

WATER QUALITY MODELING USING MATHEMATICAL FORMULATION IN  
QUAL2E

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For  
mak and ayah  
I really tried my best

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## ABSTRACT

The importance of river in the global development of mankind is undeniable since most of the early urban settlements in the history of human civilization were discovered near rivers. This development has resulted in wide spread exploitation of the river in many ways such as industries water supply, transportation purpose, domestic usage and also waste disposal. Understanding the negatives effect in long term an improvement of river management and one of the convenient ways is to manage water using water quality model. In this study, QUAL2E a one dimensional water quality model is proved using finite difference of advection dispersion equation. Since the focus of this study is on mathematical formulation, hydraulic data and river characteristics are taken from Tiung (2003). The result of the mathematical calculation is compared with the validated data obtained from this QUAL2E model. Using assumptions to obtain the value of external source, result are obtained in three different ways which are in linear, quadratic and cubic assumptions. The observation shows that the cubic assumptions is the most accurate among other assumptions since the error is small after comparison with data obtained from Tiung (2003). This study shows how the mathematical formulation is used to obtain the value of element's concentration required.

## ABSTRAK

Kepentingan sungai dalam pembangunan global manusia tidak dapat dinafikan lagi. Inikerana kebanyakan penempatan awal bandar yang bersejarah dalam tamadun manusia ditemui berhampiran sungai. Perkembangan ini telah menyebabkan eksploitasi meluas sungai dalam pelbagai cara seperti bekalan air industri, pengangkutan, penggunaan domestik dan juga pelupusan sisa. Memahami kesan negatif dalam jangka masa panjang, berlakunya peningkatan pengurusan sungai dimana salah satu cara yang mudah untuk menguruskan air adalah dengan menggunakan model kualiti air. Dalam kajian ini, QUAL2E model kualiti air satu dimensi yang dibuktikan dengan menggunakan beza sehingga menggunakan persamaan penyebaran adveksi. Oleh kerana fokus kajian ini adalah kepada permodelan matematik, data hidraulik dan ciri-ciri sungai adalah diambil dari Tiung (2003). Hasil pengiraan matematik dibandingkan dengan data sah yang diperolehi daripada model QUAL2E ini. Menggunakan andaian untuk mendapatkan nilai sumber luar, hasilnya diperolehi dalam tiga cara yang berbeza yang ada di dalam andaian linear, kuadratik dan kubik. Pemerhatian menunjukkan bahawa andaian kubik adalah tepat berbanding andaian lain kerana peratus kesilapan yang kecil selepas perbandingan dengan data yang diperolehi dari Tiung (2003). Kajian ini menunjukkan bagaimana pembentukan matematik digunakan untuk mendapatkan nilai kepekatan unsur yang diperlukan.

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## LIST OF SYMBOLS

$A$	- Cross-Sectional Area Of Flow
$C$	- Cross-Sectional Average Concentration
$d^1$	- Distance
$d$	- Depth
$D$	- Longitudinal Dispersion Coefficient
$K$	- Dispersion Constant
$K_1$	- BOD Decomposition Rate
$K_2$	- Reaeration Rate
$K_3$	- BOD Settling Rate
$K_4$	- Sediment Oxygen Demand
$L$	- Carbonaceous Bod
$M$	- Mass
$n$	- Manning Roughness Coefficient
$o$	- Dissolved Oxygen Concentration
$o_s$	- Dissolved Oxygen Saturation Concentration
$p_i$	- Internal Constituent Sources And Sinks
$Q_{i-1}$	- Flow From The Upstream Element
$Q_{x,i}$	- Lateral Flow Into (Positive) or Out of (Negative) The Element
$Q_i$	- Outflow From The Element
$r_0$	- Pipe Radius
$r_i$	- First Order Rate Constant
$S$	- Source
$t$	- Time

$u^*$	- Shear Velocity
$U$	- Cross-Sectional Average Velocity
$x$	- Direction Of Mean Flow Velocity/Distance
$y$	- Wall Coordinate
$n_A$	- Mass Flux Vector
$\tau_0$	- Boundary Shear Stress
$\rho$	- Mass Fluid Density
$\Delta$	- Del Operation

## LIST OF ABBREVIATIONS

BOD	- Biochemical Oxygen Demand
<i>BOD</i> <sub>5</sub>	- Biochemical Oxygen Demand (5-day)
CBOD	- Carbonaceous Biochemical Oxygen Demand
CWQM	- Center for Water Quality Modeling
DO	- Dissolved Oxygen
MAPE	- Mean of Absolute Percentage Error
MISG	- Mathematics In Industry Study Group
NBOD	- Nitrogeous Biochemical Oxygen Demand
<i>NO</i> <sub>2</sub>	- Nitrite
<i>NO</i> <sub>3</sub>	- Nitrate
NORG	- Organic N Concentration
<i>NH</i> <sub>4</sub>	- Ammonia
<i>PO</i> <sub>4</sub>	- Orthophosphate Concentration
QUAL2E	- Enhanced Stream Water Quality Model
QUAL2E-UNCAS	- Enhanced Stream Water Quality Model with Uncertainty Analysis
SEMCOG	- Southeast Michigan Council of Governments
WRE	Water Resources Engineer, Inc.

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## **CHAPTER 1**

### **INTRODUCTION**

#### **1.1 Introduction**

This chapter is an introductory chapter to prepare the reader of what this study is about. With six sections, this chapter comprises of the study's background, statement of problems, objectives of the study, scopes, significance of this study, and the report's layout.

#### **1.2 Background of the Study**

The importance of river in the global development of mankind is undeniable since most of the early urban settlements in the history of human civilization were discovered near rivers. Same goes to Malaysia, all of the early cities that were discovered such as Kuala Lumpur, Alor Star, Kuching, Bandaraya Melaka just to name a

few are founded in the area of rivers where the land is fertile (Andaya and Andaya, 1992; Haliza, 2007).

This development has resulted in wide spread exploitation of the river in many ways such as industries water supply, transportation purpose, domestic usage and also waste disposal. However, the quality of river is contrary proportional to the amount of pollutants in it thus; most of rivers today's are negatively affected by human activities.

Since river is still important for water supply and recreation, water quality modeling is one of the most convenient way to manage water (Mohamed, 2004). The main objective of river water quality modeling is to describe and predict the observed effects of a change in the river system. The usual application of a water quality model is for forecasting changes in water quality parameters resulting from changes in the quality, discharge or location of the point or non-point sources (Crabtree et al., 1986; Mohamed, 2004).

Streeter and Phelps are the first to develop water quality modeling in 1925 by focusing on the urban wasteload allocation problem where the impact on dissolved oxygen conditions is studied using biochemical oxygen demand (BOD) to describe the bacterial decomposition of organic carbon. This approach has led to the discoveries of two-state variable model that contain settling rate of the particulate matter and the sediment oxygen demand as parameter. In 1970s, the increased concern of society towards the environment has broadened the horizon of quality issue to include mechanistic representation of biological processes into the model. The third state variable was then discovered after an extension between carbonaceous BOD (CBOD) and nitrogenous BOD (NBOD) was made as seen in Reicher et al (2001).

Qual I was the first stream water quality model developed by F.D. Masch and Associates with the Texas Water Development Board (1971) and the Texas Water Development Board (1970) before it was modified and extended by Water Resources

Engineer, Inc. (WRE) in 1972 to produce Qual II under contract to the U.S. Environmental Protection Agency (EPA).

The Southeast Michigan Council of Governments (SEMCOG) contracted with WRE has made further modifications in 1976 besides combining the best features of the existing versions into a single model before it was later reviewed and revised by the EPA Center for Water Quality Modeling (CWQM) to be maintained. The model was only renamed to Qual2E after corrections and modifications in 1985. The enhanced model is able to assist user in model calibration and verification, improved in computational efficiency.

This model was then enhanced to Qual2E-UNCAS that allows modeler to perform uncertainty analysis on the steady state water quality simulations with three options sensitivity analysis, the order error analysis and montecarlo simulations (Brown 1987). This model can simulate up to 15 water quality constituents in any combination such as dissolved oxygen and factors affecting dissolved oxygen's concentration which are biochemical oxygen demand, temperature, algae as chlorophyll a, organic nitrogen, ammonia, nitrite, nitrate, organic phosphorus, coliforms, arbitrary nonconservative constituent and three conservative constituents.

### **1.3 Statement of the Problem**

National Straits Times published on October 2008, an article, Unloved Rivers specially dedicated to Malaysian with disappointing attitude towards rivers. Reported that even with improved waterways, rehabilitating spending on polluted rivers and enhanced public awareness, the outcome is still remain frustrating. It is also reported that dead river has becomes a fact of life in states proud to be developed like Johor, This is

true based on report by Johor State Government in Mathematics In Industry Study Group(MISG) 2011 held in UniversitiTeknologi Malaysia, Johor. It is reported that Sungai Tampoi with other five rivers has been assessed as class IV(appendix A). This call for a serious effort to improve the river quality.

Polluted river caused long-term consequences that are sometimes expensive to reverse. Sewage that is produced can affect human or animal life through water drinking causing diseases such as cholera and typhoid fever that can sometimes be fatal. Besides contaminating aquatic life, suffocation of aquatic can even occur when organic matter and nutrients increased the amount of aerobic algae causing depletion of oxygen when the concentration of nutrients such as phosphate and ammonia increase in the river. While for suspended solid, it is accepted as an extremely important cause of water quality deterioration leading to aesthetic issues, higher costs of water treatment, a decline in the fishery resource and serious ecological degradation of aquatic environments described in Brazzier&Bilotta(2008). Water modeling can be one of the catalysts to overcome this problem. Tiung (2003) has undergone a study on Sungai Tebrau branch, Sungai Tampoi to understand the concept of river modeling and water management that is beneficial for the country. Thus, this study aims to use the model mathematically using numerical method to obtain the concentrations of constituents in the river such as BOD and DO, common water constituents.

#### **1.4 Objectives of the Study**

The objectives of this study are:

- 1) To predict the concentration of constituents, BOD in the river.
- 2) To prove simulated result using QUAL 2E model by numerical method

## **1.5 Scope of the Study**

The development of QUAL2E and its mathematical model formulation will be study in this report. Numerical scheme of this model will also be carried out to prove the simulation result obtain using QUAL2E. Since there are no chemical experiments conducted throughout this study, the sample obtained from Tiung (2003) on Sungai Tampoi will be used. This study will only focus on the variables that are required for numerical modeling where the coding and computerized method of QUAL2E is therefore neglected.

## **1.6 Significance of the Study**

Numerical solution obtained using the mathematical modeling in QUAL2E will show how the result obtained using QUAL2E software mathematically. Besides enhancing the understanding in quality water modeling, the significance of the study can help in guiding and improving engineering and management decision concerned with the appropriate usage of the river. This can also prevent the additional cost for water treatment which can lead to the economy instability.

## **1.7 Layout of the Report**

There are six chapters presented in this study, including the present introductory chapter. Chapter 1 is comprises of background of study, statement of problem, objectives, significance and scope of the study. Chapter 2 reviewed the previous studies on the application of QUAL2E, procedure in developing computing model, longitudinal dispersion, advection dispersion equation and mass transfer. Next chapter presented the numerical method used, formulation of the model and description of study area. Chapter 4 will provide readers with the numerical method used in this study. However, in this chapter this focus will only be given on reach 1 since the method is the same for all reaches. Chapter 5 will discuss the result and discussion for this study. Finally, chapter 6 left for discussion, summary and conclusion of this study and recommendations for future study.

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