

TWO-DIMENSIONAL MATHEMATICAL MODEL NAMED TUNA-WQ FOR WATER QUALITY ANALYSIS

by

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LIST OF ABBREVIATIONS

1-D	One-dimensional
2-D	Two-dimensional
3-D	Three-dimensional
BOD	Biochemical oxygen demand
BOD-DO	Biochemical oxygen demand-Dissolve oxygen
COD	Chemical Oxygen Demand
DHI	Danish Hydraulic Institute
DO	Dissolved oxygen
DOE	Department of Environment
DOFM	Department of Fisheries Malaysia
E. Coli	Escherichia coli
EIA	Environmental Impact Assessment
EQA	Environmental Quality Act
FDM	Finite difference method
FPSO	Floating Production, Storage and Offloading
GDP	Gross domestic product
IOC	Intergovernmental Oceanographic Commission
NKEA	National key economic area
OGE	Oil, gas and energy
SNP	Siakap-North Petai
SS	Suspended solids
SWE	Shallow water equations
UN	United Nations
USEPA	United States Environmental Protection Agency

VCE	Vatnaskil Consulting Engineers
WASP	Water Quality Analysis Simulation Program
WQI	Water Quality Index

LIST OF SYMBOLS

α	Rate of decay
β	Aeration rate
η	Water elevation above mean
η_0	Initial condition for water elevation above mean
σ	Wave frequency
Δt	Temporal grid size
Δx	Spatial grid length in x -direction
Δy	Spatial grid length in the y -direction
A	Surface area
a	Wave amplitude
C_{BOD}	Concentration of BOD
$C_{\text{BOD},0}$	Initial condition for BOD
C_{DO}	Concentration of DO
$C_{\text{DO},0}$	Initial Condition of DO
C_s	Oxygen saturation constant
d	Water depth below mean sea level
E_x	Dispersion in x -direction
E_y	Dispersion in y -direction
g	Gravitational acceleration
H	Mean water depth
h	Total water depth
i	Finite difference spatial node in x -direction
j	Finite difference spatial node in y -direction
k	Finite difference time node

K	Wave number
n	Manning Friction coefficient
P	Wetted perimeter
Q	Flow rate
s	Longitudinal slope of channel
S	Concentration of parameter
S_0	Initial concentration of parameter
t	Time
u	Velocity component in x -direction
u_0	Initial condition for u
V	Volume
v	Velocity component in y -direction
v_0	Initial condition for v
v_s	Settling velocity
W	Loading
W_{BOD}	BOD Loading

MODEL MATEMATIK DUA-DIMENSI BERNAMA TUNA-WQ UNTUK ANALISIS KUALITI AIR

ABSTRAK

Tujuan utama kajian ini adalah untuk membangunkan model kualiti air dua-dimensi, yang diberi nama TUNA-WQ, sebagai alternatif kepada model kualiti air sedia ada yang sukar disediakan dan terhad dalam penggunaannya ataupun dilesenkan. Terdapat banyak model kualiti air yang sedia ada, masing-masing dengan ciri-ciri tersendiri yang menentukan kemudahan dan kesesuaiannya dalam simulasi pelbagai badan air. Model TUNA-WQ disahkan melalui perbandingan dengan penyelesaian analitikal sedia ada dan model kualiti air AQUASEA sebelum digunakan untuk simulasi kepulan pepejal terampai dalam air laut disebabkan pelepasan keratan gerudi dari pelantar penerokaan minyak dan gas luar pesisir di Medan Kikeh Siakap-Utara Petai, yang terletak di Laut China Selatan. Hasil simulasi menunjukkan bahawa kepekatan pepejal terampai dan kesan yang dihasilkan oleh pelepasan keratan gerudi tidak membimbangkan dari segi pengangkutan dan kegigihan pepejal terampai. Model TUNA-WQ juga digunakan untuk menyiasat kesan kumbahan yang dilepaskan oleh ladang akuakultur udang marin di Sungai Setiu, Terengganu. Pengangkutan pepejal terampai, kemasinan, *E. coli* dan dinamik Keperluan Oksigen Biokimia-Oksigen Terlarut (BOD-DO) di Sungai Setiu disebabkan oleh pembuangan efluen ladang akuakultur udang marin telah disimulasikan. Hasil simulasi menunjukkan bahawa pelepasan kumbahan ladang udang marin akan meningkatkan kepekatan pepejal terampai, kemasinan, *E. coli* dan keperluan oksigen biokimia dalam air sungai berhampiran lokasi pelepasan. Walaupun kepekatan pencemar ini agak rendah berbanding piawaian batas maksimum kepekatan parameter yang

ditetapkan untuk Kelas 1 Klasifikasi Indeks Kualiti Air Malaysia, namun, adalah penting untuk memastikan rawatan yang mencukupi dijalankan ke atas kumbahan bagi mengurangkan kesan kepada kualiti air di sungai.

TWO-DIMENSIONAL MATHEMATICAL MODEL NAMED TUNA-WQ FOR WATER QUALITY ANALYSIS

ABSTRACT

The main purpose of this study is to develop an in-house two-dimensional water quality model, codenamed TUNA-WQ, as an alternative to currently available water quality models, which are often either difficult to set up and limited in their application or are licensed. There are numerous water quality models available, each with their own characteristics, which determines its ease and suitability in simulating various water bodies. The in-house TUNA-WQ model is validated through comparisons with available analytical solution and the water quality model, AQUASEA before being used to simulate suspended solids plumes in marine water due to discharge of drill cuttings from an offshore oil and gas exploration platform in the Kikeh Siakap-North Petai field, located in the South China Sea. Simulation results indicate that the suspended solid concentration and impact generated by the discharge drill cuttings are not a concern in terms of suspended solid transport and persistence. The TUNA-WQ model is also applied to investigate the effects of effluent released from a marine shrimp aquaculture farm on Setiu River, Terengganu. The spatial temporal transport of suspended solids, salinity, *E. coli* and Biochemical Oxygen Demand-Dissolved Oxygen (BOD-DO) dynamics in the Setiu River due to the discharge of effluent from a marine shrimp aquaculture farm are simulated. Simulation results show that the discharge of effluent from the marine shrimp farm will increase the concentration of suspended solids, salinity, *E. coli* and biochemical oxygen demand in the river's water near the discharge location. Although the concentration of these pollutants is relatively low compared to the maximum limit of

the specified parameter concentration for Class 1 of Malaysian Water Quality Index Classification, it is important to ensure sufficient treatment of the effluent to reduce its impact on the receiving river's water quality.

CHAPTER 1

INTRODUCTION

1.1 Introduction to Water Quality

Water is a vital resource that is important for a healthy ecosystem and the survival of humanity itself. The growing demand for water resources has a major impact on social, economic and environmental health. This pressure on supply is influenced primarily by economic and population growth, pollution, climate change amongst many other factors. Almost half of our wetlands have vanished due to the rapid development of the planet, leading to large scale degradation in the quality of natural water resources around the world. This in turn will lead to an increase in the cost of water treatment, as well as threatening the health of people and ecosystems.

Water resources are finite and can only be renewable if well-managed. If a water resource is managed well and efficiently, it can play an important role in strengthening social, economic and environmental systems during periods of rapid changes and development. Water is one of the most important components in sustainable development, which is defined as “development that meets the needs of the present without compromising the ability of future generations to meet their own needs.” (UN, 1987). Sustainable development focuses on three key aspects of human well-being—economic, socio-political and environment conditions—with the basic premise of putting in place strong measures for economic and social development while ensuring environmental integrity is sustained for future generations. Increasing demand for water, coupled with decreasing resources create challenges in providing

sustainable sources of potable water. It is therefore vital to protect our existing waters from pollution while achieving sustainable development.

The term 'water quality' refers to the water's chemical, biological, physical and radiological characteristics and is a measure of the state of the water relative to its uses or purposes (Johnson et al., 1997). Water standards are set based on the water purposes and uses that are mainly divided into three categories: human consumption, industrial and domestic use, and environmental water quality. For human consumption, water must be treated from contaminants such as microorganisms, inorganic contaminants, organic chemicals and other pollutants that may affect the health and well-being of humans. Industrial and domestic use of water on the other hand, requires water that has less dissolved minerals. The presence of dissolved minerals such as ions of calcium and magnesium may affect industrial machineries as well as domestic water heaters or boilers (Babbitt & Doland, 1949).

The disposal of waste and effluents from various industrial activities will affect the water quality of receiving water bodies. Thus, a standard for the environmental water quality is important. An environmental water quality standard for rivers, lakes estuaries and oceans is needed in order to maintain its quality. The presence of pollutants such as toxic substances, microorganisms, biochemical oxygen demand (BOD) and suspended solids (SS) could be a hazard for recreational uses involving body contact such as aquatic sports and fishing. Poor water quality in natural water bodies could potentially affect the surrounding sensitive aquatic species as well as wildlife which use the water for drinking. This could potentially harm the surrounding habitat and disrupt the water body's ecosystem. Therefore, water quality laws are put in place in different jurisdiction to ensure the retention of good water quality standards depending on the water body classes and their uses.

In Malaysia, water quality standards are set under the Malaysia's Environmental Law, Environmental Quality Act (1974) and the Malaysia Environmental Quality (Industrial Effluent) Regulations 2009. The Malaysia's Environmental Quality Act is implemented and enforced by the Department of Environment (DOE). These are important bases for the preservation of water bodies through the continuous improvement and maintenance of the country's current quality and standards. Development projects near water bodies must not have an impact on the water bodies' quality such that its standards are greatly affected. Environmental management decisions must be made to ensure sustainability of the planned development projects.

Water quality models are useful tools for simulation and prediction of the levels, distributions and risks of pollutants discharged into a certain water body. These model-predicted impacts and mitigation measures provide a basis for environmental management agencies to make the right decisions. Many of these water quality models have been developed to evaluate environmental impacts and to propose mitigation measures. There are several well-known models available for water quality simulation, but these models are either difficult to setup and limited in their application or are licensed. This compelled us to develop an in-house two-dimensional (2-D) water quality simulation model named TUNA-WQ that could be readily adapted and customized to serve a particular problem.

1.2 Water Quality Standards in Malaysia

Malaysia has several water quality standards from the Environmental Quality Act (EQA, 1974) which includes the Water Quality Index (WQI), Malaysia Marine

Water Quality Criteria and Standard, and the Sewage and Effluent Discharge Standards. The details of these standards are given in Appendix A. Since 1978, the DOE has been conducting river monitoring to develop a base quality of standards as well as to detect changes in the water quality of rivers in Malaysia. The monitored and collected water quality data were used to determine the status of the river's water quality where it can range from clean, slightly polluted to polluted. The water quality of a river can be categorized into Classes I, II, III, IV and V based on the WQI for Malaysia as seen in Table A1 in Appendix A. The WQI is based on the parameters of BOD, chemical oxygen demand (COD), ammoniacal nitrogen, pH, dissolved oxygen (DO) and SS. Other parameters such as heavy metals and bacteria are monitored based on specific site requirements.

Aside from river monitoring, DOE also monitors marine and coastal water quality. Malaysia's coastal areas and surrounding seas are naturally abundant in aquatic resources. The protection of these aquatic resources is an important factor in ensuring sustainability and thus, the quality of marine needs to be kept to standard. Rapid and major developments on coastal areas and islands have significantly impacted the surrounding sensitive marine environment. To make sure that these sensitive aquatic resources are well managed and protected, monitoring of the marine water quality is important. The Malaysia marine water quality criteria and standard is divided into Class 1, 2, 3 and E as seen in Table A2 in Appendix A, where each of the class has its own specified limit of the water quality parameters and intended beneficial use of these marine water quality classes.

The Malaysia sewage and effluent discharge standards are established to monitor the quality of effluents discharged from treatment plants into receiving waters. The

acceptable upper limit of the various water quality parameters of discharge is classified into Standards A and B, as listed in Table A3 in Appendix A. Ensuring that effluents discharged into receiving waters conform to the effluent discharge standards helps to enforce compliance by treatment plants and provides a cleaner and safer environment for all.

1.3 Objectives of Thesis

The objectives of this thesis include:

1. To develop an in-house 2-D water quality simulation model named TUNA-WQ.
2. To validate TUNA-WQ by means of comparison of its simulation result with analytical solution and AQUASEA.
3. To simulate SS concentration generated by onsite discharge of drill cuttings from an offshore oil and gas platform in Kikeh Siakap-North Petai Field by means of TUNA-WQ.
4. To study the impact of water effluent discharged from an aquaculture farm in Setiu River on the water quality of the receiving river by means of TUNA-WQ.

1.4 Scope and Organization of Thesis

This thesis starts with a brief introduction to water quality and its importance for sustainable development in Chapter 1. The water quality standards and guidelines for Malaysia are then briefly discussed to give a better understanding of the national

governance and limitation on water quality standards. The objective as well as the scope and organization of this thesis are then presented.

In Chapter 2, a relevant literature review on water quality model is presented starting with an overview on the developments of water quality models over the years. This is followed by a discussion on two common sub-models that made up a water quality model: the hydrodynamic model and the transport model. We then briefly review a few available and commonly used water quality models and the water quality studies that were conducted using these models. Motivation for the development of TUNA-WQ are discussed, along with the characteristics that are to be achieved. A short discussion on the application of TUNA-WQ for water quality study are then presented.

Chapter 3 presents the development of the 2-D water quality model TUNA-WQ. Discussion on the governing equations and numerical solution used in the hydrodynamic model, single pollutant transport model and Biochemical Oxygen Demand-Dissolved Oxygen (BOD-DO) transport model which made up the TUNA-WQ model is presented. TUNA-WQ is then validated through comparisons with available analytical solution and the water quality model, AQUASEA.

Offshore oil and gas exploration and production is an important part of Malaysia's development. Offshore drilling, the process where a wellbore is drilled into the seabed to extract oil and petroleum, is known to impose environmental risk if not managed properly. In Chapter 4, we present the simulations of SS concentration generated by the disposal of drill cuttings from an offshore oil and gas platform in the Kikeh Siakap-North Petai (SNP) Field. The in-house model TUNA-WQ is used

in this simulation. The simulated results are then presented and discussed in the chapter.

In Chapter 5, we study the impact of water effluent discharged from an aquaculture farm on the water quality of the receiving river. TUNA-WQ is used to simulate on the effects of effluent discharge from the aquaculture farm, iSharp on the water quality of the nearby Setiu River. The critical parameters considered in this simulation study are SS, DO, BOD, E. coli and salinity. The results of the simulation are presented and discussed in this chapter.

This thesis ends with some concluding remarks and future research direction in Chapter 6.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

A water quality model is an important tool to study the fate and transport of pollutants in different water bodies. The simulated results of water quality model under different pollutant loading scenarios allows for the exploration of mitigation measures for reducing the impact of these pollutants. Site experiments for the study of pollutant loading scenarios is irrational and impractical as it would directly pollute the experimental site. Thus, water quality models can be used as a mean to identify water environmental pollution and the fate and transport of pollutants in water bodies (Wang et al., 2009). The simulated results from water quality models allow support for proper management and mitigation plans to be chosen and executed.

2.2 Development of Water Quality Models

The development of water quality models has progressed substantially over the years since the creation of the first water quality model developed by Streeter and Phelps (1925) for the control of water pollution on the Ohio River. In the early twentieth century, there was significant recognition of the need for wastewater treatment to sustain a reasonable quality of life. Human impact on water quality in urban areas was noticed, prompting the need for wastewater treatment to be installed in such areas. However, optimal design and installation of such a facility depend

significantly on the natural assimilative capacity of the receiving environment. This drove Streeter and Phelps to form the first model of dissolved oxygen and organic carbon in the waters. However, the model then was limited to only a single point source and the flow needed to be steady and uniform. Despite these limitations, its simple analytical solution and validity as an approximate model gave rise to its application for many years. After the introduction of the first water quality model, subsequent studies by O'Connor (O'Connor, 1960; O'Connor, 1967) further developed the Streeter-Phelps Model, allowing the evaluation of DO concentration in streams and estuaries.

In developed countries, motivations arose for the development of more accurate and applicable models. These motivations came from a few factors such as the emergence of new pollutants, the improvement of drinking water standards, the formation of water quality regulation bodies, and improvements in wastewater treatment technology. New water quality pollutants and new evidence on their impact – both environmentally and socially – are considered during the advancement of water quality models. Thus, water quality standards became more specific in developed countries. As drinking water standards have improved, the complexity and cost of water treatment facilities have also increased. An important part of water quality regulation requires the determination of the natural assimilative capacity of water bodies. National government bodies were formed in developed and developing countries to enforce water quality regulation. Thus, the importance of water quality models for regulatory and management purposes became more significant, driving the need for its continuous improvement and development.

During the 1960s, when digital computers became more widely available, major developments were made in water quality model as numerical solutions became feasible. Thomann (1963) involved numerical expression into the analytical framework of the models. This allowed the extension of the one-dimensional (1-D) model into the 2-D model systems. Coupling of the hydrodynamic model was done as well. In the early 1970s, the United States Environmental Protection Agency (USEPA) funded a water quality model called QUAL2, which allowed the simulation of nitrogen oxygen demand and river systems of steady and unsteady flow. During this period, focus on the development of water quality models was given on the topic of eutrophication. The extreme growth of algae has severely damaged many lakes in developing countries, prompting the need of eutrophication modelling. Nonlinear models were developed during this period which includes relationships between zooplankton, nutrients, biological growth rate, sunlight and temperature (Yih & Davidson, 1975).

Water quality models started to include more state variables and progressed into three-dimensional (3-D) models after 1975. Development on the role of solid matters along with their settling and suspending characteristics on the transport and fate of toxicants was highlighted (Thomann & Di Toro, 1983; Chapra & Reckhow, 1983). Watershed models were introduced into water quality models to reflect nonpoint source pollution input as a variable. Nonpoint source pollution refers to pollution resulting from many diffuse sources instead of only a single source. With the introduction of nonpoint source simulation and more constraint conditions, water quality management policies were improved during this period. In the 1980s and 1990s, national bodies and commercial organizations fully recognised and employed the use of water quality models. The emergence of water quality models with

improved user-interfaces has made them more marketable with a variation of modelling tools and application available. Examples of such models include QUAL model (Brown & Barnwell, 1987), MIKE model (Danish Hydraulic Institute DHI, 1993), WASP model (Ambrose et al., 1988) and AQUASEA (Vatnaskil Consulting Engineers VCE, 1998). Although these models have common elements, each of them has its own distinctive features, which are discussed in a later section of this chapter. Other distinct and more specific models that are generally not integrated into water quality models were also developed. Examples of these specific models include the micro-pollutant modelling (Chapra, 1991), oil slick modelling (Shen & Yapa, 1993), and sediment-water interactions (Di Toro & Fitzpatrick, 1993).

Due to robust and detailed regulation in developed countries, nonpoint source pollution has been reduced. Focus on the development of water quality models then shifted on to atmospheric deposition such as heavy metals, nitrogen compounds and organic compounds which has an effect on water quality of rivers (Poor et al., 2001; Morselli et al., 2003). These pollutants can be deposited onto the land surface of a watershed and then transferred by runoff to nearby water body. Air pollution models were later integrated with water quality models to simulate atmospheric pollution deposition (Esterby, 1996).

With advancements in analytical and numerical methods, such as the increase in spatial refinement and computer power, previously unrecognised pollutants have been documented in water bodies. An emerging water quality concern is the effect of personal care products on the environment and ecosystems. Many personal care products such as toothpaste, soap and cleansers contain tiny synthetic plastic particles called microbeads. These microbeads are too tiny to be removed during

wastewater treatment and are often non-biodegradable, resulting in the discharge of these microbeads into nearby waters (Fendall & Sewell, 2009). These microbeads are a threat to aquatic life and public health once they have made their way into the aquatic environment. Mistaken for food, the microbeads enter the food chain through fish, shellfish, marine mammals and birds that consumes the microbeads (Setälä et al., 2014; Lusher et al., 2013). The risks of microbeads in the aquatic environment and food chain are still not fully understood, which is why water quality models are shifted towards the simulation of this pollutant. Nonetheless, measures have already been taken in developed countries to ban the use of microbeads in cosmetic products.

2.3 Water Quality Model Components

Water quality of water bodies depends significantly on the characteristics of the water flow, the water depth and the water temperature (Thomann & Mueller, 1987). Water quality models focusing on the fate and transport of a pollutant in a water body will commonly have two sub-models: hydrodynamic model and transport model. These two sub-models form a simple water quality modelling tool that allows quantification of pollutant levels and distribution in a water body.

2.3.1 Hydrodynamic Model

To successfully simulate the water quality of a water body, the hydraulic state of the water body is an important condition that must be firstly characterised. The hydrodynamic model is usually governed by the Navier-Stokes equation, a set of

equations used to define the motion of fluids. Most water quality models generally divide the water body into a number of segments. Rivers are usually well mixed over their depth and width and thus the common method is to divide the river into segments lengthwise, giving a 1-D model. In water bodies where there is a significant flow in more than one direction such as estuaries and offshore, 2-D or 3-D segmentations are required (Watanabe et al., 1983). A 2-D or 3-D segmentation is important as well in providing a more accurate simulation results, particularly for water quality parameters which requires a more thorough analysis (Rutherford, 1994). A discretised solution of the Navier-Stokes equation is required at this point to model the hydrodynamic flow of water bodies. With suitable supporting data of the channel characteristics, the discretised solution allows for the accurate simulation of unsteady flow conditions. The solution of unsteady flow conditions is most helpful in water quality modelling involving unsteady flows such as tidal flow or pollutant spills. However, such models, particularly those involving complex boundary conditions are computationally hard to solve. A more refined discretisation is required for numerical stability as well as for accuracy standards. The discretised solution can be found using several methods whereby two classes of numerical methods is most common, the structured grid approaches such as the finite difference algorithms, and the unstructured grid approaches such as the finite element or finite volume method.

2.3.2 Transport Model

The transport and fate of a pollutant in a water body is simulated using the transport model. Pollutant transport in a water body is influenced mainly by the advection,

which is the movement of the pollutant carried by water flow. Aside from advection, another significant factor influencing the transport of pollutants in water bodies is dispersion, which is the dispersing of pollutants at a rate proportional to its spatial concentration gradient due to turbulent eddies. Other factors that effects the pollutant transport in a water body includes, the dead zones where eddies behind obstructions will entrap the pollutants, the transient storage zones where there is a temporary pollutant sorption to plants or sediments, and the non-uniform velocity over the width and depth of the water body. The usual method is to represent the pollutant transport model using the advection and dispersion process, while ignoring the dead zones, the transient storage zones, and the non-uniform velocity over the width and depth of the water body which are less significant in influencing the pollutant transport process (Camacho, 2000). The discretised solution of the advection-dispersion equation is used to model pollutant transport in a water body with the hydrodynamic model incorporated to provide the water flow information. A variety of water quality determinants can be modelled such as SS, BOD, DO, oils, nitrogen, phosphorus, pathogens and metals. Review has been done by Thomann & Mueller (1987) and Chapra (1997) on the processes transforming the state of these determinants.

2.4 Water Quality Models

Extensive reviews on the available water quality models have been done over the years as shown by Wang et al. (2013) and Gao & Li (2014). Here we briefly review some well-known water quality models, namely WASP, QUAL2E/2K, MIKE and AQUASEA.

2.4.1 WASP

The Water Quality Analysis Simulation Program (WASP) was developed by the USEPA in 1983. WASP allows for the simulation of 1-D, 2-D, and 3-D systems and a variety of pollutant types, including nitrogen, phosphorus, DO, BOD, sediment oxygen demand, organic chemicals, algae, metals, mercury, temperature and pathogens. The WASP model is suitable for water quality simulation in rivers, lakes, estuaries, coastal wetlands and reservoirs. Since WASP does not have a hydrodynamic sub-model, it is strictly used for the simulation of pollutant transport and reaction. However, hydrodynamic flow data can be incorporated from an external hydrodynamic model or by importing data files from external linkage files such as text files, spreadsheets or the hydrodynamic model interface information. Further, WASP can also be coupled with watershed models, allowing for multi-year analysis under varying environmental conditions.

WASP has been widely used in the United States and around the world. An example of water quality studies using WASP is the volatile organic pollution of the Delaware Estuary (Ambrose, 1987). Ambrose (1987) used WASP to simulate the upstream migration of seven volatile organic chemicals from a waste water effluent to a drinking water treatment plant in Philadelphia, Pennsylvania. Comparison of the simulated concentrations to the observed concentrations indicates a similar result and therefore the adequate performance of the WASP model. It was suggested that though the existing model is adequate, it could be improved through refinement and recalibration. Ambrose et al. (2005) also used the WASP model to analyse airborne mercury deposited on the Ochlockonee River watershed in Georgia. Atmospheric deposition monitoring and source attribution data were used along with simulation

models to calculate the fate and transport of mercury in the river. Results from the simulations suggest that almost 67 % of the atmospherically deposited mercury in the watershed is returned to the atmosphere, about 10 % is transported to the river while the remaining mercury is retained in the watershed. A reasonable agreement was shown from the comparison of the simulation results and the limited survey data. This concluded that though the WASP model is appropriate for the study of acceptable loading levels of mercury to the atmosphere, model calibration is needed to support new state variable for the accurate modelling of total or specific environmental mercury.

Caruso and Bishop (2009) applied the WASP model into the study of metal in Upper Tenmile Creek, Montana. In their study, WASP was used to model the resulting variation of total and dissolved metal loads with distance along the mainstream for two seasons. Results from the study show that high load of metals in the river is associated with higher erosion and increased transport from the stronger flow season.

Moses et al. (2015) used the WASP model in their study to predict daily variations in water quality parameters such as DO, BOD, nitrate, and chlorophyll concentrations in a tropical lake system. The tropical lake was divided into eight segments with the flow of the river and concentrations of the respective parameters being the model input. Results from the study suggest that precipitation greatly affects water quality whereby polluted water from drains will enter the lake system. Findings from the study confirm that specific and generalized conclusions can be accomplished with the use of the WASP model.

2.4.2 QUAL2E/2K

The USEPA developed the QUAL2E river and stream water quality model (Brown & Barnwell, 1987) which can simulate up to sixteen water quality parameters along a river. The QUAL2K model was later developed and intended to represent the modernized version of QUAL2E, where improvements include the expansion of computational structures and addition of more variables. QUAL2K is a 1-D, steady-state model of in-stream flow and water quality. The model divides the river into several segments of equal length with assumptions that the advection transport is based on the mean flow, the water quality parameters are completely mixed over the segment, and that the dispersive transport is associated with the concentration gradient. The QUAL2K model is suitable for simulation of dendritic river and nonpoint source pollution. The QUAL2K model will divide the river system into (a maximum 50) segments, where each segment is then divided into (a maximum 20) computational elements of equal length. Data requirements for the QUAL2K model include the flow data and hydraulic terms, initial conditions and reaction rate coefficients. QUAL2K is freely available for download from its website and is also advantageous in requiring only partial hydraulic data for simulations to begin. Nonetheless, the QUAL2K is limited in terms of its 1-D simulation and limited computational element number (maximum 50 segments $\times$ 20 elements) which confines the accuracy and sensitivity of the simulated water quality concentrations.

QUAL2K model is also widely used in water quality simulation. Some examples include the water quality modelling in the Bagmati River (Kannel et al., 2007). QUAL2K was used to model the water quality of the Bagmati River in Nepal, which receives wastewater containing organics and nutrients. The QUAL2K model was

applied to simulate several water quality management strategies during crucial periods to achieve the targeted water quality criteria of minimum DO at or above 4 mg/L and maximum BOD at or below 3 mg/L. The simulated maximum BOD is at 8.5 mg/L, which is much higher than the targeted water criteria of 3 mg/L. This is justified as reasonable by Kannel et al. (2007) by stating that Nepal is a developing country and the targeted European water quality criteria is difficult to achieve. Results from the simulations are found to be quite accurate compared to the field data with some exceptions. From the simulated results, the suggested mitigation measures were found to be suitable in achieving the water quality management goals for a developing country. Suggestions were given to improve on the simulation accuracy by using a 2-D or 3-D models.

Zhang et al. (2012) applied the QUAL2K to model the water quality of the Taihu Lake Basin, China. Due to pollution in the Taihu Lake Basin, water quality improvement programs were suggested to improve the water quality of the lake for sustainable development. Selection of a suitable optimal water quality improvements program is important to ensure its effectiveness and efficiency. The QUAL2K model was used to study the effects of a variety of water quality improvement program scenarios in the lake to facilitate the selection of the most optimal program. Results from the study indicated the most optimal scenario comprised of an oxidation system upstream followed with an ecological floating bed and a moveable ecological bed downstream. This scenario could reduce the BOD, ammonia nitrogen, total nitrogen, and total phosphorus by 49.50 %, 32.81 %, 35.94 %, and 45.27 %, respectively.

Hadgu et al. (2014) used the QUAL2K to model the dispersion of pollutants in River Ngarugu, Kenya. QUAL2K was calibrated with the collected data on flow, BOD,

DO and Nitrate of the river. The performance of the water quality model was assessed by comparing the simulated result with the observed data. The model was found to reflect the field data quite well with some minor exceptions. Though there exist minor differences between the simulated results and the field data, the model is accepted particularly given that financial resources for frequent monitoring and higher accuracy data analysis is limited, especially in developing countries.

2.4.3 MIKE

The Denmark Hydrology Institute (DHI) developed the MIKE models for water quality modelling. For water quality models, the models available from DHI include MIKE 11 (DHI, 1993), MIKE 21 (DHI, 1996a) and MIKE 3 (DHI, 1996b). MIKE 11 is a 1-D model that can simulate water flow and water quality transport in rivers, irrigation canals, flood plains and other inland water bodies. The model requires a large amount of data and is well suited for complex systems. The hydrodynamic model of MIKE 11 simulates dynamic flows in river with the assumption that the flow is homogenous within the river channel. The advection-dispersion model combined with the hydrodynamic model of the MIKE 11 allows for the appropriate simulation of first order decay of pollutants. Moreover, the MIKE 11 model allows more complex simulations such as the reaction of nitrate and ammonium on BOD. Data on hydrodynamic, advection-dispersion and water quality parameter can be entered from the interface of the model. The flow simulation is first performed followed by the simulation of pollutant transport. MIKE 21 can simulate flow, waves, sediments and ecology in rivers, estuaries and coastal areas in 2-D while MIKE 3 enables simulations of coastal regions, estuaries and lakes in 3-D.

These MIKE models are among the most advanced water quality models and are used worldwide in the application of water quality studies. However, it might not be financially viable for individual researcher without institutional support to maintain the license of the MIKE software due to its high cost. Example of the use of MIKE11 in water studies is the application of the MIKE11 model for the Euphrates River in Iraq (Kamel, 2008). MIKE11 was used to model the unsteady flow along a stream channel with length of 1.6 km, with the results compared to observed hydrograph. The results from MIKE11 was found to compare well with the observed data.

Menendez et al. (2013) studied the water quality of a coastal zone in the Inner Plata River in Argentina using the MIKE21 water quality model. The Plata River is one of the largest estuaries in the world with an estuarine area estimated at 35000 km². The limited water use zones of the Plata River are identified through a combination of the simulated results and the water quality criterion. A project scenario, the Remediation Master Plan is evaluated with the model to assess the benefits and costs from the changes of the limited water uses zones. The study gave an indication of the usefulness and validity of the water quality model in evaluating the water quality in coastal zone as well as its use in supporting proper mitigation plans to be implemented.

Shakibaeinia et al. (2014) used the MIKE11 model to model a 200-km reach of the Athabasca River, Alberta. Simulation of the river is done using a river-ice model (CRISSP-1D) (Shen, 2005) to replicate the ice conditions during the cold seasons where the effect of frozen river surface on the chemical and physical process of the river system is taken into consideration. The MIKE11 model is then used to simulate the transport of DO in the river with the data evaluated and validated using available

field measurements. Results of the simulation study gave understandings into the spatial and temporal variation of DO in the Athabasca River as well as the importance of ice cover on the DO concentration.

2.4.4 AQUASEA

AQUASEA is a water quality model developed by the Vatnaskil Consulting Engineers (VCE) in 1985 and is designed to solve the shallow water equation (SWE) and transport equation using the finite element method. Constantly upgraded since 1985, the AQUASEA software consists of two models, the hydrodynamic flow model and the transport model. The hydrodynamic flow models allow for the simulation of water flows in estuaries, bays, lakes, rivers and coastal areas. The transport model of AQUASEA is designed to solve the equation of mass and heat transport under the effect of the hydrodynamic flow and dispersion. The equations are solved using a Galerkin finite element method on triangular elements. AQUASEA can simulate pollutants of any kind such as inorganic or organic salt, DO, inorganic phosphorus, nitrogen as well as SS and heat transport. Though it can simulate transport of DO, AQUASEA is unable to simulate the BOD-DO reaction process in water, thus it is unable to study the effects of BOD concentration on the DO concentration of water bodies.

Irtem et al. (2011) used the AQUASEA model for simulating the water flow movement in Ayvalik Bay, Turkey. The water flow movements in the Ayvalik Bay were investigated along with the effect of the landfill road on these flows. The study shows that higher flow velocity is recorded in the polluted areas after the removal of the present landfill road, giving a positive effect on the water circulation of the

Ayvalik Bay. Thus, the results of the study are a vital input into the pollution prevention efforts for the Ayvalik Bay.

AQUASEA has been used to simulate the water flow in Manzala Lake, Egypt (El-Naggar, 2016). The lake has deteriorated due to an increase in contaminants from effluent inflow and intensive aquaculture, prompting a need to study the effects of hydrodynamic on pollutant transport from drains and inspect potential mitigation measures. The hydrodynamic flow model of AQUASEA was used to simulate and display the effect of water flow on the pollutant dispersion in Manzala Lake. The simulated flow result from the study is then used to assess any proposed engineering solution for conserving the habitat of the lake.

2.5 TUNA-WQ

Water quality models with their numerous application in water quality analysis helps in determining the appropriate mitigation actions to be carried out in reducing the impact of pollutants on water bodies. While there are numerous water quality models available as mentioned above, each of these water quality models has their respective characteristics, such as dimension, parameters, numerical methods, and computational algorithm, which all determines the complexity of the model as well as its ease of use and suitability in simulating different water bodies. A summary on the available models and their respective characteristics is shown below in Table 2.1. As shown in Table 2.1, there are several well-known models available for water quality simulation, but these models are either difficult to setup and limited in their application or are licensed.

Table 2.1: Available water quality models and their characteristics.

Models	Numerical method	Model dimension	Sub-models	Advantages & limitations
WASP	Finite difference method	1-D, 2-D and 3-D	Transport model	- Needs to be linked with external hydrodynamic model. - Able to simulate BOD-DO dynamic - Freely available for download and use.
QUAL	Finite segment	1-D	Hydrodynamic model, Transport model	- Able to simulate BOD-DO dynamic. - Allows only 1-D steady-state simulation.
MIKE	Finite difference method	1-D, 2-D and 3-D	Hydrodynamic model, Transport model	- Able to simulate BOD-DO dynamic - Powerful water quality model and widely used by researchers. - High cost for licensing rights.
AQUASEA	Finite element method	2-D	Hydrodynamic model, Transport model	- Allows 2-D simulation - Unable to simulate BOD-DO dynamic. - Limited to 10000 computational elements.

Although the WASP model is freely available for download and use, it is difficult and tedious in terms of the model set-up particularly for 2-D and 3-D variable flow. The QUAL model on the other hand is easy to use and set up due to its simplicity but is limited in terms of accuracy as it only allows for 1-D simulation. Powerful water quality models such as MIKE are popular due to their advanced hydrodynamic model and ability to simulate pollutant transport in complex river systems, but such models are expensive due to high licensing costs. AQUASEA can simulate 2-D models and is less costly as compared to MIKE, but the AQUASEA model is unable

to simulate two constituents. Thus, the AQUASEA model is not able to simulate the BOD-DO dynamic.

To overcome the limitations in the above-mentioned water quality models, we were motivated to develop an in-house 2-D water quality simulation model named TUNA-WQ. The characteristics for the TUNA-WQ model are listed in Table 2.2. The TUNA-WQ model is currently able to simulate up to 2-D as well as up to two constituents, mainly the BOD-DO dynamic. TUNA-WQ consists of 2 sub-models, the hydrodynamic model and the transport model.

Table 2.2: TUNA-WQ water quality model’s characteristics.

Models	Numerical method	Model dimension	Characteristics
TUNA-WQ	Finite difference method	1-D and 2-D	Able to simulate two constituents (BOD-DO dynamic). Easily adaptable and customizable.

For the hydrodynamic model, the discretised solution of the Navier-Stokes equation is based on the Explicit Staggered Finite Difference Method from Intergovernmental Oceanographic Commission IOC (1997). In this method, the Navier-Stokes equation is simplified into the SWE which is then solved numerically using the finite difference method (FDM). The numerical method adopted from IOC (1997) is briefly discussed in Chapter 3.

Similarly, the numerical solution for the advection-dispersion equation is obtained using the Explicit Staggered Finite Difference Method. In this thesis, the transport model is classified into (i) a one constituent model, namely, the pollutant transport model and (ii) a two-constituent model, namely, the BOD-DO transport model. The