs into the water-quality model. A new fourth-order scheme and a Saulyev scheme are simultaneously employed in the water-quality model. In [18], the hydrodynamics model coupled with water quality is established by MIKE21FM software to simulate the current situation of Erhai Lake. The water quality is also simulated by the two-dimensional hydrodynamics and water-quality coupled model. The simple explicit schemes have the advantages of simplicity in computing without losing more accuracy and these schemes are precedent for several model applications. To identify the best one of these simple schemes, comparative studies of these are necessary.

The collected field data is not suitable to input into a mathematical model. The data is varied by time. The time-dependent distributions of discharged pollutant concentration and water flow velocity are required. It is complicated work if we input them into computer implementation while a given function has a simpler operation. The object of this research is to propose an interpolation technique to all of the collected field data such as water pollutant concentration at the released polluted water point and the water flow velocity along the considered water stream. The revision shows good agreement solutions. The proposed technique is suitable to be used in several real-world problems because it is easy to program and because of the straightforwardness of the implementation. According to field water-quality data, the data will be implemented to be a function of the boundary condition. The Lagrange interpolation technique is used to synthesize their boundary conditions as required. A simple advection-diffusion-reaction numerical simulation is proposed using the Saulyev scheme. The proposed numerical technique uses an unconditionally stable method. A large or small time step and/or grid size can be employed in the proposed techniques. We apply the method to two problems with different data for obtaining the right and left boundary conditions. The results of the model show that the calculated results are reliable approximations.

2. One-Dimensional Water-Quality Model

2.1. The Governing Equation. In this section, we consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one-dimensional advection-diffusion-reaction equation (ADRE):

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} - KC, \quad 0 < x < L, \ 0 < t \leq T. \quad (1)$$

2.2. Initial and Boundary Conditions. The initial condition is

$$c(x, 0) = f(x), \quad 0 \leq x \leq L, \quad (2)$$

and boundary conditions are

$$\begin{aligned} c(0,t) &= g(t), \quad 0 \le t \le T, \\ c(L,t) &= h(t), \quad 0 \le t \le T, \end{aligned} \tag{3}$$

where x is the longitudinal distance along the stream, t is time, T is the last time, and $f(x)$, $g(t)$, and $h(t)$ are interpolated functions, while $c(x,t)$ is the concentration averaged in depth at the point x and at time t, $u(x,t)$ is the water flow velocity in the $x$direction for all $x \in [0,L]$ at time t, D is the dispersion coefficient, and K is the mass decay rate.

3. Numerical Technique

3.1. An Explicit Finite Difference Technique. The solution domain of the problem is covered by a mesh of grid lines. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0,1,2,\dots,M$ and $t_n = n\Delta t$ for all $n = 0,1,2,\dots,N$ in which M and N are positive integers, where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid spacing are $\Delta x = L/M$ and $\Delta t = T/N$.

Consider the following approximations of the derivative in the advection-diffusion equation which incorporate time weights θ as follows [10]:

$$\begin{aligned} \frac{\partial c}{\partial t} &= \frac{c_i^{n+1} - c_i^n}{\Delta t}, \\ u\frac{\partial c}{\partial x} &= u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right], \\ D\frac{\partial^2 c}{\partial x^2} &= D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] \\ &\quad + D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i+1}^n - 2c_i^n + c_{i+1}^n\right], \end{aligned} \tag{4}$$

where θ is the weighting factor. Substituting (4) into (1), we get [10]

$$\begin{aligned} &\left[1 + \frac{\text{Cr}}{2} + \theta\left(\frac{\text{Cr}}{\text{Pe}}\right)\right]c_i^{n+1} - \left[\frac{\text{Cr}}{2} + \theta\left(\frac{\text{Cr}}{\text{Pe}}\right)\right]c_{i-1}^{n+1} \\ &\quad = \left(\frac{\text{Cr}}{\text{Pe}} - \theta\left(\frac{\text{Cr}}{\text{Pe}}\right)\right)c_{i-1}^n \\ &\quad + \left[1 + \frac{\text{Cr}}{2} - 2\left(\frac{\text{Cr}}{\text{Pe}}\right) + \theta\left(\frac{\text{Cr}}{\text{Pe}}\right) + K\Delta t\right]c_i^n \\ &\quad + \left[\frac{\text{Cr}}{\text{Pe}} - \frac{\text{Cr}}{2}\right]c_{i+1}^n \end{aligned} \tag{5}$$

for $1 \le i \le M-1$ and $1 \le n \le N-1$, where $\text{Cr} = u\Delta t/\Delta x$ is Courant number and $\text{Pe} = u\Delta x/D$ is Peclet number.

Although (5) does not seem explicit, because c_{i-1}^{n+1} and c_i^{n+1} are on the left-hand side, a suitable use of the equation makes it explicit.

Therefore, (5) can be written in the following form:

$$\begin{aligned} c_i^{n+1} &= \frac{1}{\left[1 + \text{Cr}/2 + \theta(\text{Cr}/\text{Pe})\right]}\left\{\left[\frac{\text{Cr}}{2} + \theta\left(\frac{\text{Cr}}{\text{Pe}}\right)\right]c_{i-1}^{n+1}\right. \\ &\quad + \left[\frac{\text{Cr}}{\text{Pe}} - \theta\left(\frac{\text{Cr}}{\text{Pe}}\right)\right]c_{i-1}^n \\ &\quad + \left[1 + \frac{\text{Cr}}{2} - 2\left(\frac{\text{Cr}}{\text{Pe}}\right) + \theta\left(\frac{\text{Cr}}{\text{Pe}}\right) + K\Delta t\right]c_i^n \\ &\quad \left. + \left[\frac{\text{Cr}}{\text{Pe}} - \frac{\text{Cr}}{2}\right]c_{i+1}^n\right\}. \end{aligned} \tag{6}$$

For the advection term, we apply the scheme of either $u > 0$ or $u < 0$. Thus, the scheme is restricted to single-direction velocity fields, with c being transported from left to right by the flow, so the Saulyev scheme is the appropriate choice for discretizing the advective term. In (6), the term at time level $n+1$, c_{i-1}^{n+1}, has already been computed at spatial point $i-1$ by marching in the direction of increasing i. This scheme is an explicit finite difference method. In this case, only a single value, c_i^{n+1}, will be unknown. This scheme is known as Saulyev's formula and the main advantage of it is that it is unconditionally stable and explicit [10].

3.2. Iterative Method for the Initial and Boundary Conditions

Interpolation

Theorem 1 (Weierstrass approximation theorem, [19]). *Suppose that f is defined and continuous on $[a,b]$. For each $\varepsilon > 0$, there exists a polynomial $P(x)$, with the property that $|f(x) - P(x)| < \varepsilon$, for all x in $[a,b]$.*

The Taylor polynomials agree as closely as possible with a given function at a specific point, but they concentrate their accuracy near that point. A good interpolation polynomial needs to provide a relatively accurate approximation over an entire interval, and Taylor polynomials do not generally do this. The Taylor polynomials are [19]

$$P_n(x) = \sum_{k=0}^{n}\frac{f^{(k)}(1)}{k!}(x-1)^k = \sum_{k=0}^{n}(-1)^k(x-1)^k. \tag{7}$$

For the Taylor polynomials, all the information used in the approximation is concentrated at the single number x_0, so these polynomials will generally give inaccurate approximations as we move away from x_0. This limits Taylor polynomial approximation to the situation in which approximations are needed only at numbers close to x_0. For ordinary computational purposes, it is more efficient to use methods that include information at various points. The primary use of Taylor polynomials in numerical analysis is not for approximation purposes, but for the derivation of numerical techniques and error estimation.

Lagrange Interpolating Polynomials. The problem of determining a polynomial of degree one that passes through the (x_0, y_0) distinct points (x_0, y_0) and (x_1, y_1) is the same as approximating a function f for which $f(x_0) = y_0$ and

$f(x_1) = y_1$ by means of a first-degree polynomial interpolation, or agreeing with the values of f at the given points. Using this polynomial for approximation within the interval given by the endpoints is called polynomial interpolation. Define the functions

$$L_0(x) = \frac{x - x_1}{x_0 - x_1}, \qquad L_1(x) = \frac{x - x_0}{x_1 - x_0}. \tag{8}$$

The linear Lagrange interpolating polynomial through (x_0, y_0) and (x_1, y_1) is

$$\begin{aligned} P_n(x) &= L_0(x) f(x_0) + L_1(x) f(x_1) \\ &= \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1). \end{aligned} \tag{9}$$

Note that

$$\begin{aligned} L_0(x_0) &= 1, \\ L_0(x_1) &= 0, \\ L_1(x_0) &= 0, \\ L_1(x_1) &= 1, \end{aligned} \tag{10}$$

which implies that

$$\begin{aligned} P(x_0) &= 1 \cdot f(x_0) + 0 \cdot f(x_1) = f(x_0) = y_0, \\ P(x_1) &= 0 \cdot f(x_0) + 1 \cdot f(x_1) = f(x_1) = y_1. \end{aligned} \tag{11}$$

Then, P is the unique polynomial of degree at most one that passes through (x_0, y_0) and (x_1, y_1). In this case, we first construct, for each $k = 0, 1, \ldots, n$, a function $L_{n,k}(x)$ with the property that $L_{n,k}(x_i) = 0$, when $i \neq k$ and $L_{n,k}(x_k) = 1$. To satisfy $L_{n,k}(x_i) = 0$ for each $i \neq k$, it is required that the numerator of $L_{n,k}(x)$ contains the term $(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)$.

To satisfy $L_{n,k}(x_k) = 1$, the denominator of $L_{n,k}(x)$ must be this same term but evaluated at $x = x_k$. Thus,

$$\begin{aligned} &L_{n,k}(x) \\ &= \frac{(x - x_0) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)}. \end{aligned} \tag{12}$$

Theorem 2 (see [19]). *If $x_0, x_1, \ldots, x_n$ are $n + 1$ distinct numbers and f is a function whose values are given at these numbers, then a unique polynomial $P(x)$ of degree at most n exists with $f(x_k) = P(x_k)$, for each $k = 0, 1, \ldots, n$.*

This polynomial is given by

$$\begin{aligned} P(x) &= f(x_0) L_{n,0}(x) + \cdots + f(x_n) L_{n,n}(x) \\ &= \sum_{k=0}^{n} f(x_k) L_{n,k}(x), \end{aligned} \tag{13}$$

where, for each $k = 0, 1, \ldots, n$,

$$\begin{aligned} &L_{n,k}(x) \\ &= \frac{(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0)(x - x_1) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)} \\ &= \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{(x - x_i)}{(x_k - x_i)}. \end{aligned} \tag{14}$$

We will write $L_{n,k}(x)$ simply as $L_k(x)$ when there is no confusion as to its degree.

Theorem 3 (see [19]). *Suppose $x_0, x_1, \ldots, x_n$ are distinct numbers in the interval $[a, b]$ and $f \in C^{n+1}[a, b]$. Then, for each x in $[a, b]$, a number $\xi(x)$ (generally unknown) between $x_0, x_1, \ldots, x_n$, and hence in (a, b), exists with*

$$\begin{aligned} &f(x) \\ &\quad = P(x) \\ &\qquad + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} (x - x_0)(x - x_1) \cdots (x - x_n), \end{aligned} \tag{15}$$

where $P(x)$ is the interpolating polynomial given in (13). The error formula in (15) is an important theoretical result because Lagrange polynomials are used extensively in numerical differentiation and integration methods.

The error in applied mathematics is the difference between a true value and an estimate, or the approximation of that value. In numerical analysis, round-off error is exemplified by the difference between the true values of the irrational number. The approximation error in some data is the discrepancy between an exact value and some approximation to it. An approximation error can occur because the measurement of the data is not precise because instruments and approximations are used instead of the real data. In (14), it is implied that the error in linear interpolation is $|f(x) - P(x)|$, where $\tilde{f}(x)$ is the interpolating polynomial.

Interpolating the nth Lagrange interpolation polynomial can be described in a simpler form as $L_k(x)$. It is difficult to interpolate a river channel, because it has unknown functions of initial conditions and boundary conditions. The interpolation of field data uses (15) for interpolating (6). Use every 3 nodes $x_0, x_1, \ldots, x_n$ that are distinct numbers in the interval $[a, b]$ by an iterative explicit finite difference technique to find the second Lagrange interpolation polynomial for $f(x) \approx P(x)$, where $P(x)$ is the interpolating polynomial [19].

4. Numerical Experiments

Suppose that the measurement of pollutant concentration c in a nonuniform flow stream is aligned with longitudinal distance, 1.0 (km) total length and 1.0 (m) depth. There is a plant which discharges wastewater into the stream and the pollutant concentrations at the discharge point are $c(0, t) = g(t)$ (mg/L) and $c(1, t) = h(t)$ (mg/L) at $0 \leq x \leq 1$ for all $t > 0$ and $c(x, 0) = f(x)$ (mg/L) at $t = 0$. The analytical solution to

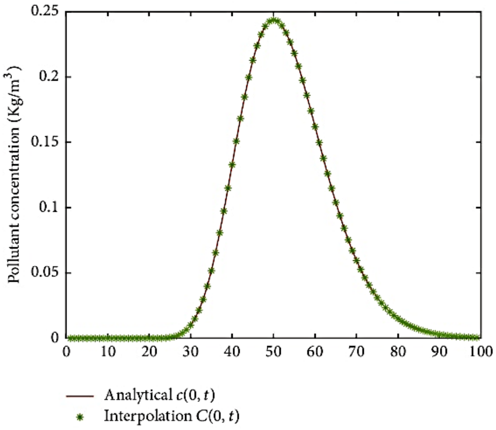

FIGURE 1: Comparison of analytical and interpolated left boundary conditions $c(0,t)$ (kg/m^3) ($\Delta x = 0.0500$, $\Delta t = 0.0100$, Pe = 5.0).

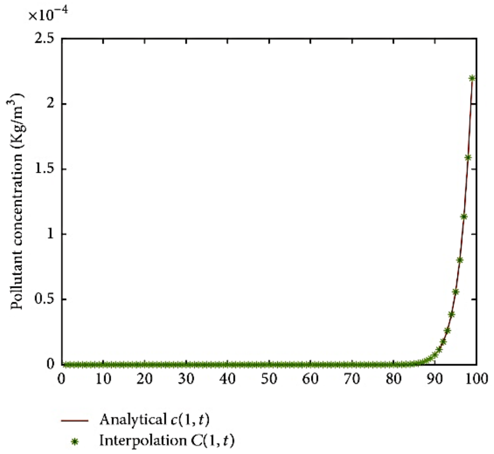

FIGURE 2: Comparison of analytical and interpolated right boundary conditions $c(1,t)$ (kg/m^3) ($\Delta x = 0.0500$, $\Delta t = 0.0100$, Pe = 5.0).

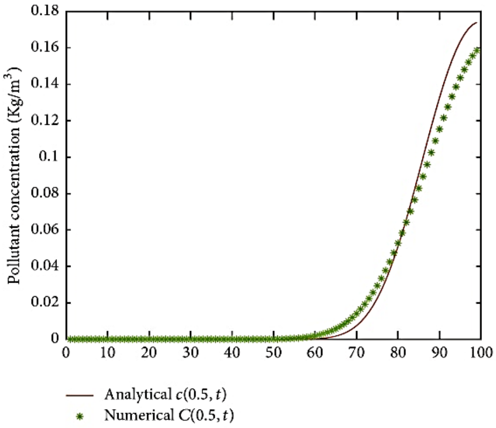

FIGURE 3: Comparison of analytical and approximated pollutant concentrations $c(0.5,t)$ (kg/m^3) ($\Delta x = 0.0500$, $\Delta t = 0.0100$, Pe = 5.0).

the one-dimensional advection-diffusion equation at $0 \le x \le 1$ is given as

$$c(x,t) = \frac{0.025}{\sqrt{0.000625 + 0.02t}} \exp\left[-\frac{(x+0.5-t)^2}{(0.00125+0.04t)}\right]. \tag{16}$$

Prediction of field data at the boundary can be obtained using a quadratic interpolated initial and boundary condition (see (13)). The interpolation is used to interpolate the right boundary condition, the left boundary condition, and the initial condition:

$$\begin{aligned} c(0,t) &= \tilde{g}(t), \\ c(1,t) &= \tilde{h}(t), \end{aligned} \tag{17}$$

for all $t \in [0, 1.0]$ and

$$c(x,0) = \tilde{f}(x) \tag{18}$$

at $x \in [0, 1.0]$, where $\tilde{g}(t), \tilde{h}(t)$, and $\tilde{f}(x)$ are interpolated functions.

The approximation of pollutant concentrations c is obtained using a Saulyev finite difference technique (see (6)) with the interpolated initial-boundary condition functions (see (17) and (18)). The calculated results are shown in Tables 1–3 and Figures 1–6.

5. Discussion

In this research, the approximation of the pollutant concentrations of a simple advection-diffusion reaction numerical simulation using the Saulyev schemes is shown in Tables 1–3 and Figures 1–6. The numerical techniques are proposed for three θ values: 0, 0.5, and 1, respectively. The case of $\theta = 0$ gives a smooth solution compared to other values. Increasing the mass decay rate affects the maximum concentration level. The interpolation results must be crude mesh as field data. The numerical results can be fine mesh or crude mesh. In Table 1 and Figures 1–5, we can see that the maximum errors of approximated pollutant concentration are reducing while the Peclet numbers are decreased. The maximum error of analytical and interpolation technique is shown in Table 2; the right boundary condition is 3.1640×10^{-08}, the left boundary condition is 3.3258×10^{-08}, and the initial condition is 2.836181×10^{-10}. Comparison of the analysis and interpolation technique is shown in Figures 1–6. The proposed

Table 1: The maximum error of approximated pollutant concentration at $x = 0.25, 0.50$, and 0.75, for all $t \in [0, 1]$.

Δt	Δx	Cr	Pe	Maximum error $x = 0.25$	 $x = 0.50$	 $x = 0.75$
0.0100	0.0500	0.2000	5.0000	1.97×10^{-2}	1.99×10^{-2}	0.63×10^{-2}
0.0100	0.0250	0.4000	2.5000	5.40×10^{-3}	5.80×10^{-3}	2.00×10^{-3}
0.0100	0.0125	0.8000	1.2500	6.63×10^{-4}	7.35×10^{-4}	2.80×10^{-4}

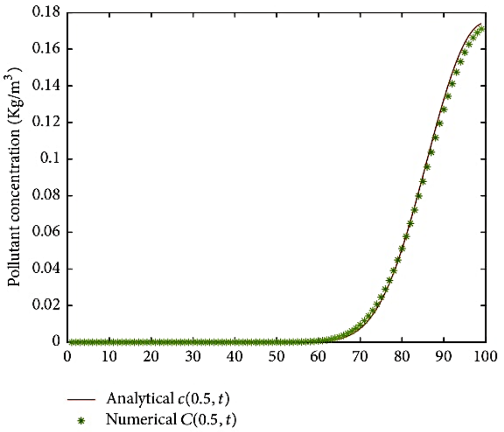

Figure 4: Comparison of analytical and approximated pollutant concentrations $c(0.5, t)$ (kg/m^3) ($\Delta x = 0.0250$, $\Delta t = 0.0100$, Pe $= 2.5$).

Table 2: The maximum error of interpolated boundary condition functions to the analytical solution (see (16)). $E(T_g) = \max|g(t) - \bar{g}(t)|$ and $E(T_h) = \max|h(t) - \bar{h}(t)|$, for all $0 \leq t \leq 1$.

t	$E(T_g)$	$E(T_h)$
[0.0, 0.2]	3.16406×10^{-10}	0.0000
[0.2, 0.4]	4.4625×10^{-10}	0.0000
[0.4, 0.6]	2.3796×10^{-10}	3.8500×10^{-10}
[0.6, 0.8]	0.03314×10^{-10}	3.3258×10^{-10}
[0.8, 1.0]	0.02461×10^{-10}	3.3258×10^{-10}
Maximum error	0.031640×10^{-10}	0.033258×10^{-10}

Table 3: The maximum error of interpolated initial condition functions to the analytical solution (see (16)). $E(T_f) = \max|f(x) - \bar{f}(x)|$, for all $0 \leq x \leq 1$.

x	$E(T_f)$
[0.0, 0.2]	$0.0002836181 \times 10^{-10}$
[0.2, 0.4]	0.0000
[0.4, 0.6]	0.0000
[0.6, 0.8]	0.0000
[0.8, 1.0]	$0.0002836181 \times 10^{-10}$
Maximum error	$0.0002836181 \times 10^{-10}$

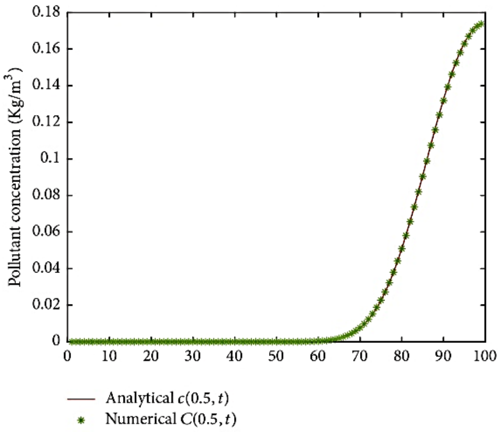

Figure 5: Comparison of analytical and approximated pollutant concentrations $c(0.5, t)$ (kg/m^3) ($\Delta x = 0.0125$, $\Delta t = 0.0100$, Pe $= 1.25$).

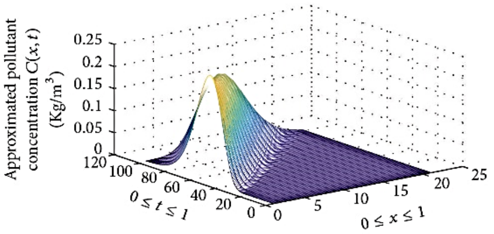

Figure 6: The Saulyev finite difference solution with quadratic interpolation $c(x, t)$ (kg/m^3) ($\Delta x = 0.0500$, $\Delta t = 0.0100$, Pe $= 5.0$).

numerical interpolation technique gives good agreement results. The accuracy of the Lagrange interpolation technique is used to predict their initial and boundary conditions as needed.

6. Conclusion

The proposed Saulyev finite difference scheme with the quadratic interpolation to the initial-boundary conditions technique is an unconditionally stable finite difference method. A large or small time step and/or grid size can be employed in the proposed techniques. The numerical experiment shows that the calculated results are reasonable approximations. The revision shows good agreement solutions. The proposed interpolation technique is suitable to be used in the real-world problem because it is easy to computer-code and because of the straightforwardness of the computer implementation. According to the collected water-quality data, functions that satisfy boundary conditions must be implemented. The computed results are verified by the numerical accuracy. The proposed technique gives reliable solutions to these processes.

Conflicts of Interest

The authors declare no conflicts of interest.

Acknowledgments

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The Saulyev Scheme for an Advection-Diffusion-Reaction Equation

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Abstract : The one-dimensional advection-diffusion-reaction equation is a mathematical model describing the transport and diffusion of pollutants and suspended matter in a river. If the flow of the river is non-uniform the model cannot be theoretically manipulated, therefore special numerical techniques are required. The objective of this research is to propose a simpler advection-diffusion-reaction technique, which is an unconditionally stable scheme of Soulyev. It is the large or small of time step and/or grid size can be employed in this technique. Examples are calculated for three of weighted parameter θ. The case of $\theta = 0$ gives a smooth solution comparing to the another values of $\theta's$. Increasing the mass decay rate affects the maximum concentration level. The numerical experiments have shown the expectable results.

Keywords : advection-diffusion -reaction equation; saulyev schemes; non-uniform.
2010 Mathematics Subject Classification : 76R50; 39A14; 35Q30; 35L51.

1 Introduction

Models are used to express the characteristics of reality which are considered important and to neglect those which seem secondary. These simplifications, good models allow to obtain an easily understandable, mathematically calculable image of the real world. A model is formulated with the aid of mathematical relation that is a mathematical model. A model is a set of rules, or formulas, which try to represent the behaviour of a given phenomenon. Several classes of mathematical models three classes appear: Models which come from laws of physics, this is the case for gravitation laws, Maxwell equations. Navier - Stokes equations, and so on; Model which come from empirical laws, such as air resistance for a movement.

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Model which come from statistical laws, for instance that fit a line between several points and assume the response to be linear. There are three reasons that why we build mathematical models. It gives a better understanding of the phenomenon, which leads to a more precise tuning of the parameters; It warns you get off limits for instance, An empirical knowledge usually is not enough to answer the questions. It allows you find the values of the parameters, which lead to a given result. So building a mathematical model usually means better control upon the phenomenon, which, in turns, mean more precision, cheaper results and better quality output. Those are the reasons to use mathematical model and how different from the fieldwork.

In [1], the Parabolic partial differential equations with nonstandard initial condition, feature in the mathematical modeling of many phenomena. While a significant body of knowledge about the theory and numerical methods for parabolic partial differential equations with classical initial condition has been accumulated, not much has been extended to parabolic partial differential equations with nonstandard initial condition. The Saulyev's explicit schemes are an economical implement to use. These unconditionally explicit schemes are very simple to program and compute. The new explicit schemes developed are very efficient and they need less CPU time than the implicit methods. The explicit finite difference schemes are very easy to implement for similar higher dimensional problems. In [2], a user friendly and a flexible solution algorithm is proposed for the numerical solution of the one-dimensional advection-diffusion equation (ADE), explicit spreadsheet simulation (ESS) technique is used instead of computer code. In the numeric solution of ADE by using finite differences, either the small values of a Courant number such as 0.05-0.10 is used for oscillation free results or an artificial diffusion is used in order to reduce oscillation. In order to provide for small Courant numbers, it is necessary to choose a small time step and/or grid size; however this increases the computer time. While the proposed ADEESS solution technique uses an unconditional stable Saulyev scheme, it is gives highly accurate results even for the values of the Courant numbers as high as 2-3. By changing only the values of the temporal weighted parameter(θ) are solved three θ values, 0, 0.5 and 1, respectively. The model results for the values of $\theta = 0$ are in good agreement with the analytical solution.

In [3],a better finite difference scheme to solve the dynamic one dimensional advection-dispersion-reaction equations (ADRE) is focused, and the effect of nonuniform water flows in a stream is considered. There are two mathematical models used to simulate pollution due to sewage effluent. First, is a hydrodynamic model for numerical techniques, we used the Crank-Nicolson method. Second, is a advection-dispersion-reaction model, we used explicit schemes. The revised explicit schemes are modified from two computation techniques of uniform flow stream problems, forward time central space (FTCS) and Saulyev schemes for dispersion model. A comparison of both schemes regarding stability aspect is provided so as to illustrate their applicability to the real-world problem.

The dispersion model that provides the pollutant concentration field. A modified MacCormack method is subsequently employed in the dispersion model. This proposed a simply remarkable alteration to the MacCormack method so as to make it more accurate without any significant loss of computational efficiency. The results obtained indicate that proposed modified MacCormack scheme does improve the prediction accuracy compared to that the tradition MacCormack method [4]. We propose and explores the simple revision to the MacCormack and Saulyev schemes that improve their accuracy for high Peclet number problems, which are named the Saulyevc and MacCormack schemes respectively, greatly improved the prediction accuracy over the original ones [5]. We propose a new scheme that guarantees the positivity of the solutions for arbitrary step sizes. We develop for one advection-diffusion reaction equation in one spatial dimension with constant velocity and diffusion and state how to generalize it [6]. The simple explicit schemes have the advantages of simplicity in computing without losing more accuracy and these schemes are precedent for several model applications. To identify the best one these simple schemes, comparative studies of these are necessary.

The object of this research is to propose a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes. The proposed numerical technique uses an unconditionally stable method. It is the large or small of time step and/or grid size can be employed in the techniques. We apply the method to three problems with different derivative right boundary conditions. The results of the model are show that the calculated results are reasonable approximations.

2 The Governing Equation

In this section, we consider the parabolic equation. The mathematical model describing the transport and diffusion processes is a one-dimensional advection-diffusion-reaction equation (ADRE)

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} - KC, \quad 0 < x < L, 0 < t \leq T, \tag{2.1}$$

with initial conditions

$$c(x,0) = f(x), \quad 0 \leq x \leq L, \tag{2.2}$$

and boundary conditions

$$c(0,t) = g(t), \quad 0 \leq t \leq T, \tag{2.3}$$

$$\left.\frac{\partial c}{\partial x}\right|_{x=L} = h(t), \quad 0 \leq t \leq T, \tag{2.4}$$

where x is the longitudinal distance along the stream, t is time, T is the last time, $f(x)$ and $g(t)$ and $h(x)$ are known functions, while $c(x)$ is the concentration averaged in depth at the point x and at time t, the function c is unknown, $u(x,t)$ is the velocity of the water in the x direction for all $x \in [0,1]$ at time t, D is the dispersion coefficient and K is the mass decay rate. We will consider the model with the following conditions, that $u(x,t)$ and D are positive constant values. The initial conditions $c(x,0) = f(x)$ at $t = 0$ for all $x > 0$. The boundary conditions are $c(0,t) = g(t)$ at $x = 0$ and $\partial c/\partial x = 0$ at $x = 1$.

3 Numerical Technique

The solution domain of the problem is covered by a mesh of grid-lines. The grid point (x_i, t_n) is defined by $x_i = i\Delta x$ for all $i = 0, 1, 2, ..., M$ and $t_n = n\Delta t$ for all $n = 0, 1, 2, ..., N$ in which M and N are positive integers, where x_i and t_n are parallel to the space and time coordinate axes. The constant spatial and temporal grid-spacing are $\Delta x = L/M$ and $\Delta t = T/N$.

Consider the following approximations of the derivative in the advection - diffusion equation which incorporate time weights θ as follows

$$\frac{\partial c}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{3.1}$$

$$u\frac{\partial c}{\partial x} = u_i^{n+1}\left(\frac{1}{2\Delta x}\right)\left[c_i^{n+1} - c_{i-1}^{n+1} + c_{i+1}^n - c_i^n\right], \tag{3.2}$$

$$\begin{aligned} D\frac{\partial^2 c}{\partial x^2} =& D\left(\frac{\theta}{(\Delta x)^2}\right)\left[c_{i-1}^{n+1} - c_i^{n+1} + c_{i+1}^n - c_i^n\right] \\ &+ D\left(\frac{(1-\theta)}{(\Delta x)^2}\right)\left[c_{i+1}^n - 2c_i^n + c_{i+1}^n\right], \end{aligned} \tag{3.3}$$

where θ is the weighting factor. Substituting the Equation (3.1) - (3.3) into the Equation (2.1).

$$\begin{aligned} &\left[1 + \frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_i^{n+1} - \left[\frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1} \\ &= \left(\frac{Cr}{Pe} - \theta\left(\frac{Cr}{Pe}\right)\right)c_{i-1}^n + \left[1 + \frac{Cr}{2} - 2\left(\frac{Cr}{Pe}\right) + \theta\left(\frac{cr}{Pe}\right) + K\Delta t\right]c_i^n \\ &+ \left[\frac{Cr}{Pe} - \frac{Cr}{2}\right]c_{i+1}^n, \end{aligned} \tag{3.4}$$

for $1 \leq i \leq M-1$ and $1 \leq n \leq N-1$, where $Cr = \frac{u\Delta t}{\Delta x}$ and Courant number and $Pe = \frac{u\Delta x}{D}$ is Pelet number.

Although the Equation (3.4) does not seem explicit, because c_{i-1}^{n+1} and c_i^{n+1} are on the left-hand side, a suitable use of the equation makes it explicit.

Therefore, Equation (3.4) can be written in the following form

$$\begin{aligned} c_i^{n+1} =& \left\{\left[\frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^{n+1} + \left[\frac{Cr}{Pe} - \theta\left(\frac{Cr}{Pe}\right)\right]c_{i-1}^n\right. \\ &+ \left.\left[1 + \frac{Cr}{2} - 2\left(\frac{Cr}{Pe}\right) + \theta\left(\frac{Cr}{Pe}\right) + K\Delta t\right]c_i^n + \left[\frac{Cr}{Pe} - \frac{Cr}{2}\right]c_{i+1}^n\right\} \\ &/\left[1 + \frac{Cr}{2} + \theta\left(\frac{Cr}{Pe}\right)\right]. \end{aligned} \tag{3.5}$$

This scheme is explicit. In this case, only a single value, c_i^{n+1} will be unknown. This scheme is known as Saulyev's formula and the main advantage of it is that it is unconditionally stable and explicit.

4 Application to a Stream Water Assessment Problem

Suppose that the measurement of pollutant concentration C in a non-uniform flow steam is aligned with longitudinal distance, 1.0 (km) total length and 1.0 (m) depth. There is a plant which discharges waste water into the stream and the pollutant concentration at the discharge point is $C(0,t) = C_0 = 2 + sin(t)(mg/L)$ at $x = 0$ for all $t > 0$ and $C(x,0) = 2 + x(1-x)(mg/L)$ at $t = 0$. The approximation of pollutant concentrations C of all schemes is show in Tables 1, 2 and 3 and Figure 1. The comparison of among 3 schemes.

Case 1: There is not rate of change of pollutant concentration at $x = L$. These means that $\frac{\partial c}{\partial x} = 0$.

Case 2: If the rate of change of pollutant concentration at $x = L$ is increase. These can be assumed that $\frac{\partial c}{\partial x} = 0.05$.

Case 3: If the rate of change of pollutant concentration at $x = L$ is decrease. We can be assumed that $\frac{\partial c}{\partial x} = -0.05$.

Table 1: Pollutant Concentration $c(x,t)(kg/m^3)$ of case 1.

Sec$(t)\backslash x$	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2400	2.1600	2.0000
5	1.0411	2.8222	2.1687	2.2387	2.2588	2.1997
10	1.4560	1.7149	2.1427	2.1112	2.2332	2.2726
15	2.6503	1.0077	2.6532	2.1862	1.3591	2.2192
20	2.9129	1.74088	1.4384	3.0381	1.3591	2.2164
25	1.8676	2.8574	1.0617	2.3877	2.5125	1.0404

5 Discussion and Conclusion

In this research, the approximation of the pollutant concentrations of a simple advection-diffusion-reaction numerical simulation by using the Saulyev schemes is shown in Table 1, 2 and 3 and Figure 1. The numerical techniques are proposed for three θ values, 0, 0.5 and 1, respectively. The case of $\theta = 0$ gives a smooth

Table 2: Pollutant Concentration $c(x,t)(kg/m^3)$ of case 2.

Sec$(t)\backslash x$	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2500	2.1600	2.0000
5	1.0411	2.8222	2.1382	2.1985	2.2588	2.2122
10	1.4560	1.7149	2.9803	2.1546	2.2398	2.2852
15	2.6503	1.0077	2.6532	1.0615	2.0994	2.2318
20	2.9129	1.74088	1.4384	1.5235	1.3658	2.2290
25	1.8676	2.8574	1.0640	2.7136	2.5191	1.0530

Table 3: Pollutant Concentration $c(x,t)(kg/m^3)$ of case 3.

Sec$(t)\backslash x$	0	20	40	60	80	100
0	2.0000	2.1600	2.2400	2.2400	2.1630	2.0050
5	1.0411	2.8222	2.1382	2.2387	2.2588	2.2121
10	1.4560	1.7149	2.9803	2.1112	2.2266	2.2849
15	2.6503	1.0077	2.6532	2.1861	2.0859	2.2316
20	2.9129	1.74088	1.4384	3.0344	1.3524	2.2288
25	1.8676	2.8574	1.0594	2.3840	2.5060	1.0528

solution compare to another values. Increasing the mass decaying rate affects the maximum concentration level. The proposed numerical technique uses are unconditionally stable methods. It is the large or small of time step and/or grid size can be employed in the techniques. The numerical experiments show that the calculated results are reasonable approximations. The revision shows good agreement solutions. The proposed technique is suitable to be used in the real-world problem due to it easily to program and the straight forwardness of the implementation.

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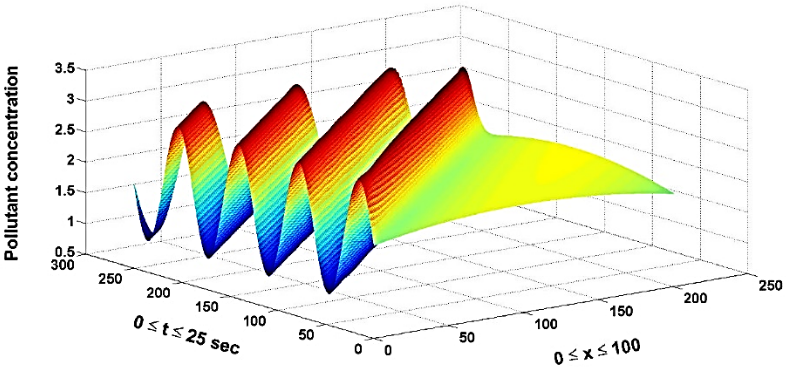

Figure 1: Pollutant Concentration $c(x,t)(kg/m^3)$ of case 1.

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Academic Publication(s)

1. Samlerk, P and Pochai, N. 2018 "Numerical Simulation to a One-dimensional Water-Quality Model in a Stream using a Saulyev Technique with Quadratic Interpolated Initial-Boundary Conditions" *Abstract and Applied Analysis*. Article ID 1926519. : 7 pages.
2. Samlerk, P and Pochai, N. 2018 "The Saulyev Scheme for an Advection- Diffusion-Reaction Equation." *Thai Journal of Mathematics.* : 7page. (Accepted)