FIELD INVESTIGATION AND MODELING OF METAL TRANSPORT AND FATE IN A COASTAL WATERSHED BY DYNHYD5 AND WASP

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Field Investigation and Modeling of Metal Transport and Fate in a Coastal Watershed by DYNHYD5 and WASP

by

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Abstract

Water pollution in coastal watersheds due to the introduction of toxic substances from industrial discharges, land, and storm drains has been a growing concern for both the public and governments. Over the years, great efforts have been paid by engineers and researchers to study the transport and fate of pollutants within a watershed in order to evaluate the impacts of water pollution on human and aquatic life. However, fewer studies have been undertaken to investigate the applications of water quality models to coastal watersheds, particularly to model the transport and fate of metals. This research proposed an integrated water quality monitoring and modeling approach for coastal waters. The approach is applied to the Nut Brook and Kelligrews River, a local watershed in Newfoundland. Intermittent field monitoring and sampling have been conducted in a number of sites within the watershed since 2006 for pollution source identification and data collection. In order to compensate the limitations existing in the intermittent field sampling and monitoring, a hydrodynamic model (DYNHYD5) and a water quality model (WASP) were utilized for hydrodynamic and water quality simulation of metals in the watershed. The selected models are found to be quite effective in simulating the trends of concerned pollutants levels over the entire study time period. Based on the results from field investigation and water quality monitoring and modeling, a number of recommendations were made to the local authorities for facilitating water pollution control and quality management practices.

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CHAPTER 1 INTRODUCTION

1.1 Introduction

Coastal watersheds, which are critical to the survival of birds, mammals, fish, and other wildlife, are vulnerable to the introduction of toxic substances such as metals from industrial discharges, land runoff, and storm drains. These substances concentrate and cumulate in the water, sediment, and local aquatic life. Pollution of coastal watersheds causes the loss of habitat and wildlife, as well as a reduction in fisheries. Aquatic plants and animals, as well as humans, can also be harmed through the consumption of contaminated fish and water. Therefore, there has been growing public concern and an increased awareness of coastal watershed pollution problems, particularly in regards to water pollution. Over the years, there have been numerous water quality studies using monitoring and modeling as a tool to examine the pollutant transport and fate and to evaluate human impacts upon a natural river or lake system. However, most of these studies (Caruso, 2004; Libelli and Giusti, 2008) focus on the pollution of inland river basin systems and only a small proportion of studies (EFDC, 2003; Lung and Nice, 2007) investigated the applications of water quality models to coastal watersheds. An integrated approach to identify and address water quality pollution problems within coastal watersheds becomes significantly important to support the local authorities in pollution control and watershed management. Compared to inland rivers, the water quality modeling of coastal waters is more challenging due to the introduction of marine debris from storm sewers and tides. Among these coastal watershed studies, most are focused on the modeling of eutrophication, nitrogen compounds, and coliforms (Renick, 2001; Hammond, 2004; Lung and Nice, 2007). Few studies have been conducted to investigate

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the metal transport and fate in coastal watersheds. However, in recent years, more and more coastal watersheds are polluted by industrial sewage from terrestrial activities due to industrialization worldwide. Those industrial sewage often contain high levels of industrial chemicals and heavy metals (e.g., Cadmium and Lead). Therefore, there has been a growing importance and need to study the metal pollution problems in coastal watersheds. Subsequently, this study proposed an integrated water quality monitoring and modeling approach for coastal waters. The proposed approach is tested by its application to a local watershed in Newfoundland, the Nut Brook and Kelligrews River watershed. The integrated approach provides valuable information for coastal watershed management and could be useful for other coastal watershed studies in the future.

In Newfoundland, conservation of coastal watersheds is extremely important because these watersheds not only support valuable biological resources but are also meaningful to the development of local recreation and tourism. The Nut Brook and Kelligrews River watershed is one of the coastal watersheds in Newfoundland, located at the west of St. John's and across the town of Conception Bay South. The drainage area of the watershed is approximate 14.83 km². The Nut Brook is approximately 5 km long and located in the west end of St. John's, and flows northwest joining the 6 km long Kelligrews River. The Kelligrews River flows across a residential area in the town of Conception Bay South and then discharges into the sea.

Nut Brook has been contaminated by wastewater containing toxic substances from the various industrial and commercial activities midway along its path in an industrial zone. Particularly, the expansion of industrial activities and quarry areas on Incinerator Road contributed to the increase of surface runoff to the watershedy, and thus resulted in a gradual deterioration of water quality in the watershed. Public concerns arise from the fact that Nut Brook is the main head-water tributary of the Kelligrews River. The degradation of water quality in the Nut Brook and Kelligrews River could pose a potential threat to the flora and fauna in that area. The Kelligrews River is meaningful for local recreation and tourism development, and it supports valuable biological resources. Downstream of the Kelligrews River serves an important habitat for a wide variety of plant life and animals such as fish, seaweeds, mussels, and other sea life.

One major purpose of this study is to investigate the pollution problems within this particularly watershed, as well as to provide valuable recommendations to local authorities for pollution control and watershed management. To investigate the change of water quality in the watershed, intermittent field monitoring and samplings have been conducted since 2006 in a number of sites along the Nut Brook and the Kelligrews River. The collected water, sediment, and soil samples were analyzed for various physicalchemical parameters in order to determine the types and extent of water contamination.

However, the data obtained from grab samples and monitoring is limited and can not fully characterize the water quality, particularly considering that the data is limited in types of contaminants measured and does not capture seasonal impacts on water quality. The number and breadth of sampling and monitoring required to fully characterize the "health" of the water body in the study area is costly both in terms of dollars and time. To compensate these limitations existing in the sampling program and to develop a predicting tool, water quality modeling tools must be applied to the study area with the purpose of providing a better interpretation and prediction of water quality responses to natural and anthropogenic pollution in the watershed. Therefore, a number of existing hydrodynamic and water quality models (e.g., EFDC, CE-QUAL-W2, and QUAL2K) were reviewed in order to select the best-fit models for the study. The EFDC refers to the Environmental Fluid Dynamics Code and it is a state-of-the-art hydrodynamic model. The QUAL2K refers to a river and stream water quality model. The CE-QUAL-W2 is a water quality and hydrodynamic model in two dimensions for rivers, estuaries, lakes, reservoirs and river basin systems. Those models are introduced in detail in the model review section.

After carefully reviewing applicable water quality models, an one-dimensional hydrodynamic model (DYNHYD5) and a water quality model (WASP) - both developed by USEPA and have been extensively applied to various water quality studies- were utilized for hydrodynamic and water quality simulation of contaminants, particularly metals, in the study area. The major reason for the selection of the DYNHYD5 and WASP models is that the models are capable of modeling the toxicant transport and have been extensively applied to different environmental studies, including simulation of pollutants in coastal waters (DRBC, 2003; Hammond, 2004). Other reasons include the availability of existing data, the manpower and time constraints of this study, as well as the accessibility of model software and technical supports from model developers. The modeling results can be further used to guide local water quality monitoring and

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sampling efforts in the future. After performing the field investigation and water quality modeling, a number of recommendations were made to the local authorities for facilitating water pollution control and quality management practices.

1.2 Study Objectives

In summary, the major objectives of this study include:

- · To develop a sampling and monitoring program for data collection
- · To propose an integrated water quality modeling approach for coastal watersheds
- · To test the proposed approach in the Nut Brook and Kelligrews River watershed.
- To solve the practical problem of pollution control and mitigation in the watershed.
- · To provide recommendations to the local authorities to watershed management.

To fulfill these objectives, the major tasks for this study can be summarized as follows:

- · To collect and analyze background information and baseline data.
- · To monitor regular water quality parameters.
- To characterize the extent of pollution and identify the possible sources of pollution in the study watershed (i.e. Nut Brook and Kelligrews River watershed).
- To review and examine candidate hydrodynamic and water quality models to determine the models that best fit the current study.

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- To calibrate the selected hydrodynamic model against the observed water levels to achieve the goal of hydrodynamic model parameterization and validation.
- To link the hydrodynamic model to the selected water quality model, estimate concentrations of metals of concern, and compare the results with observed data in order to ensure the satisfactory performance of the model in simulating metal transport and fate.
- · To discuss modeling limitations and possible improvements in the future.
- To propose recommendations for pollution control and water quality management in the study watershed.

1.3 Organization

Chapter 2 presents a detailed literature review on the historical development of water quality models as well as a discussion on the selected hydrodynamic and water quality models. Chapter 3 describes the conducted field work for collection of sampling, monitoring, and modeling data. Chapter 4 introduces the DYNHYD5 and WASP model theories, as well as the input data required for a successful running of theses models. Chapter 5 and 6 include the application of DYNHYD5 and WASP models to the study area, respectively. Chapter 7 presents the conclusions of this study and recommendations to the local authorities.

CHAPTER 2 LITERATURE REVIEW

This Chapter summarizes development of water quality models and reviews existing hydrodynamic and water quality models, such as WASP and DYNHYD5 in detail. The reasons for seleceting the DYNHYD5 and the WASP models for this study are also discussed.

2.1 Development of water quality models

River water is polluted when hazardous substances such as heavy metals, nutrients and pesticides enter into water and dissolve or physically mix with the water. These substances may be carried by rivers and transported miles away from the pollution source, and thus pose a significant threat to ecosystems and human health. For this reason, water quality management and modeling tools were utilized worldwide with the purpose of pollution control and examination of pollutant transport and fate in aquatic systems. In fact, water quality modeling has become an essential part of the process of developing and evaluating alternative scenarios for water quality management. A variety of mathematical models have been used to help explain scientific phenomena and predict outcomes and behaviors in the circumstance that field observations are limited or even unavailable (Ambrose et al., 2009). In particular, a water quality model incorporates a number of equations that represent physical and chemical reactions as well as biological processes that have occurred within the water body. It allows the users to understand and assess the hydraulic conditions in the water body, and thus evaluate human and environmental impacts upon a natural or modified river and lake system (Environmental Canada, 2010).

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In the past decades, there has been an increasing trend of using computer models for predicting water quality characteristics in various water systems, such as rivers, lakes, and oceans. These water quality models are essential and have been widely used for various purposes in environmental management. For example, many governments across the world require water quality modeling for the assessment of the environmental impact caused by any future construction designs before the project is carried out (Elliott and Thomas, 2009). Some of the water quality models have been adopted by authorities, such as the U.S. Environmental Protection Agency (USEPA), as important tools to assess the compliance of environmental guidelines (Falconer, 1992).

Water quality model development started in the early 1920s. Stimulated by a growing need to control water pollution, a comprehensive study was conducted to investigate the sources of pollution in the Ohio River as well as the impacts on the domestic water supply. The Streeter-Phelps solution, popularly known as the oxygen sag equation, was developed as an analytical expression for characterizing the oxygen balance in river (Streeter and Phelps, 1925). The Streeter-Phelps equation was inherited and further developed by researchers for several decades. Among the first useful water quality models, Thomann (1963) developed a Delaware estuary comprehensive study (DECS) model for the Federal Water Pollution Control Administration, the predecessor of the USEPA. In the DECS model, the Streeter-Phelps equation was extended to a multisegment system so that the model can be used for variable properties of the water body and multiple point-source pollutant loads along the river. The developed model proved to be quite useful in providing a quick and quantitative assessment of alternative strategies

for water pollution control. Therefore, the DECS model was considered as one of the first decision-support tools for the water quality management, and later the model was further modified and applied by a number of other researchers (Orlob and Shubinski, 1969). Starting from the 1960s, encouraged by the development of the computer technology as well as growing public concerns, the governmental agencies started to support the water quality model development by investing in systems analysis software and hardware. Consequently, a number of water quality models emerged, many of which were largely intellectual exercises and not used for practical application. However, a few models that proved to be useful in water quality management were well documented and supported by agencies such as USEPA and Army Crops of Engineers (Orlob, 1992). For example, the QUAL-I was developed by the Texas Water Development Board (TWDB) in the early 1970s to solve the steady-state oxygen sag problem for a multi-segment river with variable coefficients and to simulate the heat-energy exchange through the air-water interface (Masch and Associates, 1971). An enhanced version of this model, the OUAL II, was developed by Water Resources Engineers, Inc. (WRE) for the USEPA in 1973. Comparing to its first version, the OUAL II can be applied to more complex physical systems and capable of evaluating the impacts of nutrients loadings on the aquatic system. As a result, the model was subsequently improved by WRE and used by the USEPA Center for Water Quality Modeling (CWQM) as a basic model for the investigations of waste allocations. Based on the modification of the QUAL II, a number of its associated water quality models (e.g., QUAL2E, CE-QUAL-R1, and CE-QUAL-ICM) were developed supported by USEPA. These models have been applied for various water quality studies by researchers and have become widely used today. On the other hand,

driven by the concerns for the effects of toxic substances in the riverine systems, another group of water quality models were developed to simulate the transport and fate of toxic substances, as well as contaminant partitioning among water column, suspended matters, and sediments (Di Toro et al., 1981; Orlob, 1992).

In summary, as indicated by Ambrose et al. (2009), modern water quality modeling can be divided into several periods characterized by the available computer technology. The first development phase of water quality models began with the availability of mainframe computers in the 1960s. This period was considered as the embryonic stage of the mathematic models. A number of models were developed especially in academia, mostly served the purposes of degree requirements, and were best understood by their developers. Most of the models were not well documented for others to use, the software was not easily transferable, and the costs were excessive (Orlob, 1992). Some of the noteworthy models developed during this period include early water quality analysis simulation program (WASP) box models, dynamic estuary model (DEM), storm water management model (SWMM), early QUAL models, MIT dynamic network (MIT-DNM), and Stanford watershed model.

In the 1970s, the situation began to improve gradually through the efforts of governmental organizations, such as the USEPA and the Army Corps of Engineers, as well as relatively small communities of dedicated adherents. The developed water quality models were refined and generalized through the application to priority water-quality problem areas in the United States. For example, the early WASP models were applied to

the Delaware Estuary for simulation of dissolved oxygen, and the Sacramento River and the Great Lakes for investigation of eutrophication processes (DRBC, 1970; Di Toro et al., 1971; Thomann et al., 1979). The early OUAL models were applied in streams for steady state dissolved oxygen study (Duke, 1973). The SWMM model was used by many municipalities in the U.S. for the simulation of the urban storm water hydrology and pollutant runoff loading (Metcalf & Eddy Inc. et al., 1971). The applications of those models contributed to the advancement of modeling technology. Another benefit was that those developed models were screened through the real-case application in order to identify and document the promising models for continuing development and application. At the same time, driven by the advancement of technology in detection of previous unrecognized toxic substances in surface and ground water, as well as the raised concerns from public and policy makers for assessing the risk of exposure to those toxic substances. new models were developed for different environmental problems, such as metals and organic toxicants. Some of the prominent models include hydrologic simulation program - Fortran (HSPF), QUAL2E, and WASP3, as well as exposure analysis modeling system (EXAMS), CE-OUAL models and Hydrologic Engineering Center (HEC) models. The HSPF model was developed using structured programming techniques. Although the code was completely new, its algorithms were derived from the Stanford watershed model, along with agriculture runoff management model (ARM) and the nonpoint source model (NPS) (Orlob, 1992; Ambrose et al., 2009). It was considered as a comprehensive watershed model for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants, such as nutrients and pesticide (Johanson et al., 1984). The QUAL2E steady-state stream model was developed from the early QUAL

models. The model code was renewed and an external uncertainty and sensitivity analysis was developed and added to the model (Brown and Barnwell, 1985). The WASP3 was developed by Ambrose et al. (1986) by linking the basic WASP modeling framework with hydrodynamic, eutrophication and toxic chemical modules. The EXAMS was developed by combining simple waste loading, transport, and chemical process algorithms. It has been primarily used in stream reaches or farm ponds to evaluate the fate, transport, and exposure concentrations of organic chemicals such as pesticides, industrial materials, and leachate from disposal sites (Burns et al., 1982). A series of CE-OUAL models were developed by the U.S. Army Corps of Engineers Waterways Experiment Station. The CE-QUAL models were applied to reservoirs at the beginning of model development and further modified for estuaries and other riverine systems. Among them, the CE-OUAL-R1 model was developed as a dynamic, one-dimensional model to simulate hydrodynamics and water quality in lakes and reservoirs (Environmental Laboratory, 1995). The CE-OUAL-W2 model is a two-dimensional, laterally averaged, hydrodynamic and water quality model that can be applied to rivers, lakes, reservoirs and estuaries (Cole and Buchak, 1995). A series of HEC models, such as HEC-RAS and HEC-HMS, were developed as hydraulic and water quality models. The Hydrologic Engineering Center's River Analysis System (HEC- RAS) can be used to perform onedimensional steady flow, unsteady flow, sediment transport/mobile bed computations, and water temperature modeling. It has been particularly used in floodplain management and flood insurance studies to evaluate floodway encroachments (Brunner, 2002). The Hydrologic Engineering Center's Hydrologic Modeling System (HEC-HMS) was developed for simulation of precipitation-runoff processes of dendritic watershed systems, and has been applied in a wide range of geographic areas to solve various problems such as flood hydrology, river basin water supply, and small urban and natural watershed runoff (Scharffenberg and Fleming, 2010).

From the 1980s to the mid 1990s, the improved access to microcomputers contributed to the third modern development of water quality models. The model databases and executables were installed on the microcomputers and the simulation can be performed locally. A number of aforementioned models were further modified and refined during this time period. For example, WASP version 4, which incorporates hydrodynamic linkage, a pre-processor, and a post-processor, was developed (USEPA, 1999). Along with the model distribution, model technical support and training courses were developed in order to better assist the general user. Furthermore, the water quality model dimensionality was extended to two-dimensional and three-dimensional. Multidimensional hydrodynamic models, such as environmental fluid dynamics model (EFDC), were developed and linked with water quality models, such as WASP (Hamrick, 1996). In the EFDC, the physical characteristics of a waterbody is represented by stretched or sigma vertical coordinates and Cartesian or curvilinear, orthogonal horizontal coordinates. It can be used to simulate the transport of material in complex surface environments, such as estuaries, lakes and offshore, in one, two, and three dimensions. The model was supported by USEPA and widely used by engineers and researchers (USEPA, 2002).

In the late 1990s to the 2000s, the improvement of computer technology, Windows operating system, and local area network linked to the internet motivated the fourth development phase of water quality models. The advance in computer technology, particularly the development of model graphical user interfaces, significantly facilitated the access to the models, as well as the analysis of observed data and model output. In addition to the model preprocessors and graphical postprocessors, geographic information system (GIS) linkages were used to better interpret the model output (Ambrose et al., 2009). For example, the aforementioned SWMM has undergone several major upgrades since it was developed, and the current edition of SWMM, version 5, is a complete rewrite of the previous release. The SWMM 5 enables the user to edit drainage area input data in Windows and view the model results in a variety of formats, including colorcoded drainage area and conveyance system maps, time series graphs and table, profile plots, and statistical frequency analyses (USEPA, 2010). In addition, the aforementioned QUAL2E model was further developed during this period to a Windows-based version, QUAL2K. The QUAL2K is implemented within the Microsoft Windows environment and Excel is used as the graphical user interface. Comparing to the OUAL2E, there are other improvements in the QUAL2K, such as the development of unequally-spaced segments, modeling of particulate organic matter, denitrification, pH, and bottom algae (Chapra et al., 2008). Another example of model improvement is the development of large-scale hydrodynamic linkage routines for the water quality model. Threedimensional hydrodynamic model, such as the EFDC model, was further developed and applied for a number of water quality studies. The EFDC model, developed as a hydrodynamic and water quality model at the Virginia Institute of Marine Science, is

capable of simulating a variety of environmental flows and pollutants transport problems in one, two, and three dimensions. The model can be applied for simulations of salinity, temperature, sediment, contaminant, and eutrophication problems. It is also capable of simulating general discharge control structures, such as culverts and spillways. The EFDC model has a long history of applications that solve a wide variety of water quality problems. For example, the model has been applied for the simulations of pollutant and pathogenic organism transport from both point and nonpoint sources, as well as the simulations of oyster and crab larvae transport in the Chesapeake Bay. The model was also used to study the salinity intrusions in the York River, Indian River Lagoon and Lake Worth, the transport and fate of pollutants in the James River and San Francisco Bay, and the eutrophication in the Peconic Bay, Christina River Basin, and Neuse River. Numerous applications of EFDC model in last decades are listed by USEPA (2002).

Currently, driven by the needs of regulations, as well as advances in computer technology, the water quality modeling has evolved significantly to better address complicated water bodies, pollutant types, and pollution management problems. A number of models were developed and have been applied for simulation of various contaminants. For example, Luo et al. (2008) developed a methodology to simulate spatial distribution of pesticides by using Soil and Water Assessment Tool (SWAT). Chen et al. (2004, 2005) applied an integrated pesticide losses model (PeLM) for simulating pesticide pollution in a watershed system. Maslia and Aral (2004) applied analytical contaminant transport analysis system (ACTS), a computational analysis platform, to assess the fate and transport of tetrachloroethylene. Ferguson et al. (2003) discussed the possibility of

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integrating pathogens within hydrologic models. Man and Tsai (2007) developed a stochastic partial differential equation-based model, based on the law of mass conservation and the Langevin equation, to simulate the transport of suspended sediment in open-channel flows. Puckett et al. (2008) developed a methodology to combine hydrologic, mineralogical, chemical, dissolved gas, and isotopic data in order to simulate the fate and transport of nitrate in the streambed.

On the other hand, the collaborations between government, academia, industry, and engineering consultants have promoted the development of water quality models. The aforementioned major contributors include the USEPA, the U.S. Geologic Survey (USGS), the U.S. Department of Agriculture, the U.S. Army Corps of Engineers' Hydrologic Engineering Center (HEC), as well as other federal and state agencies worldwide (Ambrose et al., 2009). The improvements in water quality models can be summarized as follows: improved capability in handling more detailed environmental analysis both spatially and temporally; more user friendly model interface and graphical postprocessor which enables users to calibrate the model more quickly and meanwhile better illustrate the model outputs; improved the accessibility to environmental data from on-line repositories: more robust modeling frameworks link watershed, hydrodynamics, atmospheric, and water quality models together. Currently, a number of models, such as WASP, include a Windows® interface to facilitate the editing of model input data. Some models (e.g., DYNHYD5) are developed to use free-format input instead of previous FORTRAN formatted input files in order to alleviate the data transcription errors introduced during the input compilation. The advancements in graphical postprocessor, such as the ability to animate predicted water quality dynamics on a geographical map, helped the model users to interpret the model results easier. This way the stakeholders and decision makers can better understand the capabilities and the performance of the model, and thus make appropriate decisions on management of the water resource on critical areas. On the other hand, the improved accessibility to online database helps the model users to process and utilize environmental data for model setup and calibration. For example, the USGS provides access to detailed riverine information for most watersheds in the U.S., including river channel geometry (e.g., length, width, depth, and slope), cumulative drainage area and connectivity with other channels. USGS also provides Digital Elevation Model (DEM) coverage for large rivers, streams, lakes, and reservoirs, which allows the visualization of landscape and changes in topography, as well as the delineation of watershed boundary and drainage area. In addition, time series flow and water quality data from real-time gages can also be downloaded from the USGS webpage. The increased accessibility of water quality data significantly facilitated the calibration of water quality model against observed data. The recent development on model framework also enables more comprehensive analysis of environmental problems. Water quality models were linked with a series of models, such as atmosphere, watershed, and soil models to simulate more complicated constituents transport and transformation in different environmental media. Those linkage models can be either used as stand-alone model or specialty modules for a water quality model. For instance, watershed or hydrodynamic models are normally used coupled with a water quality model to provide runoff and flow dynamics. Overall, the linkage of water quality models to external

simulation models enables model users to address more complicated environmental problems in multiple environmental media.

In the future, the water quality models are expected to be further improved on many aspects. The models should be promoted to handle more complicated water bodies and various pollutant types. The model framework should enhance the capabilities in linking with other models for efficient prediction of pollutants transfer. The connection between existing models and online databases should also be promoted to increase the accessibility of real-time monitoring data, such as water quality, meteorological, and flow data. The further development on new computer technology, as well as model solution efficiencies, would continually decrease the model simulation periods in the future. The advancement in computer technology will also improve the visualization of model output, which allows decision makers to easier understand the model predictions under alternate management options (Ambrose et al., 2009).

2.2 Water quality modeling steps

The basic steps in the water quality modeling application were established by the early 1970s and can be summarized as follows (James, 1993): 1) Formulation of modeling objectives. During this step, a clear quantitative description of system output is essential, to avoid the adoption of unsuitable models. For example, a variety of pollutants, including metals, organic matters, coliforms, and nutrients, were analyzed in this study to determine the most significant pollutants as chemicals of concern for modeling. Based on

this information, the objective of modeling becomes to simulate the transport and fate of concerned metals along the river system, 2) Review of theoretical background. This step includes analysis of processes that affect local water systems, as well as a review of any previous modeling studies that have been done in the same or similar field. For example, the water quality at the Nut Brook and Kelligrews River watershed was affected by the tides from Conception Bay. Thus, a water quality model capable of simulating tide impacts should be considered during the model selection stage. At the same time, a literature review on existing water quality models that have been applied to similar fields should be conducted in order to determine appropriate water quality models for the study area, 3) Conceptual framework for modeling. During this step, it is important to have a concept of which processes should be included during the modeling. Some chemical and biological processes (e.g., vitalization for simulating metals) that have insignificant effects on the modeling output should be eliminated to avoid the over-complication of the model. 4) Model calibration and validation are two primary elements in water quality modeling applications. One or two particular models will be selected as model candidates after reviewing contemporary studies that have been done in same or similar situations. However, those selected models have to be validated before they are accepted and used, since no model is considered as representing the local system without suitable proof. During the calibrations of models, model input parameters or coefficients, whose values were most likely determined by government agencies or previous studies, have to be experimentally re-evaluated and adjusted to give a quantitatively best fit to an observed data set. However, values of some parameters can be obtained from literature reviews if sensitivity analysis shows that it is not a crucial parameter. The calibration step is

repeated until the outputs of data are at an acceptable level of error. Sometimes if the results of output are unsatisfactory with the observed output, it would be necessary to go back to the conceptualization step to modify the structure of model. For example, some processes which significantly affect model outputs may have been incorrectly ignored during the conceptualization of the modeling (Rinaldi et al., 1979).

2.3 Model Selection

After reviewing of existing hydrodynamic and water quality models, the DYNHYD5 and WASP models were selected for this study. The reasons for selecting those two models are summarized as follows:

- The DYNHYD5 hydrodynamic model and the WASP water quality model are capable of modeling the toxicant transport and fate along the Kelligrews River.
- Those two models were both developed by the USEPA and have been extensively
 applied for different environmental studies. In particular, the models have prove
 to be effective for simulations of pollutants in coastal rivers.
- The model software and documents are accessible from the USEPA's webpage.
 The continuous technical support from model developers is also a critical reason for selecting those two models.
- The majority of the model inputs, particularly the channel geometry data, can be obtained by the research team through field work and literature reviews.
The availability of input data to this study, as well as the manpower and time constraints put on it, makes the one-dimensional DYNHYD5 and the WASP models suitable models for this study.

2.4 Review of the selected hydrodynamic and water quality models

Literature reviews have been conducted for existing water quality models, coupled with hydrodynamic models, in order to determine the best fit models for the study area. However, all of the water quality models can not be discussed in detail. Therefore, a discussion on selected models is provided in this section.

2.4.1 Water Quality Analysis Simulation Program (WASP)

The WASP model is a USEPA generalized modeling framework that simulates contaminant transport and fate in various surface waters systems, such as rivers, lakes, and estuaries. Since the WASP model is an uncoupled water quality model, an external hydrodynamic model is required to provide riverine hydrodynamics, such as flow velocity and depth. The WASP model can be used to investigate 1, 2, and 3 dimensional systems, depending on the dimensionality of the hydrodynamic linkage. The WASP model also allows users to specify time-varying model variables, such as exchange coefficients, pollutant loading rate, as well as upstream and downstream boundary concentrations. The model uses finite difference methods and is capable of automatic time stepping in order to ensure model stability. The WASP model consists of four modules: EUTRO, TOXI, HEAT, and a hydrodynamic linkage. The EUTRO module is used to simulate conventional water quality constituents, such as dissolved oxygen and eutrophication processes. The TOXI module simulates the transport and transformation of organic chemicals and heavy metals. The HEAT module is used to simulate heat transport by using the conservation equations of energy. The hydrodynamic linkage enables the linkage of the WASP model to hydrodynamic models, including DYNHYD5, EFDC, EPD-RIV1, and SWMM. The river body is represented as a series of computational segments in the WASP. Within a segment, the chemical concentrations and other environmental properties are assumed to be spatially constant. The water volume and concerned chemical constituents are tracked within segments and accounted for over time and space using a series of mass balancing equations (Wool et al., 2003).

In recent decades, the WASP model has been extensively applied to a variety of water bodies for various water quality problems. The earlier versions of the WASP model have been applied to the Great Lakes and the Potomac Estuary for simulation of eutrophication (Thomann, 1975; Thomann and Fitzpatrick, 1982). Wang et al. (1997) used the WASP model to simulate the transport and reactions of metam-sodium, a soil furnigant, and the volatile methyl isothiocyanate (MITC) in the Sacramento River. Butkus et al. (1999) applied the WASP model, coupled with DYNHYDS hydrodynamic model, to simulate annonia and dissolved oxygen concentrations along the Snohomish River. The application of the WASP model proved to be successful and contributed to the establishment of a USEPA approved TMDL for the Snohomish River. In addition to the conventional water quality problems, the WASP model was also utilized to simulate the fecal coliforms within the Back Bay of Biloxi (Renick, 2001) and Lower Appomattox River (Hammond, 2004). The Delaware River Basin Commission (2003) used the DYNHYD5 and the WASP models to simulate chloride concentrations within the Delaware River Estuary. The successful simulation of chloride concentrations contributed to the development of TMDL for the polychlorinated biphenyls (PCBs) for the Delaware River Estuary. Overall, the WASP model has a long history of applications. These numerous applications are summarized by Ambrose et al. (2009).

The current version of the WASP model (WASP7) is distributed and supported by the USEPA's Watershed and Water Quality Modeling Technical Support Center located in Athens, Georgia. The model software, manuals, and other documentations can be downloaded from the USEPA webpage. The data requirements for the WASP model can be extensive, depending on the complexity of water systems and the types of pollutants being modeled. However, the data requirements for the simulation of metal in the study area are relatively modest, which facilitates the implementation of WASP modeling in this study. Most of the input data can be collected through field investigation and measurements. Some can be obtained from literature reviews and can be further calibrated through field observations. Considering the availability of model software, documents, and technical support, as well as adequate data for the implementation of the WASP model, the model is selected for the water quality simulation portion of the study.

The detailed model formulations and data requirements for the WASP model are introduced in Chapter 5.

2.4.2 The Dynamic Estuary Model Hydrodynamics Program (DYNHYD5)

DYNHYD5 is an unsteady, uncoupled, one-dimensional hydrodynamic model that simulates water flows, volumes, and heads by using channel-junction (link-node) approach. The model solves the one dimensional equations of continuity and momentum for a branching computational network. The model can be applied to various riverine systems with moderate bed slopes, as well as tidally influenced estuaries. It is capable of handling variable tidal cycles, wind, and unsteady inflows. In the model, it is assumed that the river channels can be adequately approximated by rectangular geometry with constant top width (Ambrose et al., 1993a).

As the DYNHYD5 model is a one-dimensional model using a channel-junction modeling approach, the data requirements for implementation of the model are relatively simple, compared to other hydrodynamic models. Most of the inputs data can be obtained through field monitoring and measurements. All of the required inputs for execution of the model are contained within a single space-delimited text file. The ease of implementation, as well as the data availability, makes the DYNHYD5 model a competitive candidate for this study's selection of a hydrodynamic model. After running the DYNHYD5 model, one of the model outputs with a HYD file extension can be linked

to a water quality model to provide riverine hydrodynamics. The DYNHYD5 model is currently distributed by the USEPA's Center for Exposure Assessment Modeling (CEAM) and, like the WASP model, supported by the USEPA's Watershed and Water Quality Modeling Technical Support Center. Considering the data availability for implementation of the DYNHYD5 model, the compatibility with the WASP model, as well as accessible technical support from model developers, the DYNHYD5 and WASP model were selected for this study. The model formulations and required inputs for simulation of the DYNHYD5 model are introduced in Chapter 4.

CHAPTER 3 FIELD WORK

Chapter 3 consists of an introduction of environmental issues, previous studies at the study area, objective of field work, methodologies, as well as modelling data acquisition and processing.

3.1 Problem statement of the study area: Nut Brook - Kelligrews River Watershed

Nut Brook - Kelligrews River watershed is located between the western outskirts of St. John's and the town of Conception Bay South (Figure 3.1). The headwater of the Nut Brook is situated at the south of Trans Canada Highway. Nut Brook flows toward northwest for approximate 5km and discharge into the Kelligrews River. Similarly to other major cities, the city of St. John's and the surrounding townships have many industrial, commercial and residential regions generating different kinds of wastewater containing toxic substances. The Nut Brook stream can be impacted by some industrial activities midway along its path in an industrial zone if without appropriate treatment and management of wastewater. Another concern arises from the fact that Nut Brook is the main head-water tributary of the Kelligrews River, which flows through a dense population region. Although the Kelligrews River is not a drinking water resource, it is sometimes used recreationally for fishing and swimming. Any contamination of Nut Brook could possibly post health risks to the residences living at the downstream of the Kelligrews River, as well as flora and fauna in that area. Therefore, due to recent growing development in the watershed and environmental concerns, this study becomes essential to determine the source of pollution as well as the extent of pollution.



Figure 3 1 The Nut Brook - Kelligrews River watershed

3.2 Review of previous studies

In the summer of 2005, Northeast Avalon Atlantic Coastal Action Program (NAACAP) initiated a monitoring project on the Nut Brook stream system. The collection and analysis of water and sediment samples had been done for the purpose of collecting baseline information, which help understand and assess the impact of environmental damage caused by contaminants released from human activities in the Incinerator Road region. After that, another project - "A preliminary assessment of indicators of stress in fish from the Kelligrews river system" was carried out by Oceans Ltd. and Department of Fisheries and Oceans in 2007. In that project, some indicators (e.g., tissue histopthology and enzyme indicators) were selected to assess the fish health in the Kelligrews watershed. Many biological and biochemical parameters including gross pathology, tissue histopthology, mixed function oxygenase (MFO), acetylcholinesterase (ACHE) and vitellogenin were tested for the brook trout that collected from two sampling sites in the Nut Brook and the Kelligrews River. The report indicated that the increased level of enzyme indicator MFO is associated with presence of organic compounds such as polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCB) and dioxins. Increased level of enzyme ACHE was generally associated with agricultural pesticides use such as selected organophosphate and carbamate pesticides. Meanwhile, it was also mentioned in the report that "depression of ACHE may actually be a more general marker of exposure to neurotoxic contaminants which may, depending on concentration, include various heavy metals, hydrocarbons, detergents and organochlorines" (Mathieu et al., 2007). Both enzyme indicators were found to be similar level in the fish bodies from both

the Nut Brook and the Kelligrews River. However, as pointed out by that report, it was not possible to make a conclusion that whether the level of enzyme is abnormal, without understanding of reference level of enzyme indicators in the system. In addition, the fish study discovered that the collected fish were found with enlarged livers, a condition termed hepatomegaly, and fatty liver, a condition termed steatosis. A number of other biological effects were found such as an evident elevation of vitellogenin, eosinophilic foci, and bile duct hyperplasia. Those effects were associated with impacted water quality such as presence of chemical and biochemical byproducts (Mathieu et al., 2007).

In 2008 an environmental study -"Environmental pollution investigation and ecological risk assessment in the Nut Brook and the Kelligrews River" was carried out by a group of Memorial University students. The main purpose is to investigate the major pollution sources in the Nut Brook and Kelligrews River watershed, and to assess ecological risk caused by pollutants in the rivers. Water samples from eight sites, with three sites in Nut Brook and five in the Kelligrews River were collected and analyzed for metals as well as organic matters from 2006 to 2008. The main focus in the study was the ecological risks posed by the contaminants in Nut Brook and its tributaries. However, due to the limited information on local species, the ecological risk assessment was developed only for the most typical species in the Nut Brook and the Kelligrews River – Brook trout. The results of ecological risk assessment showed that the ecological risk from several contaminates (e.g., zine, copper, nitrogen ammonia) exceeded acceptable risk level (Chen et al., 2008).

3.3 Description of industry activities and pollution sources

Based on the analysis of historical monitoring data collected from 2005 to 2010, it can be concluded that the general water quality of Nut Brook degraded when it flows through the industrial zone located on the Incinerator Road (Ficken, 2006; Chen et al., 2008). The impairment of water quality occurring along the river was linked to the operations of industrial activities as well as the dumping sites located in the area.

Based on the digital map from the City of St. John's, the previous studies (Ficken, 2006; Chen et al., 2008), as well as the field observations in the current research, the following industry activities were identified (Figure 3.2), starting from the east of the Incinerator Road to the west. The Department of Works, Services, and Transportation, which located at the south of street; across the street, there are three adjacent companies, which are Weir's Construction, Hayward Porter's Trucking Ltd., and Maritime Oil Services Ltd. An inactive quarry located at the right side of those companies at the north of incinerator road. Around twenty minute's walk, a Disposal Services Ltd called Pardy's., which was described as the septic waste handling facility in the previous study (Ficken, 2006), is located on the south side of the Incinerator Road. The Nut Brook's tributaries flow alongside the chemical handling facility and met the downstream junction. There is an operating quarry site sitting behind the septic waste handling facility. Across the street, there is a Rothsay Concentrates Company Ltd., which refers to rendering plant in the report, located at the north side of street. This rendering plant was moved away and replaced by a new dewatering technology company in 2008. On the further west side of Disposal Services Ltd., there is a dumping site. A tepee incinerator had been operating on the dumping site for many years (Ficken, 2006). After the incinerator was moved, the wastes from incineration were left untreated and piled up. Some wastes are uncovered at the topsoil and some are buried deep in soil, which makes the whole dumping site as an uncovered landfill site. Opposite to the dumping site, there is an old car wreck depository. It has to be noted that the leachate as well as surface sediment runoff from both the landfill and the car depository can possibly carry hazard chemicals such as heavy metals and organic matters into the river system. At the west side of the dumping site, there is a large inactive quarry operation site. The main environmental issue with the operation of a quarry is that it causes soil erosion as well sediment runoff by removing vegetations from the topsoil. The minerals from the rock can enter the stream through rainfall or snow melt, and cause environmental damage to the water system (Dentoni and Massacci, 2007). At the end of the Incinerator Road, there is a firefighter's training facility, which marked as Department of Works, Services & Transportation Marine Emergencies.



Figure 3.2 The locations of industries on the incinerator road

The water pollution in the industrial zone could be mainly caused by non-point sources. The results of field investigation and sample data analysis indicated that several industrial activities could possibly contribute to the non-point source pollution in the area.

The first concern is those active and inactive quarries. Quarries are used to produce useful construction materials such as silt, sand or gravel and transport to nearby companies. Like many other man-made activities, guarrying causes a significant impact on the environment if without appropriate management. Besides the loss of wildlife habitats and the obvious visual impact, the guarries can easily increase sediment runoff and soil erosion because surface vegetation is damaged during quarrying process (Wardrop et al., 2001). In addition, quarrying involves the production of significant amounts of waste such as clay, silt and other materials. The wastes are more likely to enter streams through surface runoff. Various minerals from the rock entering the steam will lead to the increase of metal constituents in the stream. An active quarry behind the chemical handling facility is shown in Figure 3.3. The approximate river flow direction is from south to north. It can be seen that the Nut Brook flows through an active quarry site without sufficient buffer zone maintained. Quarry tailings such as gravels and sands are piled up at the east corner of the site, where adjacent to the Nut Brook. The tailings can easily enter the stream and deposit at the bottom. Once the quarry tailings accumulate on the riverbed, they change the texture of soil and sediment, which would negatively affect the flora and fauna. The environmental effects of quarrying activities on the surface water quality have been reported by a number studies (Lupankwa et al., 2006; Huang et al., 2010; Lameed and Avodele, 2010).

In addition, several man-made ponds were built on site to wash the aggregate material and then the water in the ponds was left for sedimentation (Figure 3.4). The problem is that during major storms the pool could fail in holding of wastewater. Consequently the wastewater that contains a variety of contaminants from quarrying activities could be released to the streams, and cause water quality degradation. In addition, the wastewater and storm water could also pick up minerals and waste on the ground and carry them to the streams.







Besides the quarrying operation, the abandoned landfill and car dumping site could be the other sources of pollution. During the field reconnaissance, it was found that residue from the former incinerator along with other garbage such as plastic bags and glass bottles were still left uncovered on site. The sampling analysis showed that the river water in the downstream of landfill and dumping site had an increased contaminant concentration (e.g., Copper) in comparison with the headwater in the upstream. This indicated the impacts of leachate from the sites to the downstream water quality. In addition, a number of dumped vehicles that have been heavily eroded were found on site and the leachate could be rich in heavy metals and possibly bring them to the surrounding river tributaries, especially during rainy seasons.

3.4 Objectives of field work

Field work was carried out from 2008 to 2010 to obtain required information for the current study. Meanwhile, historical monitoring data that collected by NAACAP in the study area during 2006 to 2008 were processed and used. The objectives of field work in this study can be summarized as follows:

- Water/sediment sample collection from sampling sites in the Nut Brook and the Kelligrews River.
- Monitoring of regular water quality parameters including dissolved oxygen (DO), turbidity, salinity, conductivity, pH, total dissolved solid (TDS), total coliform and feeal coliform.

- · Identification of possible pollution sources in the Incinerator Road region.
- · Collection of soil samples at abandoned landfill site.
- · Collection of river channel geometry data for hydrodynamic modeling.
- Collection of time-varying water level data and tidal height data for hvdrodynamic model.
- Determination of modeling parameters in hydrodynamic and water quality simulation.

3.5 Introduction of sampling sites

Eight sampling sites were chosen in the Nut Brook and Kelligrews River watershed from 2006 to 2008. In 2009, additional 6 sampling sites were added due to their importance in identification of pollution sources. The original 8 sampling sites were unchanged due to the concern of data consistency. The site numbers and names are listed in Table 3.1. The geographical locations of the sampling sites are shown in Figures 3.5 and 3.6.

Table 3 1 Sampling sites in the Nut Brook - Kelligrews River watershed from 2006 to 2010								
Site # (2006~2008)			Site # (2009~2010)					
		Site name/description						
	(total 8 sites)		(total 14 sites)					
	Site 1	Headwater of Nut Brook	Site 1					
		Nut Brook tributary junction	Site 2-1					
		Nut Brook tributary junction	Site 2-2					
		Nut Brook tributary at the	Site 2-3					
		downstream of landfill						
	Site 2	Nut Brook Junction	Site 2					
	Site 3	Outlet of Nut Gully	Site 3					
		Inlet of Nut Gully	Site 3-1					
	Site 4	Swimming Hole	Site 4					
	Site 5	Nugent's Field	Site 5					
	Site 6	Red Bridge	Site 6					
	Site 7	Kelliview Trail	Site 7					
	Site 8	Heart of estuary	Site 8					
		Mouth of estuary	Site 8-1					
		Sandi Pond	Site H					
		(Headwater of Kelligrews River)						



Figure 3 5 Locations of sampling sites in Nut Brook and Kelligrews River



Figure 3 6 Locations of sampling sites on the Incinerator Road

Site 1 is at the headwater of the Nut Brook, located the southeast of the Trans Canada Highway. It is a pond surrounded by boggy wetlands. This site was chosen because it is located unstream of all pollution sources, and there are rare anthropogenic activities. representing a good reference site. The water quality at this site can be used as a baseline. to compare with that at the downstream of this river, after flowing through the industrial area. Sites 2 to 5 are located at different tributaries along the incinerator road. Site 2-1 is located in the stream close to the chemical handling facility and in the upstream of the Nut Brook and its tributary junction. The water quality at this site is used to understand the impact of guarries as well as chemical handling facilities on the water body. Site 2-2 is located at a small pond, where two tributaries meet together. The water samples are collected from the outlet of the pond, to ensure that the water has been well mixed. Site 2-3 is located at the north side of Incinerator Road. The samples are collected from a stream formed by the underground seepage coming from the underneath of the landfill. Site 2 is at the junction of all tributaries in the industrial zone. The sampling site is a pool surrounded by dense weeds and trees. The site is located at downstream of the industrial area, around 15 minutes walk distance from Incinerator Road, Sedimentation is very heavy at this site, restricting flow in some places, and the area is full of dense weeds. Algae are visibly suspended on the surface of the pond, indicating a eutrophic condition, Sites 3 and 3-1 are located at the outlet and inlet of the Nut Gully, respectively. Water quality in both sites is expected to be better than those in the industrial zone due to natural degradation and dilution. The water quality at Site 3 represents water quality of the Nut Brook that flows into the Kelligrews River.

The rest of the sampling sites, Site 4 to Site 8-1 and Site H, are located in the Kelligrews River. Site 4 is the first site after the junction of the Nut Brook and the Kelligrews River. The sampling site is located at an abandoned swimming pool. The water quality at this site can be used to compare with the other sites at the downstream of the Kelligrews River, where water quality could be affected by anthropogenic activities. Site 5 is located at the downstream of Site 4, where many recreational activities occurred around this site along the river. Additionally, a facility dumping site is also located near to the river, and many deserted facilities from a former cement company were observed on site. Site 6 is located near the highway and water samples were taken under a bridge. The stream from this site further flows into the residential area. Site 7 is located in the residential area and the samples were taken from a small stream with average width of 3m. Site 8 is located in the downstream of the residential area with high population of fauna such as birds and ducks. Site 8-1 is located at the mouth of estuary where tide occurs periodically. It is suspected that water quality at site 8 is impacted by the reflux of sea water from the Conception Bay which entrains high concentrations of contaminants such as metals. Site H is located at the headwater of the Kelligrews River and water samples are taken from Sandi Pond, Similar to the headwater of the Nut Brook, this site is located in a boggy wetland and surrounded by dense woods. The water quality at this site can be used as a reference for the Kelligrews River, since rare human activities are found around this site.

3.6 Methodology

3.6.1 Summary of field work

NAACAP has started to monitor the water quality of the Nut Brook and the Kelligrews River since June 2006. A number of water parameters and contaminants have been measured and recorded. After 2008, a group of Memorial University students joined the field work to collect necessary data for their study. The sampling date and parameters, as well as testing laboratories are summarized in Table 3.2.

Year	Sampling	Sample	Type of tests	testing	Number of
	date	type(s)		laboratory	sampling
					sites
2006	July-25th	Water	Monitoring	Onsite	8 sites*
	Aug-8th		Metal	CREAIT **	
	Aug-21st		Coliform	NAACAP	
	Sep-5th		Solids	NAACAP	
			Nutrients	CREAIT	
			Hardness	NAACAP	
2007	July-23rd	Water	Monitoring	Onsite	8 sites*
	Aug-8th		Metal	CREAIT	
	Aug-28th		Coliform	NAACAP	
	Sep-22 nd		Nutrients	CREAIT	
			Hardness	NAACAP	
	Aug 28 th	Sediment	Metal	CREAIT	8 sites*
2008	July-15 th	Water	Monitoring	Onsite	8 sites*
	Nov-5 th		Metal	CREAIT	
			(Nov 5 th Sweep)		
	Nov-5 th	Sediment	Metal	CREAIT	
2009	June-23rd	Water	Monitoring	Onsite	14 sites*
	July-14 th		Metal	EC Lab***	
	Aug-11 th		TOC	EC Lab	
	Sep-15th		Nutrients	EC Lab	

			Coliform	Marine	
				Institute	
			Flow Velocity	Flow tracker/	
			/Depth/	Measuring	
			Width	tape	
			Water Level	Data logger	
		Soil	PAHs, PCB	ALS Lab****	
			Hydraulic	Infiltrometer	
			conductivity		
	July-14 th	Sediment	Metal	EC lab	
	Dec-2nd	Water	Monitoring	Onsite	
			Metal	CREAIT	
			Coliform	Marine	
				Institute	
2010	March-23rd	Water	Monitoring	Onsite	14 sites*
			Metal	CREAIT	
	Oct -15th		Retrieve data		
			logger		

Note:

*Locations of 8 sites from 2006 to 2008 and 14 sites from 2009 to 2010 are described in

Table 3.1.

**CREAIT refers to the ICP-MS Analytical Lab at Memorial University.

***EC lab refers to the Environment Canada Lab in Moncton.

****ALS lab refers the Analytical Chemistry & Testing Services in Halifax.

During the field work, regular water quality parameters were tested onsite by Hydrolab Quanta - G multiparameter water quality sonde, which is capable of measuring pH, conductivity, DO, temperature, salinity, TDS, turbidity. A catalogue data sheet was developed to record all the results of tested parameters. The tests were performed following the methods stated in the multiparameter sonde manual. Acid preservatives were added to the water samples on site before transported to the lab for analysis. For example, nitric acid was added to water samples for Inductively Coupled Plasma – Mass Spectrometry (ICP-MS) test. The addition of nitric acid leached the metals out of the solid and into solution. Samples were further filtered at the lab with 0.45 micrometer filter before ICP-MS test, as recommended by USEPA (ENCO, 2009).

The multiparameter sonde was calibrated with standard solutions before each field trip to ensure the accuracy of measured results. Besides the onsite monitoring, water and sediment samples were also collected and conserved following standard procedures. The collected water samples were sent to the corresponding labs for different tests, which were specified in Table 3.2. For example, a group of water samples were sent to Environment Canada's lab in Moneton for metal, total organic carbon and nutrients tests. Additional water samples were also sent to the lab in Marine Institute for coliform test. Soil samples were collected at landfill site for PAHs analysis due to the concern of impact from landfill residues to the nearby water body. River channel geometry data (e.g., channel profile) that required as model input were also measured along the rivers.

3.6.2 Water quality indicators

A number of regular water quality indicators were consistently monitored in each field trip. Those water quality indicators including DO, pH, conductivity, salinity, and TDS represent the "health" of the water system in the Nut Brook and the Kelligrews River. Furthermore, theses indictors have been tested in previous programs by NAACAP (Ficken, 2006) and MUN students (Chen et al., 2008). It is critical to assess the changes of those indicators with time which can indicate the trend of health and/or recovery of the system.

3.6.2.1 Dissolved Oxygen

Dissolved Oxygen is an important environmental indicator that describes the concentration of free oxygen dissolved in water. It is one of the most well-established indicators of water quality. Adequate dissolved oxygen is necessary for good water quality, since it is an essential element to all aquatic life. Reduced oxygen levels in the surface river can cause lethal and sublethal effects in a variety of organisms, especially in fish. Generally speaking, if the DO level drops below 5 mg/L, aquatic life will be in stress (CCME, 1999). According to the CCME (1999) water quality guidelines for DO in freshwater for the protection of aquatic life, for warm water, DO level of 6 mg/L is considered to be lowest acceptable dissolved oxygen concentration for early life stages, and 5.5 mg/L for other life stages. Meanwhile, DO level can also be affected by salinity, since salinity decreases the ability of water to hold oxygen (USEPA, 1993).

The results of measured DO of 14 sampling sites during 2009 and 2010 are shown in Figure 3.7. The average DO level in September 2009 and March 2010 were found higher than the average DO level in 2009 summer, which could caused by the difference of average water temperate between winter and summer. The measured average water temperate during winter was around 4 °C, while approximate 17 °C for summer. The cold water has much higher solubility of oxygen gas than warm water, which makes the overall DO level in winter are higher than summer (Michaud, 1991). The average DO level in the Kelligrews River (Site 4 ~ Site H) were found higher than that in the Nut Brook (Site 1 ~ Site 3-1) during all sampling trips, with the exception of March 2010. The improved DO level in the Kelligrews River was possibly caused by the increased flow rate leading to the increase of oxygen diffusion between water body and air. Meanwhile, it is noticed that relative lower DO level occurred in the sites around the Incinerator Road (Sites 2-1, 2-2, 2-3, and 2) and the Nut Gully (Sites 3 and 3-1). In comparison with the DO level in headwater of the Nut Brook, the drops of DO level were probably associated with the increased turbidity at these sites (Figure 3.12). The surface runoff from the Incinerator Road increased suspended particles in the water body

resulting in increased turbidity. The turbid water heated more rapidly by the sun than clearer water since suspended particles absorb sun's energy. In addition, water body loses its ability to hold dissolved oxygen once the temperate of water body increases. Therefore, the surface runoff at these sites can lead to a decrease in dissolved oxygen level (Michaud, 1991; Moreno and Neretnieks, 2006). Sites 3 and 3-1 are located at the outlet and inlet of the Nut Gully. The DO levels were relatively low at these two sites, possibly associated with heavy sedimentation at that area. The DO reading from multiple water quality sonde could have been affected by the turbid water that caused by the placement of the probe in the river, even though cautions have been taken during the measurement. Overall, the average level of measured DO meets the CCME guideline for the protection of aquatic life.





3.6.2.2 pH

pH is a measure of how acidic or basic a solution is, based on the amount of hydrogen ion presented in the solution. pH is an important water quality indicator since it is critical to survival of most aquatic lives. The change of pH level in a river system indicates an input of certain constituents from surrounding environment. pH can be affected by humanwastes, minerals from surface runoff, aerosol and dust from the air, as well as photosynthesis and respiration process by plants and animals (USEPA, 1993). Meanwhile, change of pH can also affect the solubility of some constituents in the river such as metals, which would indirectly influence the aquatic life. For example, the lowered pH level could resuspend some toxic metals in the water column (USEPA, 1993). The increase of solubility of those constituents will also result in the increase the bioavailability to acuatie life (CCME, 2003).

The results of measured pH at 14 sampling sites during 2009 and 2010 are shown in Figure 3.8. The headwater of Nut Brook (Site 1) is located in a boggy wetland, where pH level is naturally low due to the presence of natural acids (Ficken, 2006). The increase of pH level after headwater indicated an input of chemical constituents in the runoff flowing into the water body. The pH level in the Kelligrews River fluctuated between 6.5 and 8, with only a few exceptions. According to the CCME guidelines for the protections of aquatic life, the recommended range of pH in rivers in general is between 6.5 and 9.0 (CCME, 2003). Therefore, the pH level of sites located along the Kelligrews River basically fit within the guideline range. However, as mentioned above, the bioaxailability of a substance increases by lower or upper ranges of pH in water system. That means, the chemicals in Nut Brook could be more toxic to aquatic life due to the increased bioavailability, especially for the sites near the Incinerator Road where relative high metal concentrations were detected.





3.6.2.3 Conductivity, salinity and total dissolved solid

Conductivity is a measure of water's ability to conduct electricity and it indicates the ionic activity and content in the water body. Pure or distilled water is a very poor conductor of electricity. Similarly, salinity is a measure of the saltiness or dissolved salt content in water body. It is usually used to describe the levels of different salts such as sodium chloride, magnesium and calcium sulfates, and bicarbonates in the water body. Normally, conductivity increases as salinity increases, since dissolved salts and other inorganic chemicals conduct electrical current. Total dissolved solid is a measure of substances including any minerals, salts, metals, cations or anions dissolved in water. Therefore, conductivity, salinity and TDS are correlated water quality indicators (USEPA, 1993). Generally, if the water body has a high level of conductivity, then the salinity and TDS in the water body would also be high.

As seen from Figures 3.9, 3.10, and 3.11, conductivity, salinity and TDS show a similar trend among all sites. They were low at the headwater of the Nut Brook (Site 1) and the Kelligrews River (Site H), which represented the natural water condition at that area. Those indicators increased at the sites near the Incinerator Road, which indicates an input of salty substances from that area. The loading of salty substances could attribute to the surfaces runoff from streets, landfill, or quarrying sites which contains various minerals as well as other salty substances. Once those salty substances enter into the nearby stream, it increases the ionic activity and content of the river body. Sites 8 and 8-1 were found have much higher salinity, conductivity and TDS than all other sites, which could be
caused by the sea water invasion. The tide at the mouth of estuary brings back the brackish sea water to these two sites. The levels of salinity in site 8 fluctuated a lot during different sampling trips, which could be affected by the time of tide. It has to be noted that the TDS sensor on the multiple parameter sonde was replaced by a turbidity sensor during sampling trip on March 2010, thus turbidity was tested instead of TDS at that time.



Figure 3 9 Conductivity in the Nut Brook and the Kelligrews River in 2009 and 2010



Figure 3 10 Salinity in the Nut Brook and the Kelligrews River in 2009 and 2010





3.6.2.4 Turbidity

Turbidity is also a key indicator of water quality that expresses the cloudiness of water body. Turbidity is caused by suspend matters or impurities that interfere with the clarity of the water. The suspend matters can consist of silt, clay, organic and inorganic matters. In surface water, the typical source of turbidity includes surface runoff from disturbed watershed (e.g., stormwater and construction), solid waste and wastewater discharge from communities as well as industrial zones, organic compounds that produced from decay of leaves and plants, etc. (USEPA, 1999).

The results of turbidity tests from the sampling trip in March 2010 are shown in Figure 3.12. Again, the headwaters of the Nut Brook and the Kelligrews River have low turbidity with 2.2 and 3.0 NTU, respectively. After the Nut Brook flows through the industrial zone on Incinerator Road, the turbidity at the Nut Brook flows through the industrial zone on Incinerator Road, the turbidity could be a result of surface runoff from active and inactive quarry sites on the road, as well as other possible sources such as dumping site. The quarry operation itself can produce large amount of unwanted dust; meanwhile, the operation destroys the protective topsoil layer and causes soil erosion. After site 3-1, the Nut Brook flows into the Kelligrews River and gets diluted. The turbidity remained stable between Sites 4 to 6 and increased slightly at the end of estuary due to the reflux of sea water.



Figure 3 12 Turbidity in the Nut Brook and the Kelligrews River in 2010

3.6.3 Coliform

Besides general water quality monitoring, water samples were also analyzed for both total coliform and fecal coliform counts. Total coliform and fecal coliform are important bacteria indicators of possible sewage contamination. Total coliform include genera that originate in feces –"fecal coliform", as well as genera not of fecal origin – "non-fecal coliform". Total coliform used to be most widely adopted indicators for water quality; however, recent research found that total coliform could not effectively reflect fecal contamination from human or animal feces due to presence of non-fecal genera such as Klebsiella and Citrobacter. Therefore, fecal coliform are currently chosen as the best indicator for fecal contamination (Health and Welfare Canada, 1992). In the field work, water samples were collected and preserved following standard procedures. Water samples were maintained at a low temperature by using ice packs and storage in a cooler during transportation. The samples were processed in the lab of Marine Institute within 30 hours after collection, in order to avoid die-off or multiplication of coliform.

Water samples taken from June, July, September and December in 2009 were analyzed for both total coliform and fecal coliform counts. The results of coliform tests are shown in Figure 3.13. It should be noted that the maximum coliform count which was 2500 colony-forming unit (CFU) per 100 ml sample, representing that the coliform in the sample were uncountable since the dilution plates were completely covered by coliform. The comparison between the results and Canadian recreational water quality guidelines for E.coli are not performed here, as CCME guideline requires "the geometric mean of at least five samples taken during a period not to exceed 30 day should not exceed 2000 E. coli (or fecal coliforms) per liter" (CCME, 1998). However, in this study, water samples were only taken on monthly basis.





3.6.4 Metals

Concentrations of metals were also tested during every sampling trip because some metals such as Copper, Lead, and Zinc could be toxic in high levels (USEPA, 1993). Those metals can enter streams easily, especially when the Nut Brook flows though an industrial zone on the Incinerator Road. The land in the Nut Brook - Kelligrews River watershed can be contaminated with various metals due to the presence of anthropogenic activities such as transportation, construction and recreational activities. The metals were washed into the nearby water bodies through surface runoff during a rainfall or snow melt event. After that, metals can stay in water in either suspended or dissolved form. The toxicities of the metals are dependent and affected by a series of factors such as pH, hardness, and temperature (CCME, 2003).

The concentrations of various metals were consistently monitored since 2006. Starting from 2009, additional 6 sites were monitored in order to identify the sources of contamination. The locations of total 14 sites were introduced in Section 3.5.

The water quality data vary with many factors such as transport of pollutants due to biological, chemical and physical processes, spatial and temporal variations of background level and degradability of pollutants, measurement bias, and errors during sample collection and lab analysis. Using of appropriate statistical methods to analyze environmental data with different characteristics is important. Improper statistical methods could possibly lead to wrong conclusions. For example, using mean value to

estimate the average concentration of chemicals for each year could possibly cause overestimation of true concentration due to the presence of "outliers" during data analysis. Those "outliers" are normally extreme high concentrations caused by a series of factors discussed above. Considering the vast amount of sampling results, median values of all test results of each metal at each site were used to represent the average metal concentrations in the whole sampling period. Over 30 metals constituents were tested by ICP-MS, and the results of metal analysis were screened to select the concerned metals. The median concentrations of the concerned metals in 2009 and 2010 are shown in Figures 3.14 to 3.23. As seen from the figure, the concentrations of most metals (e.g., Iron, Zinc and Lead) show a similar trend. The concentrations were relative low in the headwater of the Nut Brook and the Kelligrews River, which indicated the background concentrations of metals in the watershed. The concentrations mostly increased from Site 2-1 where the Nut Brook flows into the industrial zone, and reached peak at either Site 2-3 or Site 2. The concentrations at site 4 were mostly lower than those at site 3-1, which indicated a dilution of metal concentrations by the joined water flow from the Kelligrews River. The concentrations remained approximately stable between Site 4 to Site 6 because rare human interference occurred among the sites. The concentrations of the most metals increased at Sites 7 and 8, where the Kelligrews River flows through residential area and into the Conception Bay. The increase of concentrations at these two sites could attribute to sewage discharge, surface runoff, tides, as well as other anthropogenic activities in the surrounding area.



Figure 3 14 Concentrations of Manganese in the Nut Brook and the Kelligrews River in 2009 and 2010

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CCME guideline for the protection of aquatic life (2003) was used to compare with the average concentrations of various metals to assess the compliance of guideline for the Nut Brook and the Kelligrews River. The guidelines for the concerned metals are listed in the Table 3.3. It has to be noted that some guideline values (e.g., Lead) are calculated based on average hardness or pH level of water body. In addition, a measure of spread for the test results is provided in order to indicate how much the data sample is spread out or scattered. The test results are based on 6 sampling events during 2009 and 2010. The interquartile range (IQR), the lower quartile (Q1) and upper quartile (Q3), and the size of data sample are calculated and shown in Table 3.4.

		(Source: CC	ME, 2003)		
Metals	Mn	Fe	Ca	Mg	Ni
Guideline	N/A	300 ug/L	N/A	N/A	25 ug/L
	Pb	Cu	Sr	Al	Zn
	l ug/L	2 ug/L	N/A	100 ug/L	30 ug/L

Table 3 3 Existing CCME guidelines for the concerned metals

Table 3.4 Statistical measures of data samples												
Metals	Mg				Al				Са			
Site	Q1	Median	Q3	IQR	Q1	Median	Q3	IQR	Q1	Median	Q3	IQR
1	424	500	540	115	195	239	340	145	549	770	925	376
2-1	513	916	1438	925	200	321	451	251	2971	4755	10063	7092
2-2	561	910	1655	1094	200	279	385	185	3078	5068	11068	7989
2-3	1937	2435	4488	2551	231	311	458	227	13710	17240	35880	22171
2	1717	2470	4253	2535	189	445	1008	819	11772	14986	27778	16006
3	833	1614	2915	2082	186	262	286	100	4051	6063	9348	5297
3-1	1367	2630	5268	3900	80	262	354	273	4443	9210	16998	12555
4	869	2045	2850	1981	62	127	351	173	2665	7205	9458	6792
5	922	2045	2783	1860	33	139	235	202	3362	8415	10868	7505
6	971	2400	2913	1942	17	86	215	199	3592	9725	12620	9028
7	1492	3050	6443	4950	31	179	355	323	5923	10660	14135	8212
8	1578	7330	23293	21714	67	267	338	271	7111	11555	21478	14367
Н	514	590	1720	1206	98	204	308	211	1419	2040	308	211

Metals	Mn				Fe				Ni			
Site	Q1	Median	Q3	IQR	Q1	Median	Q3	IQR	Q1	Median	Q3	IQR
1	12	18	25	13	150	206	298	148	0.04	0.30	0.30	0.25
2-1	44	60	95	52	363	470	848	484	0.30	0.60	2.40	2.10
2-2	68	164	356	287	323	695	898	575	0.34	0.70	2.15	1.81
2-3	146	332	500	354	786	1340	1775	989	0.55	1.10	1.60	1.05
2	189	460	1097	909	556	1875	4032	3476	0.85	1.20	2.60	1.75
3	54	86	175	121	371	447	557	186	0.30	0.90	3.10	2.81
3-1	75	177	218	143	240	391	723	482	0.57	0.90	1.08	0.50
4	33	36	61	27	185	254	363	178	0.33	0.60	1.10	0.77
5	29	36	84	56	103	246	373	270	0.24	0.40	0.65	0.41
6	33	67	85	52	98	207	206	163	0.33	0.40	0.55	0.23
7	145	270	472	327	330	385	592	262	0.51	1.10	1.85	1.35
8	149	249	330	181	459	568	1025	566	1.21	2.00	2.20	0.99
Н	8	17	29	21	141	300	329	188	0.11	0.20	0.28	0.17

Metals	Cu				Zn				Pb			
Site	Q1	Median	Q3	IQR	Q1	Median	Q3	IQR	Q1	Median	Q3	IQR
1	0.20	0.50	0.70	0.51	0.96	1.30	3.86	2.90	0.25	0.30	0.36	0.11
2-1	0.48	0.70	1.08	0.60	1.85	3.75	6.51	4.66	0.28	0.45	0.73	0.45
2-2	0.70	0.80	1.20	0.50	2.55	3.68	7.08	4.53	0.28	0.40	0.94	0.65
2-3	1.35	2.40	6.16	4.81	8.83	15.30	99.30	90.5	0.40	0.66	1.53	1.13
2	1.35	2.30	4.00	2.65	7.26	11.40	30.06	22.81	0.40	1.03	2.30	1.91
3	0.24	0.40	0.70	0.47	1.18	2.84	6.28	5.11	0.30	0.45	0.53	0.23
3-1	0.58	0.90	1.08	0.50	1.80	2.67	4.85	3.05	0.25	0.35	0.51	0.26
4	0.44	0.50	0.55	0.11	0.90	1.15	7.07	6.17	0.15	0.20	0.30	0.15
5	0.33	0.45	0.58	0.25	0.68	1.30	8.78	8.10	0.12	0.24	0.35	0.23
6	0.30	0.40	0.50	0.20	0.38	1.05	2.31	1.93	0.10	0.10	0.13	0.03
7	0.50	0.64	3.11	2.61	2.00	4.59	14.72	12.72	0.10	0.15	0.73	0.63
8	0.73	1.45	4.50	3.78	4.70	6.35	27.30	22.6	0.24	0.54	1.58	1.34
Н	0.20	0.20	6.65	6.45	0.71	0.90	9.93	9.22	0.09	0.20	0.68	0.59

Metals	Sr			
614-	Q1	Median	Q3	IQR
1	3.92	5.00	6.50	2.58
2-1	10.23	16.08	31.75	21.52
2-2	10.46	18.14	36.00	25.54
2-3	48.50	64.00	123.00	74.50
2	43.00	53.20	102.30	59.20
3	12.56	23.75	38.25	25.69
3-1	18.40	36.00	80.00	61.60
4	12.03	30.00	41.00	28.97
5	12.73	31.50	41.50	28.77
6	14.64	36.50	48.50	33.86
7	19.79	42.00	62.50	42.71
8	23.80	70.00	202.30	178.5
Н	6.52	9.00	11.00	4.48

Currently, there is no CCME guidelines related to Manganese, Calcium, Magnesium and Strontium in fresh water for the protection of aquatic life. However, as discussed above, the changes of concentrations of those metals can still indicate a loading of contaminants from surrounding environment or dilutions caused by headwater.

Concentrations of Iron, Aluminum and Copper exceed CCME guidelines in sites adjacent to Incinerator Road. Among them, concentrations of Aluminum were found naturally high in the headwater due to the presence of acidic water from wetland. Concentrations of Iron at most sites exceeded CCME guideline and the high readings occur at the sites adjacent to Incinerator Road. The average concentrations of copper only exceeded guideline at Sites 2-3 and 2. Iron and Copper at sites around Incinerator Road are likely due to industrial activities such as quarrying. In addition, some metals (e.g., Zinc and Lead) did not exceed guideline but show higher concentrations at the sites in the vicinity of Incinerator Road.

However, it has to be mentioned that only the median values of measured concentrations during 2009 and 2010 were compared with the guidelines in this study. The plots of results only reflected time averaged concentrations. The concentrations are a function of season, rainfall and other climatic conditions. For instance, the measured concentrations tended to increase after a rain event because the runoff could carry contaminants to the water body. Although the average concentrations of some metals at some sites (e.g., concentrations of Lead at Sites 4 and 5) were lower than the guideline, their maximum concentrations actually exceeded the guideline. In addition, limited samples were taken during 2009 and 2010. Extensive sampling and monitoring efforts with higher frequency are recommended in the future study.

3.6.5 PAHs

As mentioned above, an incinerator was previously operated at the closed landfill site. The exhaust as well as remaining residue on site could be a main source for polycyclic aromatic hydrocarbons (PAHs) contamination. PAHs are byproducts generated during incomplete combustion, and tend to remain in soil and sediment for many years due to their low susceptibility to decomposition and degradation (CCME, 2008). The PAHs in residues could possibly leachate and disperse to the surrounding environmental through surface runoff, and consequently contaminate downstream surface water and groundwater. To determine the PAHs contamination level at the landfill site, soil samples were collected during the field work for PAH analysis.

As the PAHs compounds are likely to disperse and accumulate in the prevailing wind direction during the incinerator operation period; therefore, soil samples at 20cm depth from four corners (Sites A, B, C, and D) of the landfill site were tentatively collected for PAHs analysis to determine the possible accumulation areas of PAHs (Figure 3.24).



Figure 3 24 Locations of four sampling comers at landfill site

From the results of PAHs test, it was found that the Site A had a higher concentration than other sites. Therefore, further soil sampling work were conducted at the site A, the central of landfill site (the former incinerator's location), and the river at the downstream of landfill site (Site 2-3). The river bottom sediment at site 4 was collected for PAHs analysis due to the concern of possible deposition of PAHs compounds carried by surface runoff over the landfill site as well as the exhausts from the former incinerator. In order to conduct a comprehensive analysis, soil samples at different depth (0em, 10em, 30em, 50em, and 70em) on the landfill site were collected. However, the maximum depth of site A that soil sampler auger could reach is around 50 cm due to presence of bedrock. Two sediment samples with approximate depth of 0 cm and 10 cm were taken from the riverbed. Totally 16 PAHs compounds were routinely tested by the ALS Laboratory using gas chromatography-mass spectrometry (GC-MS), and 5 of 16 PAHs compounds were detected at a measurable concentration. The result of PAHs analysis is shown in Figure 3.25. Central Point







The legend of following graph shows five different PAHs compounds, including Benzo(a)anthracene, Fluoranthene, Naphthalene, Phenanthrene, and Pyrene. The length of each bar represents the concentration of different PAHs chemicals, with unit of mg/kg marked at bottom of the figure. As shown in the figure, the concentrations of PAHs compounds at site A were even higher than the central point of the landfill, where the former incinerator located. This indicated that the PAHs compounds in the exhaust of incinerator tended to deposit and accumulates in the wind direction. Meanwhile, it is also noted that the concentrations of PAHs in soil show a decreasing trend as the soil depth increases, which indicated that the source of pollution derived from top soil and pollutants tended to diffuse to deeper soil layer.

The results of PAHs test at the landfill were used to compare with the Canadian soil quality guidelines for the protection of freshwater life for industrial land use (CCME, 2010) due to the concern of aquatic life in the downstream. The measured concentrations of Naphthalene and Phenanthrene at various depths were found higher than the guideline and their magnitude of exceedances were 16.2 and 7.4, respectively (Table 3.4).

	Tabl	e 3 5 Results of	PAHs test for soil samples a	at landfill site		
PAH(s)	Number	Ranges of	CCME soil quality	Magnitude of exceedances		
	of soil	measured	guideline for the	(ratio of max observed		
	samples		ns protection of	concentration to CCME		
		(mg/kg)	freshwater life a	guideline)		
Naphthalene	15	0.05~0.211	0.013 ^b	16.2		
Phenanthrene	15	0.05~0.339	0.046 ^b	7.4		

a: Canadian Soil Quality Guidelines for the Protection of Freshwater Life for Industrial

Land Use (CCME, 2010).

b: The value is applied based on a site-specific basis where potential impacts on nearby

surface waters are a concern (CCME, 2010).

However, it has to be noted that limited number of soil samples were collected and tested in this study. More extensive soil sampling is recommended at the landfill site and adjacent riverbed in the future study to further investigate the contamination of PAHs as well as its potential impacts to the downstream. Future toxicity study is also suggested at the river located at the downstream of landfill to assess the stress of contaminants to the fish habitats. The results will help support the future decision and clean up actions in the landfill site.

3.6.6 Model input data collection and processing

A number of input data are required for the simulation of DYNHYD5 model and WASP model. Among these inputs data, some data such as continuous and time variable tidal heights should be collected during field work.

Therefore, in this study, HOBO[®] water level data loggers were deployed and used to record time-varying water level changes during the simulation period. Totally 5 data loggers were deployed in the Kelligrews River at Site H (headwater), Site 3 (Nut gully), Site 4 (Swimming hole), Site 7 (Kelligrews trail) and Site 8-1 (mouth of estuary). The data logger has a pressure transducer and a temperate senor inside which can measure instant absolute pressure and temperate changes with time. Each data logger was calibrated on site before put in use. For instance, the data logger was placed at water surface for 10 seconds to measure atmospheric pressure, and then at water depth of 5cm, 10 cm, and 15 cm for 10 seconds respectively to measure the absolute pressure change can be
defined using a regression equation. Considering the data logger memory capacity as well as the length of simulation period, the record interval was set as 10 minutes. In other words, the deployed data logger at these sites could record instant water level every 10 minutes. An example of processed water level data from data logger deployed at Site 7 (Kelliview Trail) is shown in Table 3.6.

Table 3.6 Sample processed water level data			
Time	Pressure	Calibrated	
	(psi)	water level (m)	
09/12/11 02:50:46	14.5183	0.58	
09/12/11 03:00:46	14.5183	0.57	
09/12/11 03:10:46	14.5167	0.57	
09/12/11 03:20:46	14.5167	0.56	
09/12/11 03:30:46	14.5167	0.55	
09/12/11 03:40:46	14.5149	0.55	
09/12/11 03:50:46	14.5149	0.55	
09/12/11 04:00:46	14.5167	0.54	

Meanwhile, river channel geometry and flow characteristics were also measured during the field work. The water depth and water velocity were recorded at 0.5 meter's width interval, starting from the left bank to the right (Figure 3.26). An example of observed river channel geometry data at Site 7 (Kelliview Trail) on March 27th, 2010 is shown in Table 3.6. The average velocity and depth in each section of a stream were measured, and thus flow at subsection can be calculated. The total discharge was calculated by summing up flows in each subsection. The water velocity at each rectangular subsection was measured by placing a flow meter at about 6/10ths of the total depth. The channel width was also recorded on site by using a measuring tape along the river.



Figure 3 26 The cross section of a river channel

(Source: Andrews, 2006)

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Width (m)	Measure	Velocity	Subsection flow
(left to right)	depth (cm)	(m/s)	(m ³ /s)
0~0.5	25	0.25	0.03
$0.5 \sim 1$	28	0.3	0.04
$1 \sim 1.5$	37	0.6	0.11
$1.5 \sim 2$	31	0.5	0.08
$2 \sim 2.5$	42	0.5	0.11
2.5 ~ 3	51	0.4	0.10
3~3.5	48	0.7	0.17
$3.5 \sim 4$	35	0.7	0.12
$4 \sim 4.5$	32	0.4	0.06
$4.5 \sim 5$	29	0.5	0.07
$5 \sim 5.5$	26	0.4	0.05
$5.5 \sim 6$	14	0.1	0.01
$6 \sim 6.5$	14	0.1	0.01
Average depth		31.7 cm	
Total cross section flow		0.96 m ³ /s	

Table 3 7 Measured river channel geometry data at Site 7 (Kelliview Trail) on March 27th, 2010

In the DYNHYD5 model, such irregular channel cross-sections were assumed that can be represented with hydraulically equivalent rectangular cross-sections. Therefore, the measured depths at each subsection were averaged to determine the average depth of each cross-section. Meanwhile, the results of data logging were further calibrated against the averaged depth of cross section to ensure that the measured depth by data logger could well represent the average depth. Other model input collection and processing will be discussed in the Chapter 5 of model application to the study area.

CHAPTER 4 DYNHYD5 HYDRODYNAMIC MODEL AND WASP WATER QUALITY MODEL

Chapter 4 introduces DYNHYD5 hydrodynamic model and WASP water quality model theory, architecture as well as required model input file used for supporting this study. The objective of using DYNHYD5 model is to simulate water hydrodynamics and generate an output file that can be linked to Water Quality Analysis Simulation Program (WASP) and to provide the flow and volumes to water quality modeling.

4.1 Overview of DYNHYD5 model

The hydrodynamics model DYNHYD5 is derived from an original Dynamic Estuary Model and enhanced to simulate water velocity, flow, volume, and head by using a channel junction (link-node) approach. It is an unsteady, uncoupled, continuous simulation, one-dimensional hydrodynamic model that solves the one-dimensional equations of continuity and momentum for a branching or channel-junction computational network. The simulation interval of the model can be varied and typically proceed at 1 to 5 minutes. The resulting unsteady hydrodynamics including water velocity and water depth are averaged over larger time intervals and stored as input for later use of water quality models such as WASP. The model is more applicable for shallow river systems with moderate bed slope as well as tidally influenced estuaries. However, as stated in the model manual, it can be applied in most natural flow conditions such as larger rivers and estuaries, but not small mountain streams or dam-break situations (Ambrose et al., 1993a).

4.2 Model Equations

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Overall, the DYNHYD5 model simulates the propagation of a long wave through a shallow river system while conserving both energy and mass by solving one-dimensional equations. Water velocity and flow are predicted by using the equation of motion that based on the conservation of momentum; meanwhile, water depths and volumes are predicted by using the equation of continuity that based on the conservation of volume. In the DYNHYD5, flow is mostly idealized as one dimensional and river channels can be approximately represented by a constant top width with a variable hydraulic depth. Other model assumptions include wave length is significantly greater than the depth, Coriolis and other accelerations normal to the direction of flow are negligible, and river bottom slope are moderate (Ambrose et al., 1993a; DRBC, 2003).

Since the DYNHYD5 model uses link and node method to simulate hydrodynamics, the water flow and volume are simulated individually by solving one dimensional equation of momentum and continuity, respectively. A number of dominant equations used in DYNHYD5 model are introduced below.

4.2.1 The equation of continuity

In the DYNHYD5 model junctions are considered as volumetric units that receive and store water from their adjoining channels. The equation of continuity is given by (Ambrose et al., 1993a):

$$\frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial x}$$

Where,

A = cross sectional area (m²),

 $Q = flow rate (m^3/sec),$

t = time (sec), and

x = longitudinal channel distance (m).

In addition, DYNHYD5 assumes the irregular cross-sectional area of the river channels can be adequately represented by rectangular with a constant top width (B). Therefore, the equation can be modified as:

$$\frac{\partial H}{\partial t} = -\frac{1}{B} \frac{\partial Q}{\partial x}$$
(4.2)

Where,

H = water surface elevation or head (height above an arbitrary datum) (m),

B = channel width (m),

 $\frac{\partial H}{\partial t}$ = rate of water elevation change with respect to time (m/sec), and

 $\frac{1}{B}\frac{\partial Q}{\partial x}$ = rate of water volume change with respect to distance per unit width (m/sec).

(4.1)

4.2.2 The equation of motion

In the DYNHYD5, the transport of water are predicted in channels (links) connecting upstream and downstream junctions. The equation of motion is given by (Ambrose et al., 1993a):

$$\frac{\partial V}{\partial t} = -V \frac{\partial V}{\partial x} + a_{g,\lambda} + a_f + a_{w,\lambda}$$
(4.3)

Where,

 $\begin{array}{l} \frac{\partial V}{\partial t} = \mbox{the velocity rate of change with respect to time (m/sec^2),} \\ V \frac{\partial V}{\partial x} = \mbox{the rate of momentum change by mass transfer (m/sec^2),} \\ a_{\mu,\lambda} = \mbox{gravitational acceleration along longitudinal (\lambda) axis of channel (m/s^2),} \\ a_j = \mbox{frictional acceleration (m/s^2), and} \\ a_{\mu,\lambda} = \mbox{wind acceleration along longitudinal (\lambda) axis of channel (m/s^2).} \end{array}$

Since gravitational acceleration is determined by the slope of the water surface, therefore, the acceleration along the longitudinal axis is:

$$a_{\mu,\lambda} = -g \sin S \qquad (4.4)$$

Where,

g = acceleration of gravity (= 9.81 m/sec2), and

S = water surface slope (m/m).

In a river system with small water surface slope, the term "sin S" can be substituted as S. Meanwhile, the water surface slope is defined as the water elevation changes along the distance of channel. Therefore, the gravitational acceleration term can be modified as follows:

$$a_{g,\lambda} = -g \frac{\partial H}{\partial x}$$
(4.5)

In addition, frictional acceleration term in the equation of motion can be expressed using the Manning equation for steady uniform flow. It is worthy to mention that river system does not typically experience steady uniform flow; however, the flow can be assumed to be uniform and steady in the case of extremely small time steps. Therefore, the frictional acceleration term can be rewritten as:

$$V = \frac{1}{n} R^{2/3} S_f^{1/2}$$
(4.6)

Where,

n = Manning roughness coefficient (sec/m1/3),

R = hydraulic radius (approximately equal to the depth for wide channel) (m), and

$$S_f = energy \text{ gradient} = \frac{\partial H}{\partial x}$$
 (m/m).

A number of governing equations have been listed in the section to help understand the DYNHYD5 model. However, it is still recommend to review the User's Manual (Ambrose et al., 1993a) for more detailed descriptions of the DYNHYD5 hydrodynamic model.

4.3 Model Networks

The equations of motion and continuity at alternating grid points are solved through the link-node network. In other words, the water velocity and volume changes at each channel and junction are simulated using the link-node method during the simulation period. At each defined time step, the equation of continuity predicts the water head or pollutant concentration changes at the nodes, while the equation of motion predicts the water velocity changes at the links. Therefore, the nodes in the network are viewed as junctions storing water while the links are viewed as channels conveying water. In addition, as described above, the DYNHYD5 model idealizes irregular cross-sectional area of the river channels as rectangular with a constant top width. Meanwhile, it is assumed in the model that the wave length is significantly larger than depth (Ambrose et al., 1993a). As a result, a schematic diagram can be developed to interpret the link and node network.



Figure 4 1 Representation of DYNHYD5 model network Modified from (Ambrose et al., 1993a) As shown in the figure, each junction is a volumetric unit that used to store water that transports through connecting river channels. The sum of water volume at all junctions represents the total water volume in the river system. Each channel is a conveyor that transports water between two adjoining junctions. The starting point and ending point of each river channel are the central point of adjoining junctions. In the model, the river channels are represented as a rectangular with constant top width. Taking together, the channels represent all the water movement in the river system. Therefore, the hydrodynamics of the river system can be interpreted by overlapping of two physical networks: nodes and links. As the DYNHYD5 model connected to water quality models, the junctions are corresponding to segments which are used to calculate pollutant concentration changes. Similarly, the channels will be used to calculate mass transport between segments in the water quality model (Ambrose et al., 1993a). Overall, the link and node network can be applied to complex branching river systems with irregular shorelines and produce results with acceptable accuracy for most river studies if parameters of model are well defined (DRBC, 2003; Hammond, 2004; MDEQ, 2006).

4.4 Model Inputs

In this section, the required input groups for running of DYNHYD5 model will be introduced. The DYNHYD5 model is written by FORTRAN 77 and input data files are coded in space-delimited ASCII text. The model software package include a PREDYN preprocessor, example input files, execution files, a postprocessor, model user manuals, as well as other related documents. PREDYN is a DOS-based DYNHYD5 preprocessor which is designed to generate input data that can be used by model execution files. Each group of inputs data requires specific FORTRAN format (e.g. "15, 3F10.0, 615" format is required for junction data) which has been introduced in the manual. The PREDYN preprocessor provides an easy way to compile input data that meet the required format. Text editor software (e.g., Textpad) is used in this study instead of the PREDYN after gaining sufficient experience with the structure of the input files. The use of text editor provides significant efficiency in preparing or modifying of required data inputs, especially during the model calibration and verification.

In addition, the DYNHYDS model has been further updated by the model developers (Ambrose and Wool). However, it has not been documented yet. The updated version of DYNHYDS is obtained through personal communications of model developers and is applied in this study. The updated version of HYNHYD5 can be obtained through the author of this document (Yuan Chen, yc7762@mun.ca). The updated version of DYNHYD5 uses mostly free format input, so there must be a space between input values. Meanwhile, the required data for some input groups have been changed. For example, the first data line in the simulate control data group has new variables representing the start date for simulation, which is used in the new output postprocessor file. Further more, junctions with upstream inflow are not mapped to WASP segment 0 (i.e., a WASP boundary) in the updated DYNHYD5. Only junctions with seaward boundary should be mapped to WASP segment 0. Last but not least, a graphical post-processor (MOVEM) which was a component from WASP model has been added in the DYNHYD5 model to process the simulation results into tables or graphics. The DYNHYDS input data can be divided into 12 groups, from group A to group L. The summaries of each data group are listed below (Ambrose et al., 1993a; Hammond, 2004). Readers are recommended to review user manuals (Ambrose et al., 1993a) for detailed description of input data.

Group A: Simulation control

Simulation control data include the simulation title and description, model network parameters (total number of junctions and number of channels), simulation time step, junction and channel initial conditions as well as the beginning and ending day of simulation. It has to be noted that the size of output files vary significantly, depending on the complexity of model network, the simulation time interval as well as the length of model simulation period.

Group B: Printout control

Printout control data allow the users to specify printing options, including a number of junctions for which printouts are desired, print starting time as well as print interval. The change of printout control data will not have any influences on the results of modelling, but only changes the frequency of displayed results in output file.

Group C: Hydraulic summary

Hydraulic summary data controls how the hydrodynamic results are processed and read by the water quality model. This data group includes the date to begin storing parameters to file, the time interval for storing intermediate results in scratch file, ratio of hydraulic time steps to one quality time step, 6. Meanwhile, the option number for summary data should equal to 1, so that a permanent summary file can be generated and used by water quality models; otherwise, no summary file will be created.

Group D: Junction data

Junction data includes junction parameters for the entire network. Those parameters include junction number, initial head in reference to a horizontal model datum at each junction, junction surface area, bottom elevation above or below the horizontal model datum, channel number entering the junction (maximum number of channels is limited to 5 in updated version). If the initial depths of each junction are not defined, then the model will use bottom elevation and mean depth to calculate the initial depth internally. The surface area of a junction refers to half of the total surface areas of connecting channels. In some cases, the surface area of a junction has to be estimated by using a polygon network when more than two channels are entering into one junction (Figure 4.2). This normally happens in large river system where branching or looping are common. A number of software such as ArcGIS can be used to facilitate the measurement of junction surface area. The junction volumes are calculated internally in the model based on those junction data, and updated through the simulation by adding the product of the surface area and the change of depth to initial depth.



Figure 4 2 Definition sketch for junction surface area Modified from (Ambrose et al., 1993a)

Group E: Channel data

Similar to Group D, channel data consist of channel parameters for the entire network. Those parameters include channel number, channel length, channel width, hydraulic radius or channel depth, channel direction, manning roughness coefficient, initial mean velocity in each channel, as well as the connecting channel numbers at the higher and lower end of channel. The hydraulic radius is usually assumed to be equal to the mean channel depth in river systems where channel widths are greater than ten times of the channel depth. The channel orientation which can be measured by software such as ArcGIS, refers to the direction of the channel axis measured from true north. The channel axis in the network normally starts from lower junction number to higher junction number, which is the direction of positive flow (upstream to downstream).

Group F: Inflow data

Inflow data group is used to describe constant or variable inflow for specific junctions in the network. Constant inflow parameters include the number of constant inflows, junctions that will be receiving the inflow, as well as the value of the constant inflow. Variable inflow parameters consists of the number of variable inflows, junctions that will be receiving the following variable inflows, the number of data points for variable inflow, simulation time of various inflow data points, as well as corresponding value of the variable flow. It should be noted that the inflows are negative values while the outflows are positive ones in the DYNHYD5 network. The user can write 0 in the inflow data group when there is no inflow for the entire river system.

Group G: Seaward boundary data

Seaward boundary data are used to describe the seaward boundaries for river systems such as estuaries. There are three seaward boundary input options available in the model. The first option allows users to specify the regression coefficients for tidal cycle, tidal starting time and period. The tidal regression equation is listed as follows:

$$y = A_1 + A_2 \sin(\omega T) + A_3 \sin(2\omega T) + A_4 \sin(3\omega T) + A_5 \cos(\omega T) + A_6 \cos(2\omega T) + A_5 \cos(3\omega T)$$

$$(4.7)$$

Where,

y = elevation of tide below or above common model datum (m),

Ai = regression coefficients,

$$\omega = \frac{2\pi}{tidal \ period}$$
 (1/hr), and

T = time (hr).

Once all seven of the coefficients are specified, the single tidal function can be formed and repeated thought the simulation. Option 2 allows users to input height versus time for single tidal cycle, and those data will be fit to the tidal regression equation in the Option 1. Option 3 allows users to enter high and low tidal heights versus time for multiple tidal eycles, and the input data will be fit to half sine curves. Among three options, Option 3 is considered to be optimal way to provide tidal data when variable seaward boundary data are available. The variable seaward boundary data can be obtained by tidal stage recorders located at the model boundary or downloaded from USGS Tide tables if present. Meanwhile, there are several additional parameters in the seaward boundary data group that allows users to shift and adjust the scale of the seaward boundary data.

Group H: Wind data

Wind parameters along with channel orientation and channel hydraulic radius are required to estimate the wind acceleration to the water body. Later two parameters have been included in the channel data. The wind parameters include wind speed measured at 10 meters above the water surface, and wind direction which refers to degrees measured from true north.

Group I: Precipitation/Evaporation input

Variable precipitation and evaporation data can be specified during the simulation period. The model assumes all the junctions have the uniform precipitation and evaporation rate. Beside the time-variable precipitation and evaporation data points, users also need to input the scale factor and units conversion factor. For example, the unit conversion factor has to be 1.157 E-7 if the rainfall units are em/day. The scale factor is useful in the model calibration process. The impact of a certain parameter (e.g. precipitation/evaporation) can be identified by increase or decrease the magnitude of the values.

Group J: Junction Geometry Input

Junction geometry input data is required when the junction surface area changes along the water surface elevation. The parameter include the number of junctions with variable surface areas, junction number and change rate of junction surface area with respect to the water surface elevation.

Group K: Channel Geometry Input

Similarly, the channel geometry data allow user to specify the change of channel width with respect to water surface elevation. It should be noted that a value of zero implies that the cross-section area of channel is assumed to be rectangular. In most of cases, data group J and K are not specified useless accurate junction and channel geometry data are available.

Group L: DYNHYD Junction to WASP Segment Map

This option allows users to choose the junction numbers to be mapped to the water quality model. There are two options available for feeding hydrodynamic information to the output for the WASP model. Option 1 allows the DYNHYD to write time variant segment velocities and depths for WASP. Option 2 allows the DYNHYD only write one set of segment velocities and depths for water quality model to read. Option 2 only applies when water depth and water velocity do not change significantly during the simulation period. It should be noted that junction in DYNHYD model should correspond exactly to the WASP segment. Meanwhile, the boundary junctions in the network include headwater and tributaries should be mapped as segment 0 in the WASP. However, as mentioned above, junctions with upstream inflow are not mapped to WASP segment 0 in the updated version of the DYNHYD model.

4.5 Overview of WASP model

Since DYNHYD5 is an uncoupled hydrodynamic model, a water quality model is required to simulate the transport and fate of pollutants within the river system. Therefore, in this study WASP model is used together with DYNHYD5 model that can provide flow, depth and velocity. In this section, the model structure, theory, dominant equations and required inputs are discussed. Readers are recommended to review the user manuals (Ambrose et al., 1993 b, c; Wool et al., 2003; USEPA, 2006; Wool et al., 2008) for detailed model description.

The Water Quality Analysis Simulation Program (WASP, Version 7) used in this study is an enhancement the original WASP which has been continuously updated with the support with USEPA. The WASP model has been widely used to help users predict and

interpret water quality responses to natural and man-made pollution, and provide necessary information for pollution management decision making such as determination of Total Maximum Daily Load for various pollutants (MDEQ, 2002; MDEQ, 2006; Ernst and Owens, 2009). WASP is capable of simulating time varying processes include advection, dispersion, pollutants loading, exchange and transformation. The model can simulate various pollutants types including simple toxicant, non-ionizing and ionizing organic toxicant, and mercury in 1, 2, and 3 dimensions in a variety of water bodies as ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters. In addition, the WASP model also allows users to input time-variable exchange coefficients, advective flows, waste loads, and water quality boundary conditions. In brief, the WASP incorporates the time-varying processes of advection, boundary exchange, pollutants loading and dispersion in simulating various water systems. Furthermore, the model allows user to develop new kinetic structures without rewrite large portions of computer code, however, this requires much experience on programming on the part of the modeler (Ambrose et al., 1993 b).

WASP model consists of two sub-models that simulate conventional pollution and toxic pollution, respectively. The former sub-model deals with pollution problems involving dissolved oxygen, biochemical oxygen demand, nutrients and eutrophication. The later sub-model deals with toxic pollution problems caused by metals, organic chemicals and sediment. Once an external hydrodynamic linkage is provided, the hydrodynamic information is averaged over time and delivered to both sub-models (Ambrose et al., 1993 b; USEPA, 2006).

4.6 Model Equations

Similar to other hydrodynamic and water quality models, the basic principle of WASP is the conservation of mass and energy. The water quality constituents and water volume are tracked and accounted from the point of spatial and temporal input to its final point of export. In other words, the mass and momentum are conserved throughout time and space through a series of mass balance equations. The 3-dimensional mass balance equation used in the WASP model is listed as follows (Ambrose et al., 1993 b; Ambrose and Wool, 2009):

$$\frac{\partial C}{\partial T} = \left[-\frac{\partial(\omega C)}{\partial x} - \frac{\partial(w C)}{\partial y} - \frac{\partial(w C)}{\partial z}\right] + \left[\frac{\partial}{\partial x} (E_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} (E_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z} (E_x \frac{\partial C}{\partial z})\right] + S_L + S_R + S_R$$

(4.8)

Where,

C = water quality constituent concentration (mg/L or g/m³),

u = longitudinal advective velocity (m/day),

v = lateral advective velocity (m/day),

w = vertical advective velocity (m/day),

Ex = longitudinal diffusion coefficient (m²/day),

Ey = lateral diffusion coefficient (m2/day),

Ez = vertical diffusion coefficient (m²/day),

SL = direct/diffuse loading rate (g/m3-day),

S_B = boundary loading rate (g/m³-day), and

 $S_K = kinetic transformation rate (g/m³-day).$

The first term of the above equation describes the advective transport of pollutants between adjoining segments in longitudinal, lateral and vertical directions. The second term of equation represents the exchange of pollutants among segments caused by dispersion. The term of S_L , S_B and S_K in the equation represent the external pollutants loading, boundary loading and kinetic transformation, respectively.

The mathematical equation of dispersion used to describe the exchange of pollutant constituents in the model is derived from Fick's first law of diffusion and shown as follows:

$$Exchange = -\frac{E_{ij} * A_{ij}}{L_{ij}} (C_j - C_i) \qquad (4.9)$$

Where,

Eij = the dispersion coefficient between segment i and j (m²/day),

Aii = the cross-section area between segment i and j (m²),

Lij = The mixing length between segment i and j (m),

Ci = water quality constituent concentration in segment i (mg/L or g/m3), and

Ci = water quality constituent concentration in segment j (mg/L or g/m³).

In the current study, WASP simulation is only developed for 1-dimensional pollutants simulation due to reasons such as lacking of precise channel geometry data, advective velocity and dispersion coefficients in three dimensions. Therefore, the former 3dimensional mass balance equation can be simplified for simulation of water quality in only longitudinal direction. Meanwhile, assuming the pollutant constituents are well mixed in the water column, the equations can be further modified by multiply the crosssection area of segment (A). The mass balance equation can be rewrite as:

$$\frac{\partial (AC)}{\partial t} = \frac{\partial}{\partial x} (-uAC + E_x A \frac{\partial C}{\partial x}) + A(S_L + S_B) + AS_K \qquad (5.0)$$

4.7 Model Network

In the WASP model, a river system can be divided into a set of segments in lateral, vertical and longitudinal direction, depending on the dimensionality of the water quality simulation. (Figure 5.1). Those segments adding together represent the physical configuration of the water body. In addition, the segments in the WASP model should exactly correspond to the hydrodynamic junctions in the DYNHYD5 model when external hydrodynamic linkage is applied (Figure 5.2). The concentration of water quality constituents are tracked and calculated within those segments while the transport of water quality constituents is simulated across the interface of adioining segments.

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Figure 4 3 WASP Segmented Model Network (Modified from Ambrose et al., 1993b)



Figure 4 4 Link-node hydrodynamic network and WASP network Source: (Ambrose et al., 1993 b)

4.8 Model Inputs

Before the release of version 6.0, the WASP model uses space-delimited input data files coded with ASCII text and model programs runs under the DOS system, which is same as the DYNHYD model. Starting from version 6.0, a WASP graphical user interface was provided to assist users in developing input data sets. All the model inputs were entered in a WINDOWS-based preprocessor. Meanwhile, the model code has been converted into a series of dynamic link libraries (DLLs) instead of original FORTRAN 77 code.

There are a number of documents available for the study of the WASP model. The input datasets for WASP (before Version 6.0) are introduced by Ambrose et al. (1988; 1993 c). The manipulation of the WASP model (after Version 6.0) has been described in details in the WASP user's manual (USEPA, 2006; USEPA, 2009) as well as WASP graphical user interface user's guide (Wool et al., 2008). WASP model theory, governing equations and interpretation of process (e.g. chemical tracer transport and sediment transport) in the water quality simulation are more particularly described in model supplement documents (Ambrose et al., 1993 b ; Wool et al., 2003; Wool et al., 2008; Ambrose and Wool, 2009). In summary, the WASP model input can be divided into 10 groups according to the interface screens or options in the model (Ambrose et al, 1993 c; Hammond, 2004; Wool et al., 2008).

Group 1: Input parameterization

The data entry form for input parameterization is the first option that needs to be completed when starts a new project. In this screen, users have to specify which submodel will be simulated. Modules that available in WASP 7 are eutrophication, advanced eutrophication, simple toxicant, non-ionizing toxicant, organic toxicant, mercury, and heat. Users are able to provide comments for the new created project. The simulation start time and end time are specified in the start time dialog box. Meanwhile, users are also prompted to locate the non-point source file and the hydrodynamic linkage if any of them are used. There are four hydrodynamics options available in the WASP7: net flow, gross flow, 1-D network kinematic wave and hydrodynamic linkage. The theoretical difference between those hydrodynamics options are described in detail in the user manual. In summary, if the net flow option is selected, the model will only calculate net transport when opposed flow occurs; in other words, the flow will be 0 once the flows enter the segment equals with flows leave out. The gross flow option allows the model to calculate the opposed flow independently and move mass in both directions. The 1-D network kinematic wave is a simple but realistic option for one -dimensional, branching streams or rivers. It is a routine that uses one-dimensional continuity equation and a simplified form of the momentum equation that considers the effects of gravity and friction to calculate flow wave propagation and changes in flows, depth and velocities throughout a stream network. The input for 1-D network kinematic wave routine consists of upstream inflow, tributary inflows, outflows, manning roughness coefficient for each segment as well as segment geometry data including channel length, width, minimum depth and slope. The kinematic wave equation for each segment is solved by using 4-step Runga-Kutta numerical technique in the WASP (USEPA, 2009).

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The hydrodynamic linkage option is applied in the case that a compatible hydrodynamic model (e.g. DYNHYD and EFDC) is used to generate out put files that contain model network and flow information. The generated out put file with "hyd" extension includes time-varying segment volumes and averaged segment interfacial flows that can be used by the WASP model. However, once the hydrodynamic linkage option is used, users can not input any additional flow information. For instance, the data processor will extract segments network and simulation starting time and ending time those information from the linkage. Once the hydrodynamic linkage works successfully, the WASP has enough information to do a simple test run without defining other inputs and parameters such as pollutants loadings rates and boundary concentrations, because the model will use default values (e.g. 1 g/L for all boundary concentrations) for those undefined inputs or parameters. The rest run should obtain a result of concentration approximate to the default initial concentration. Therefore, this step is normally recommended to test the integrity of imported hydrodynamic linkage. Hydrodynamic linkage is used in this study to obtain unsteady transport in river system because adequate input data for a successful run of hydrodynamic model can be obtained through field monitoring. For example, time varying inflows can be monitored and used by the hydrodynamic model, instead of using estimated inflow time functions to define network inflows in kinematic wave routine. Meanwhile, channel directions which is idealized as straight for main stem flow path in kinematic wave routine, can be specified by using hydrodynamic linkage.

In the data entry form, user will also need to decide if a restart file should be created for next simulation, and the time step used in the simulation. Once the hydrodynamic linkage is used, the time step used in simulation is fixed by the ratio of hydrodynamic time steps to water quality time steps. For example, if the simulation time interval for hydrodynamic model is 1 minute and the ratio of hydrodynamic time steps to water quality time steps is set to 10, then the WASP model will automatically extract flow information from linkage with a time step of 10 minutes. The ratio of hydrodynamic time steps to water quality time steps is specified by the users in the hydrodynamic model, and is largely depend on the characteristics of pollution problem being analyzed (Ambrose et al., 1993b). For example, analyzing a problem involving instant toxic pollutants discharges at upstream may require a time step of minutes to hours; by contrast, analyzing a problem involving natural degradation of certain pollutants may allow a time step of hours to several days.

Group 2: Model systems

The system data entry form is used to specify which state variables will be considered in the simulation, as well as which process will be simulated. For example, users can choose the type of toxicant to be simulated, bypassed or remain constant during the simulation. In addition, users have to specify the dispersion/flow bypass option, which depends on whether the pollutant constituent will be affected by such processes. Maximum concentration should also be specified to maintain the stability of model. The simulation will stop once the results of concentration during simulation exceeded the user

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specified maximum concentration. In the end, a boundary scale and conversion factor are specified for each state variable. The scale factor are used to adjust boundary concentrations without re-entering the times series data. For example, the users can change the boundary scale factor to 2 in order to understand the effect of doubling pollutants loadings on the water quality.

Group 3: Print interval

The user can specify the time functions in which the simulation results will be written to simulation result file. The time function of print interval allows users to view output at shorter interval for specific simulation period, instead of remain constant. The print interval should consider the simulation duration and intervals as well as the size of model network.

Group 4: Segmentation

The segment data entry form consists of four tables: segment definition, environmental parameters, initial conditions and fraction dissolved.

The segment definition table requires segment specific geometry information including segment name, volume, type, length, width, minimum depth, slope, and roughness, as well as multipliers and exponents for both velocity and depth. The definition and determination of multipliers and exponents for both velocity and depth in various river
systems are detailed described in the user manual. However, users are not required to input any additional segment geometry information if external hydrodynamic linkage are used along with WASP.

In the environmental parameter table, time-varying segment parameters such as temperature, PH and bacterial concentration are defined. The environmental parameters considered in the table vary with the pollutant types being simulated.

In the initial concentration table, initial concentrations for each variable in each segment are specified to reflect the measured constituent concentration at the beginning of simulation. In the fraction dissolved table, the dissolved fractions of state variable in each segment must be specified at the beginning of simulation. For pollutants such as metals, the fraction dissolved is depending on the chemical partitions.

Group 5: Segment parameter scale factors

This option allows users to determine which parameters will be considered in the simulation as well as specify a scale factor for selected parameters. The advantage of using this feature is that the influence of each parameter can be viewed by considering or removing them. Further more, as discussed above, the scale factor for each parameter can be used to identify their effects on model results.

Group 6: Exchange

In the exchange input screen, there are two exchange field options: surface water and pore water. The former one is selected when to simulate surface water toxicant and solid dispersion; while the later one is selected when to simulate the exchange of dissolved toxicants within the river bed. Once the exchange options are defined, the users have to specify dispersion functions for each set of exchange segment pairs. Meanwhile, the interfacial mixing area of exchange segments as well as mixing length can be specified within an exchange function. In most cases, the mixing area of exchange segments equals to the cross-section area between paired segments, while the mixing length equals to the distance between the central points of the paired segments which is actually the channel length.

Group 7: Flows

The flow input screen is similar to exchange input screen. Surface water flow, pore water flow, solids transport, as well as evaporation/precipitation can be specified for each paired segments. If a DYNHYD5 hydrodynamic linkage is used, users are not able to specify any additional flow information in the WASP model.

Group 8: Boundaries

After the flow pattern is defined or an external hydrodynamic linkage is used, the model automatically determines the boundary segments in the model network. The time varying

boundary concentrations must be specified at every model boundary that receives flow inputs, outputs or exchanges from outside the model network.

Group 9: Loads

The loads data entry allows users to specify the direct and diffuse pollutants loading rates for simulated state variables within a given segment. With the load time function, the users are capable of specifying time varying loading rate (kg/day) for specific segments.

Group 10: Constants

Specific constants for the water quality constituents being simulated must be entered in this option. For example, half saturation denitrification and other nitrate nitrogen constants must be specified to simulate the eutrophication process; while decay rate must be specified to simulate coliform concentration. The determinations of model parameters such as partition coefficient are specified in the model application chapter.

Group 11: Post processor

The post processor "MOVEM" is used to process vast amount of data that produced by execution of the WASP model. After successful running of WASP model, an output file with "BMD" extension can be read by post processor. The post processor can plot the results of simulation in graphical formats. Meanwhile, the observed data can also be loaded and compare with the simulated results in a window. In addition, the post processor can also illustrate the model results on a spatial grid using various colors to represent predicted values; however, this requires an ArcGIS shapefile that can be used by the post processor.

CHAPTER 5 APPLICATION OF HYDRODYNAMIC MODEL TO THE NUT BROOK AND KELLIGREWS RIVER WATERSHED

In this Chapter, the DYNHYD5 model is applied to the study area, the Nut Brook and Kelligrews River watershed. This includes the data analysis and processing to prepare model inputs for running of the model, the determination of some model parameters, as well as the sensitivity analysis and validation of the model.

5.1 The Study Area

The drainage area of the Nut Brook and Kelligrews River watershed (Figure 5.1) is approximately 14.83 km². The Nut Brook is approximately 5 km long and located in the west end of City of St. John's, NL. The brook flows northwest and joins the 6 km long Kelligrews River. The headwater portion of the Kelligrews River is within the City of St. John's and flows through the Town of Conception Bay. South into the Conception Bay.

As outlined in Chapter 3, the water quality in the Nut Brook and Kelligrews River watershed is impacted by upstream industrial activities. A monthly water quality sampling and monitoring program has been implemented to assess the extent of pollution in the study area; however, the data obtained from grab samples and monitoring is limited and does not fully characterize the water quality. Particularly considering that the data is limited in types of contaminants measured and does not capture seasoned impacts on water quality. For example, the contaminants are diluted during rainfall events. The number and breadth of sampling and monitoring required to fully characterize the "health" of the water body in the study area is costly both in terms of dollars and time. To supplement the sampling program and develop a predicting tool, a water quality model is used in this study to interpret and predict water quality responses to natural and anthropogenic pollution in the watershed. The purpose is to simulate the transport and fate of the concerned contaminants particularly metals in the Nut Brook and Kelligrews River and to provide valuable information for water quality management. The results can be used to guide future monitoring and sampling efforts.

The major tasks can be summarized as follows:

- Review possible hydrodynamic models and water quality models and determine the models that best fit the current study;
- Collect and process the required data for running the selected hydrodynamic model and water quality model;
- Calibrate the hydrodynamic model with the observed data to ensure that it can correctly simulate the advective water movement in the concerned rivers; and
- Link the hydrodynamic model to the water quality model and calibrate and verify the water quality model with measured metal concentrations to ensure a satisfactory simulation of contaminant transport.



Figure 5 1 The study area: the Nut Brook and Kelligrews River watershed, Newfoundland

5.2 Watershed Delineation

Prior to water quality modeling. ArcGIS® was used to delineate the Nut Brook and Kelligrews River watershed and the drainage area. The size of the watershed impacts the hydrodynamic modeling parameters (e.g., channel direction) and water quality modeling results (Teegavarapu et al., 2005; Chang, 2009). The delineation of the Nut Brook and Kelligrews River watershed was implemented by ArcGIS and ArcHydro tools, based on a 5 m digital elevation model (DEM) obtained from the City of St. John's. ArcHydro tool is an add-on to ArcGIS software for extracting topologic variables from a DEM raster to build geometric networks for hydrologic analysis (Kraemer and Panda, 2009). The delineation process was completed by following a sequence of steps on the ArcHydro tool bar menu. The raw DEM is processed to fill sinks and then used to calculate flow directions by using eight-direction (D8) method and steepest flow path algorithm. After that, the flow accumulation is calculated internally. Once the threshold of a stream is defined by users, which can either be defined by the threshold areas or the number of cells, the stream laver can be generated. It must be noted that the use of small threshold values for a large DEM will require an extended processing time and lead to a significantly dense stream network. For the best representation of river channels, the threshold value to initiate a stream was set to 700 cells and the land area of each cell is 25 m². After that, stream grid cells are segmented and all the grids in the same segment are assigned with the same code. The

code is used to indicate to which catchment the grid is associated with during the delineation process. Then the grids are converted into catchment polygons through the "Catchment Polygon Processing" feature in ArcGIS. Meanwhile, the previous stream grid is converted into a drainage line feature class with the "Drainage Line Processing" function. Finally, watershed boundary can be delineated by the "Watershed Processing" command. In summary, the delineation process consists of the filling of the DEM, flow direction and grid formulation, flow accumulation, stream grid generation, links grid generation, watershed grid formation and watershed processing (Sarangi et al., 2004). The delineated boundary and stream network are shown in Figure 5.2.



Figure 5.2 The delineated watershed and stream network

Another set of river stream network data was also extracted from the DEM data package that was requested from the City of St. John's (Figure 5.2). The points in the figure contain the elevation data at 5-meter interval. The stream network in the figure was delineated and artificially calibrated against the local topographic map by the City of St. John's. As can be seen from Figure 5.2, the delineated stream channels in the study well match with the river streams that were delineated by the City of St. John's. As a result, the stream network data delineated and calibrated by the City of St. John's was used during the modeling, because the data set has higher resolution and has been calibrated with the local topographic map. Therefore, a number of channel data, such as river width and directions, were obtained and used for modeling.

5.3 Input Preparation

The data sets required for running of the DYNHYD5 model were collected and compiled for supporting the simulation. The required input files and their format have been specified in Chapter 4. The collection and processing of those input files for the DYNHYD5 model will be introduced in the following sections. The generated model junction data and channel data did not vary through the DYNHYD5 model calibration, verification and linkage to water quality model. Meanwhile, the determinations of some parameter values for the DYNHYD5 model were also introduced. Due to the vast amount of inputs for the DYNHYD5 model, some examples of key model inputs and parameters are presented in this chapter.

5.3.1 Model segmentation

One of the major concerns at the beginning of the model application is the choice of model dimensionality. A number of factors should be considered and researched for the selection of appropriate model and model dimensionality. The selection of appropriate model dimensional capability for DYNHYD5 model will depend on a number of factors including the type of pollution problem that being simulated, the availability of bathymetry data, observed data or collected data, channel geometry data, and channel velocities in longitudinal, lateral, and vertical directions. As outlined above, the main purpose of this study is to interpret and predict water quality responses to natural and manmade pollution, by simulating the transport and fate of pollutants especially metals along the Nut Brook and the Kelligrews River. The Nut Brook and the Kelligrews River are relative narrow and shadow rivers, compare with other tidally influenced rivers that have been previously studied by using DYNHYD5 and WASP model (Hammond, 2004; EFDC, 2003). The water velocity as well as pollutant concentrations in the both rivers are considered to be laterally and vertically averaged, and the water flow as well as pollutant concentrations were measured in the centre of both rivers. Therefore, a one-dimensional DYNHYD5 model and WASP model were selected for this study.

In the DYNHYD5 model, a river network is represented by a series of segments. The model segmentation should be implemented before running the DYNHYD5 model. To best present the modeling, guidelines from Ambrose et al. (1993a) were used. First of all, the upstream boundary of the model network was chosen after the junction of the Nut

Brook and the Kelligrews River due to a lack of channel profile and flow data for the Nut Brook portion. This is because the Nut Brook is a relatively small stream that flows across a wetland, and its river channel paths and flows are difficult to determine, especially during dry seasons. As there is no historical gauging data available for the Nut Brook, the upstream boundary was selected at the Swimming Pool (Site 4) which is the first sampling site after the junction of the Nut Brook and the Kelligrews River. Other reasons for choosing this site as the upstream boundary include availability of consecutive water stage data as well as concentrations of the concerned contaminants. In addition, the Swimming Pool is located far away from the Conception Bay which eliminates any backwater or tidal effects on the stream flows. The downstream boundary was extended to the Conception Bay so that the seaward boundary data could be obtained as model inputs. In addition, a number of junctions were chosen at the existing sampling stations (e.g., Site 7), where water quality data is available for the calibration and verification of the water quality model. Finally, the total number of model segments was limited to an acceptable level to avoid over complexity of the model network.

In the DYNHYD5 model, a river system is represented by a number of junctions and channels. As a result, 11 junctions were chosen along the Kelligrews River in this study. After the determination of junctions, 10 channels were automatically generated by ArcGIS. It has been noted during the model segmentation that the sudden change of junction spacing (channel length) will cause the instability of the DYNHYD5 model (Ambrose et al., 1993a). Therefore, model junction spacing was held relatively constant through the model network in this study in order to ensure model stability. The locations of the junctions and channels are shown in Figure 5.3.



5.3.2 Junction data

As introduced in Chapter 4, a series of junction data, including junction numbers, initial heads, junction surface area, bottom elevation above or below datum, and channel numbers entering the junction, are required as model inputs. The bottom elevation of each junction was read from the DEM obtained from the City of St. John's. A handheld GPS was also utilized during the field work to take elevation readings at each junction to verify the elevation data extracted from the DEM. The initial head of each junction was calculated by adding the initial water depth at each junction to the junction bottom elevation. The initial water depth at each junction corresponds to the water surface elevation at the beginning time of model simulation and was measured during the field work. The average water level at most junctions at the beginning of the simulation period were lower than 1.5 meter. Thus, the water levels at those junctions can be measured by holding a flow tracker in the middle of river. It was observed during the model calibration that the initial depth approached to an accurate solution rather quick after the running of the DYNHYD5 model and normally occurred within an approximately 6-hour simulation period. In addition, the river profile at each junction was measured on site with the aid of a measuring tape and flow tracker. The procedure for measurement of river profile has been introduced in Chapter 3.

The surface area of each junction corresponds to the sum of one-half the surface area of all channels that entering and exiting the junction. The surface area of each channel was estimated by the AreGIS tools based on the aerial photos from the provincial mapping

agency. To ensure the accuracy of the aerial photo, the river channel width from the aerial photo at each junction was compared with the field measurements. The results showed a reasonable agreement with offset value less than 1 meter. After the determination of surface area at each junction, the channel numbers that entering and exiting each junction were determined (Figure 5.3) and specified in the input file. In the current version of the DYNHYD5 model, the numbering convention works from upstream to downstream which corresponds to the positive flow direction. A summary of the junction data used for the DYNHYD5 model calibration and verification is shown in Table 5.1.

Junction	Initial	Surface	Bottom	Channel e	nter and
number	head (m)	area (m²)	elevation (m)	exit jur	rction
1	42.7	324	42.1	1	0
2	33.2	1152	32.7	1	2
3	27.3	1565	26.7	2	3
4	24.5	2368	24.0	3	4
5	18.8	2447	18.1	4	5
6	15.9	1559	15.3	5	6
7	2.5	1421	1.8	6	7
8	1.7	9255	1.2	7	8
9	1.0	19387	0.0	8	9
10	1.0	11383	0.0	9	10
11	0.8	573	0.0	10	0

Table 51 Summary of the Junction data in the DYNHYD5 model

5.3.3 Channel data

Similarly, a series of channel data, including channel length, width, direction, hydraulic radius, initial velocity, upstream and downstream connecting junctions and Manning's roughness coefficient, are required for the simulation of the DYNHYD5 model. In the DYNHYD5, the channel length corresponds to the distance between the central points of adjoining junctions, which can be estimated with the aid of ArcGIS. The DYNHYD5 model assumes the river channel with irregular cross-sectional area can be adequately represented by rectangular with constant top width. Therefore, the channel top-width was obtained along the length of channel by the ArcGIS to calculate the average top-width for each channel. The channel width at a number of junctions (e.g., Junctions 1, 5, and 7) were measured on site to verify the estimated channel top-width in ArcGIS. Beside the channel length and width, the channel direction, which refers to the direction of the channel axis in degrees from true north, was also measured with the aid of an angle measuring tool in ArcGIS. As discussed above, the DYNHYD5 assumes that the cross section of river channels can be represented with hydraulically equivalent rectangular, which means the hydraulic radius remains approximately constant along the length of each channel. The hydraulic radius is normally assumed to be equal to the mean channel depth in the cases that channel widths are ten times greater than its depth. However, this is not applicable in this study area because the width to depth ratio of most channels are lower than 10. Instead, the hydraulic radius for each river channel was calculated by equation 5.1 (Ambrose et al., 1993a):

$$R = \frac{BD}{B+2D}$$
(5.1)

Where,

R= hydraulic radius (m),

B= channel width (m), and

D= channel depth (m).

The channel width was measured in ArcGIS and the mean depth of each river channel was estimated by averaging the adjoining junction depths. Therefore, the hydraulic radius for each river channel was determined. The initial velocity for each channel was assumed to be 0 m/s due to the lack of velocity measurements for all river channels at the beginning of the simulation time period. Similar to the initial depth, the DYNHYD5 simulated the river velocity to an accurate solution after an approximate 6 hours' model warm-up period. The upstream and downstream connecting junctions for each river channel were also specified (Figure 5.3).

The Manning's roughness coefficient is an important factor for flow calculations in a natural channel and can vary significantly due to the variability of channel surfaces. Therefore, the Manning's roughness coefficient for each channel served as the key parameter for the calibration of the DYNHYD5 model. The estimate of initial values for the Manning's roughness coefficient was introduced by Cowan (1956) and McCuen (1998). The value of Manning's roughness coefficient is first determined by the general type of river channel and then modified on the basis of various descriptors of the channel and its surface. In other words, the Manning's roughness coefficient value is the sum of base roughness coefficient and various modifiers, including irregularity, cross section, obstructions, vegetation and meandering modifier (McCuen, 1998). The base roughness coefficient, which is affected by the character of channel, plays the most important role during the determination of the Manning's roughness coefficient (Table 5.2).

Character of channel	Basic value	
Channel in earth	0.02	
Channels cut into rock	0.025	
Channels in fine gravel	0.024	
Channels in coarse gravel	0.028	

Table 5.2 The determination of base roughness coefficient for the Manning's roughness coefficient Source: (McCuen, 1998)

The river bed and bank vegetation along the Kelligrews River was observed during the field work in order to obtain a reasonable initial value for the Manning's roughness coefficient. As a result, the initial Manning's roughness coefficient values for all river channels along the Kelligrews River were determined and used in the model sensitivity analysis. A summary of the river channel data used for DYNHYD5 calibration is shown in Table 5.3.

Lonoth	Table 5. Width	3 Summary of t	he Channel d	ata in the DYNI Manning's	Twittel	Tunotion	Innation
=	IIIII AA	nyurauuc	DIFECTION	Mannings	1211111	nuction	nononu
		radius		roughness	Velocity	at	at
-	(m)		(degrees)		(m/s)	lower	higher
						end	end
5	2	0.38	11	0.025	0	2	-
9	9	0.50	356	0.025	0	ŝ	7
5	5	0.48	335	0.025	0	4	ω
90	7	0.51	350	0.025	0	5	4
0	5.1	0.49	350	0.025	0	9	5
5	3.5	0.52	345	0.025	0	7	9
52	ŝ	0.52	340	0.025	0	8	7
55	47	0.96	340	0.025	0	6	8
80	115	86.0	325	0.025	0	10	6
1	9	0.75	315	0.025	0	11	10

5.3.4 Inflow data

Constant or time-varying inflow and outflow data for specific junctions in the network are required for the simulation of the DYNHYD5 model. However, in real cases, the measurement of time-varying flow is difficult and relatively expensive. A common method used to obtain time-varying flow is to derive flow from water level using the site specific relationship between the measured water level and flow. The Swimming Pool (Junction 1) is the only surface inflow for the Kelligrews River after the junction of the Nut Brook and the Kelligrews River. Therefore, water levels and flows at the Swimming Pool were measured on site on December 2, 2009, March 27, 2010 and October 22, 2010 (Table 5.4). The measured water flow and water depth at the Swimming Pool is plotted in Figure 5.5.

Date	Table 5 4 Calculated channel flow at the Swimming Pool Channel width Average depth Velocity Flow				
	(m)	(m)	(m/s)	(m ³ /s)	
12/02/2009	2	0.28	1.7	0.95	
3/27/2010	2	0.30	1.9	1.14	
10/22/2010	2	0.43	1.7	1.46	



Water level (m)

Figure 5.4 Mathematical relationships between the water level and flow

From Figure 5.4, the time-varying inflow of 10 minute intervals at the Swimming Pool can be calculated based on the measured water level, as well as the relationship between the water level and flow. Due to the vast amount of inflow data, only an example of inflow data on December 4, 2009, for the DYNHYD5 model is shown in the Table 5.5. In the DYNHYD5 model the inflows are represented by negative values while the outflows are represented by positive values.

Date	Inflow	
	(m ³ /s)	
12/04/2009 12:01:43 AM	-0.74	
12/04/2009 12:11:43 AM	-0.75	
12/04/2009 12:21:43 AM	-0.76	
12/04/2009 12:31:43 AM	-0.75	
12/04/2009 12:41:43 AM	-0.77	
12/04/2009 12:51:43 AM	-0.74	
12/04/2009 01:01:43 AM	-0.75	
12/04/2009 01:11:43 AM	-0.76	
12/04/2009 01:21:43 AM	-0.74	
12/04/2009 01:31:43 AM	-0.73	
12/04/2009 01:41:43 AM	-0.73	
12/04/2009 01:51:43 AM	-0.72	
12/04/2009 02:01:43 AM	-0.73	
12/04/2009 02:11:43 AM	-0.73	
12/04/2009 02:21:43 AM	-0.71	
12/04/2009 02:31:43 AM	-0.72	

Table 5.5 An example of inflow data at the Swimming Pool for DYNHYD5

The recorded water level at Junction 1 (the Swimming Pool) approached to zero, sometimes even showing negative results, especially during the time period from February 3 to 19, 2010. Such low readings of water level were caused by the frozen water in the Swimming Pool during that period, which affected the absolute pressure underwater resulting in errors in the pressure transducer. The freezing of surface water is validated by the measured water temperature from the data logger which approached to 0°C during this period. In order to maintain model stability, a minimum water level (0.1 meter) was used to replace the negative readings during the simulation period. The determination of minimum water level (0.1 meter) was based on the minimum water level before the freezing of surface water occurred and it proved to be reasonable during the calibration. As a result, a minimum water inflow at the Swimming Pool during that period was calculated, based on the relationship between water level and flow, and used throughout the model calibration and verification.

5.3.5 Seaward boundary data

Seaward boundary data is also required as an input for the DYNHYD5 model. The downstream model boundary was chosen at the mouth of estuary (Junction 11) where the Kelligrews River flows into the Conception Bay. A data logger was deployed at the site from December 2, 2009, to March 26, 2010, in order to record time-varying tidal height data. As introduced in Chapter 3, the data logger was calibrated against various water depths before it was used to record data. The frequency of data logging was set to 10 minutes. As a result, a vast amount of tidal height data with respect to sea-level datum were obtained and plotted in Figure 5.5.

The collected tidal height data were processed to obtain high and low tidal heights for multiple tidal circles. High and low tidal heights versus time were specified and used as seaward boundary data inputs for the DYNHYD5 model. An example of the processed seaward boundary data for the DYNHYD5 model is shown in Table 5.6.



Figure 5.5 Collected tidal height data at the seaward boundary from December 2, 2009, to March 26, 2010

Date

Date	Hour	Minute	Tidal height
			(m)
12/03/2009	2	29	0.14
12/03/2009	8	29	1.18
12/03/2009	16	49	0.18
12/03/2009	20	39	0.85
12/04/2009	3	49	0.10
12/04/2009	8	59	0.97
12/04/2009	16	29	0.24
12/04/2009	21	29	0.65
12/05/2009	4	19	0.31
12/05/2009	10	19	0.99
12/05/2009	19	9	0.27
12/05/2009	22	19	0.75
12/06/2009	4	59	0.19
12/06/2009	10	9	1.19
12/06/2009	17	39	0.02
12/07/2009	0	29	0.80
12/07/2009	4	19	0.16
12/07/2009	10	19	1.10

Table 5.6 An example of processed seaward boundary data for the DYNHYD5 model

In this study, wind and precipitation/evaporation effects were not taken into account due to the lack of meteorological data in the study watershed. In addition, junction and channel geometry options in the DYNHYD5 model, which are used to describe the change of river channel profiles with respect to the change of water level, were not utilized due to the lack of detailed bathymetry data for the Kelligrews River.

5.3.6 Simulation control, Printout control, and Hydraulic Summary

The total number of junctions and channels were specified as 11 and 10, respectively, in the simulation control data group. The model simulation interval was tentatively set to 30 seconds for a test run. However, it was found during the model calibration that the model became unstable at the time step of 30 seconds. The model instability was caused by the sudden drop of river bottom elevations at several river channels. Such instability can be solved by decreasing the time step. In our case, the time step was reduced to 1 second for model calibration and verification, leading to a much stable run.

In the study, the model calibration period was chosen from December 3, 2009, to February 2, 2010. The model verification period was chosen from February 20, 2010 to March 26, 2010. The time period between Feb 3 and Feb 19, 2010 were not included in the model calibration and verification due to the fact that the measured inflows at the Swimming Pool approached zero, or showed negative values during that time period. The simulation results for all junctions and channels during the calibration and verification period were printed out every 30 minutes. The observed water level data from the deployed data logger were averaged every 30 minutes in order to facilitate the comparison between the observed results and the modeled results for model calibration and verification. The DYNHYD5 model generates three output files were generated with the file extensions of OUT, RST, and HYD, respectively. The OUT file includes a summary of input data, as well as error messages encountered during the running of the DYNHYD5 model. The RST file contains the junction volumes and channel flows at the end of simulation and can be used by the DYNHYD5 model for continuing simulation. The HYD file contains averaged hydrodynamic variables and is used by water quality models.

The hydraulic summary data is used to process the generated hydrodynamic results to be used by the water quality model, WASP. The time interval for storing intermediate results in a scratch file was set to 12.5 hours, as recommended by the model manual (Ambrose et al., 1993a). The frequency with which to store hydraulic data on the scratch file was set to 10 seconds. The ratio of hydraulic simulation time steps to water quality ones was set to 30. As a result, the water quality model time step was fixed at 30 seconds. In addition, the option number of the hydraulic summary was set to 1 in order to create a permanent summary file that can be read by the water quality model, WASP.
5.3.7 DYNHYD5 Junction to WASP Segment Map

The DYNHYD5 junctions are mapped to segments in the WASP model when the hydrodynamic linkage is used by the WASP model. In the current version of the DYNHYD5 model, only junctions with seaward boundary are mapped to segment 0 in the WASP. Therefore, the DYNHYD5 Junction to WASP segment map used in this study is shown in Table 5.7.

Junction	Segment
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	0

Table 5 7 DYNHYD5 Junction to WASP Segment Map DYNHYD5 WASP

5.4 Sensitivity Analysis of the DYNHYD5 Model

Sensitivity analysis was performed to quantify the impacts of model input parameters on model results and the model stability before the calibration of the DYNHYD5 model. The time period selected for the sensitivity analysis was chosen from December 3, 2009, to February 2, 2010, which is the same as the model calibration period. Three key model inputs were chosen: inflows, Manning's roughness coefficient, and tide height scales. The input parameters were adjusted at \pm 5% and \pm 15%, respectively, to determine impacts of their variations on model results. The sensitivity analysis of tidal effects was facilitated by adjusting the tidal scale factor in the seaward boundary data group instead of reentering the seaward boundary data. However, the inflow data and the Manning's roughness coefficient were calculated and reentered as the model input during the sensitivity analysis. It is important to note that the study used One-Factor-at-a-Time method for the sensitivity analysis. The parameters are studied individually and no interactions between parameters are considered due to the manpower and time constraints on the study.

The modeled water level results at two specified junctions (Junctions 7 and 9), due to the variations of model parameters, were compared with the simulation results using the preestablished initial inputs values (e.g., 0.025 for Manning's roughness coefficient) for sensitivity analysis. In practice, the modeled water level due to the variations of model parameters divided by the initial ones using the pre-established model parameters, in order to evaluate the impacts of change in different model parameters. Figures 5.6 to 5.11 quantified the instantaneous changes in water level, compared against pre-established base line values at both Junctions 7 and 9 due to the variations of model input parameters. In order to summarize the impacts of model input parameters, the modeled time-varying water level at Junctions 7 and 9 were averaged and compared with the initial model results. The averaged percent changes of water level at Junctions 7 and 9, due to the variations of model parameters, are summarized in Figures 12 and 13.

As shown in Figures 12 and 13, the percent change of inflow and Manning's roughness coefficient impacted the modeled water level at Junctions 7 and 9. The modeled water level at Junction 7 was more affected by the inflow and Manning's roughness coefficient: however, Junction 9 was more affected by the changes of tidal scale factor. The modeled water level at Junction 7 was negligibly affected by the tidal scale factor due to its relatively higher elevation (1.8 m). The peaks in Figure 5.8 indicated that the water level at Junction 7 was occasionally affected by the tides during the high tide period. By contrast. Figure 5.9 showed that the water level at Junction 9 was affected by the tide heights throughout the simulation period. Meanwhile, the changes in water level at Junction 7, due to the variations of Manning's roughness coefficient, remained approximately stable; however, the changes at Junction 9 varied significantly during the simulation period. Overall, the change of inflow and Manning's roughness coefficient had relatively large impact on the modeled water level at Junction 7 but less impact on Junction 9. The change of tidal scale factor hardly affected the modeled water level at Junction 7; by contrast, it caused considerable impact on the modeled water level at Junction 9.





----- +5% Inflow



Date

Figure 5.7% change of modeled water level at Junction 9 with variations of inflow











+15% Mannings -5% Mannings -15% Mannings

Figure 5 10% change of modeled water level at Junction 7 with variations of Manning's roughness coefficient



Figure 5 11% change of modeled water level at Junction 9 with variations of Manning's roughness coefficient







Figure 5 13 Averaged % change of modeled water level at Junction 9 with variations of model parameters

The results obtained from the model sensitivity analysis indicated which input parameters have significant impacts on results and should be optimized in order to obtain a satisfying model result during model calibration. However, the observed model input parameters, such as inflow, can not be optimized and should be treated separately in comparison with the tidal scale factor and the Manning's roughness coefficient. The model user should refine the observed inflows by calibrating the pressure transducer with the observed water depth, as well as increasing the time of measurements on water velocity, water depth, and flows, in order to have high degree of confidence on the input parameters.

5.5 Calibration of the DYNHYD5 model

The model calibration period was chosen from December 3, 2009, to February 2, 2010. The reason for choosing this time period for model calibration has been discussed earlier in this chapter. As mentioned above, the results obtained during model sensitivity analysis were used to determine the model parameters to be modified in order to obtain reasonable model results. As a result, the model input parameters, including Manning's roughness coefficient and tide scale factor, were adjusted until the model results converged with the observed results. The observed water level at Junction 7, where a data logger was deployed to record time-varying water level, was used to compare with the modeled water level throughout the model calibration period. In addition, the modeled results were plotted against the observed results at Junction 7 and a linear regression analysis was used to produce a goodness-of-fit (r^2) value. A 45° line is also plotted to show the line of perfect agreement between the observed and modeled results. By this way, the plot can show to what extent the modeled results are biased on the high or low side during the model calibration and verification. As the r^2 value approaches 1, the relationship between the modeled and observed results fits the linear regression well.

A comparison between the modeled results and the observed ones at Junction 7 is shown in Figure 5.14. It indicated that the modeled water level basically fit with the observed values. It has to be noted that the modeled water level remains stable at a minimum water level occasionally. This is because a constant minimum inflow was used as model input, to replace the zero or negative water levels measured by the transducer at the Swimming Pool. The reason for obtaining zero or negative measured water level and the process of generating minimum inflow to replace those values were discussed earlier in this chapter. It is also found that the DYNHYD5 model was unable to accurately simulate the high water level that occurred in Junction 7. A satisfying goodness-of-fit value (r^2 =0.936) was obtained for the linear regression between the observed and modeled results (Figure 5.15). As can be seen from the figure, the model tended to underestimate the water level in the cases of high water level period. As a result, the optimized model parameters remained unchanged for the model verification.





Figure 5 14 Modeled versus observed water level at Junction 7 for model calibration



Figure 5 15 Goodness-of-fit test for the modeled and observed water level at Junction 7 during the model calibration period

5.6 Verification of the DYNHYD5 model

The time period for the model verification was chosen from February 20, to March 26, 2010. The selection of this time period for model verification has been discussed earlier in this chapter. The model parameters which have been optimized through model calibration process remained unchanged throughout the model verification. In comparison with model calibration, a different set of inflow and seaward boundary data were processed and used for the model verification. As a result, the modeled water level at Junction 7 was plotted against the observed water level during the verification time period (Figure 5.16). It indicated that the modeled water level did not exactly correspond to the observed water level. The overall modeled water level during the verification period was slightly higher than the observed water level. This discrepancy may be attributed to the overestimate of inflows during the verification period. As discussed above, the inflows were approximately estimated based on the mathematical relationship between the measured water level and flow on site. However, the approximation was based on limited onsite measurements and may not accurately represent the actual relationship between the measured water level and flow. The relationship between the measured water level and flow might vary during dry and wet seasons. The observed and modeled results were plotted to obtain a linear regression, as shown in Figure 5.17. A satisfying goodness-of-fit value (r2=0.949) was obtained for the linear regression between the observed and modeled results.



Figure 5 16 Modeled versus observed water level at Junction 7 during the model verification period





A linear regression analysis was also used to determine the overall goodness of fit value for both model calibration and verification period, as shown in Figure 5.18. As a result, a r² value of 0.923 was obtained for the entire simulation period. As can be seen from the plotted figure, the modeled water level generally corresponded well with the observed water level during the entire simulation period, leading to a satisfactory simulation. Meanwhile, it also indicated that the DYNHYD5 was more capable of representing the relatively low water level rather than the high water level during the simulation period.



Figure 5 18 Goodness-of-fit test for the modeled water level and observed water level at Junction 7 during the entire simulation period

In summary, this chapter discusses the application of the hydrodynamic model-DYNHYD5 model to the study area. The processing and generation of the DYNHYD5 model input were specified and the determinations of the key inputs and parameters were also discussed in this chapter. Three specific model input parameters were selected for the model sensitivity analysis and impacts on model results due to their variations were evaluated. To successfully implement the DYNHYD5 model, the model parameters were optimized through the model calibration and utilized for model verification. The observed water level at a specific junction was used to compare with the modeled water level from December 3, 2009, to March 26, 2010. A relatively satisfying agreement was obtained between the modeled results and the observed ones during the entire simulation period. Consequently, the results from the hydrodynamic model were used in the water quality model.

5.7 Prediction of the DYNHYD5 model

After the calibration and verification of the DYNHYD5 model, there is confidence to apply the model to predict the streamflow in the Kelligrews River. It was observed during the sensitivity analysis that the streamflow from Junctions 1 to 7 were mainly affected by the upstream inflows as well as Manning's roughness coefficient, given that river segment and channel data remained unchanged during the whole simulation period. By contrast, the streamflow at Junctions 8 to 10 were largely affected by the tidal height (tidal scale factor) at the seaward boundary. The streamflow in the Kelligrews River were further predicted during the period from July 25, 2006, to December, 2, 2009, during which time the historical water quality data were available for calibration and verification of the WASP model.

In order to obtain time-varying inflow data at the Swimming Pool during the simulation period from July 25, 2006, to December 2, 2009, the approximate time-varying water level at the Swimming Pool during that period were estimated through the relationship between the weekly averaged precipitation and water level change at the Swimming Pool. The daily precipitation data were obtained from Environment Canada and processed to obtain weekly averaged precipitation. The measured water level data during the time period from December 3, 2009, to August 12, 2010, were obtained by the deployed transducer at the site and were averaged to obtain weekly averaged water level changes. The weekly averaged water level change versus the weekly averaged precipitation was plotted in Figure 5.19. A linear regression analysis was performed between the weekly averaged water level change and precipitation. A relatively satisfying goodness-of-fit value (r²=0.744) was obtained for the approximation (Figure 5.20).

In addition, the initial water level at the Swimming Pool on July 25, 2006, was measured on site in previous study (Ficken, 2006). Therefore, the weekly averaged change of water level at the Swimming Pool during the period from July 25, 2006, to December 2, 2009, can be roughly estimated based on the relation curve as well as the precipitation data during that time period. It must be noted that the approximation of water level assumes that the change of water level at the Swimming Pool was mainly caused by the change of precipitation and such approximation could be only performed on a weekly averaged

basis. As a result, the estimated water level at the Swimming Pool during the time period from July 25, 2006, to December 2, 2009, can be obtained. The estimated water level was used to generate weekly averaged water flow based on the relationship between the water level and flow at the Swimming Pool (Figure 5.21). The approximated relationship between the water level and flow at the Swimming Pool has been discussed in Section 5.3.4 of this chapter. The generated water flow at the Swimming Pool was further processed as inflow data for the DYNHYD5 model. As a result, the streamflow at Junctions I to 7 were modeled after the successful running of the DYNHYD5 model.













Figure 5 21 Estimated water inflow at the Swimming Pool for the time period from July 25, 2006, to December 2, 2009

In summary, after the sensitivity analysis, calibration, and verification of the DYNHYD5 model, the model was further used to predict the water level of Junctions 1 to 7 in the Kelligrews River where the stream flows were mainly affected by the upstream inflows and Manning's roughness coefficient. The model results during the prediction period were combined with the results from the model calibration and verification period to be further used for water quality modeling. Meanwhile, in order to maintain the stability of the DYNHYD5 model, a minimum inflow at the Swimming Pool was estimated for the time period between February 3, and 20, 2010, during which time the measured water inflow approached zero or negative due to the frozen surface at that time period. As a result, the stream flows during the time period from July 25, 2006, to March 26, 2010, were simulated by the DYNHYD5 model. A summary of the time period used for model sensitivity analysis, calibration, verification, and prediction is shown in the Table 5.8.

Table 5 8 A summary of the time periods used for model simulation	
	Time periods
Sensitivity analysis	December 3, 2009~ February 2, 2010
Calibration	December 3, 2009~ February 2, 2010
Verification	February 20, 2010~ March 26, 2010
Prediction	July 25, 2006~ December 2, 2009

5.8 Modeling Limitations

Although the DYNHYD5 model produced reasonable results in simulating the streamflow in the Kelligrews River, the performance of model simulation in this study was limited by the data availability at the model parameter calibration and verification. The predictive capability of the hydrodynamic model utilized in this study could be further improved once those limitations are addressed. The encountered limitations are summarized as follow:

> Use of one-dimensional hydrodynamic model and water quality model for the study area

A major concern during the model set up is the choice of model dimensionality. In this study, the dimensionality of the water quality model was limited by using onedimensional hydrodynamic model. The rationales for selecting the one-dimensional hydrodynamic model, DYNHYD5 model, for the study area have been discussed in Chapter 2. In general, the data sets required for simulation of a two-dimensional or threedimensional model are highly extensive. For example, the three-dimensional hydrodynamic model (e.g., EFDC model) uses a grid of cells to represent waterbody geometry instead of a number of channels and junctions. In that case, the physical properties of each cell, including length, width, initial water depth, bottom bed elevation, roughness height, and vegetation type, must be specified as one of the model inputs (USEPA, 2002). Meanwhile, the data and time required to calibrate and validate a twodimensional or three-dimensional model are much greater than a one-dimensional hydrodynamic model. Considering the characteristics of the Kelligrews River, the available data of river geometry, and the time constraints placed on this study, the onedimensional DYNHYD5 model was selected to reproduce the hydrodynamics of the Kelligrews River in this study.

Lack of historical inflow data (or gauging stations) at the upstream and seaward boundary

In the DYNHYD5 model, the inflow and outflow data are required to describe the receiving inflow at the model upstream and other model boundaries, as well as the outflow at the seaward boundary. In this study, the model upstream segment was selected at the Swimming Pool in the Kelligrews River, where consecutive water levels were measured by the deployed pressure transducer and data logger. As mentioned in Chapter 4, direct measurement of time-varying inflow is difficult and expensive. A common method to obtain time-varying flow is to derive flow from the measured water level, using the site specific mathematical relationship between the measured water level and flow. However, due to the limited time and manpower on this project, only three sets of water level and flow data were measured at the Swimming Pool during 2009 and 2010 to develop the relation curve between the measured water level and flow.

In addition, during the DYNHYD5 model prediction, weekly averaged inflow at the Swimming Pool between 2006 and 2009 were estimated based on the approximated

regression between the observed water level change and rainfall during December 2009 and August 2010. The approximated water flow at the Swimming Pool between 2006 and 2009 was estimated on a weekly averaged basis, and was not capable of reflecting daily changes of water flow. Consequently, the daily changes of pollutant concentrations may not be reflected in the model results between 2006 and 2009. However, the consecutive water level with 10 minute intervals was obtained by the deployed data logger on site since December 2009, and the data was further processed to obtain daily averaged inflow as the model input. Thus, the daily concentrations of pollutants were simulated during the time period between December 2009 and August 2010. This was reflected from the model results that the concentrations of pollutants during December 2009 and August 2010 fluctuate more frequently than the time period between July 2006 and December 2009 due to the use of daily flow rather than the weekly averaged flow as model input.

On the other hand, the high and low tidal heights for multiple tidal circles at the seaward boundary are required as model input to determine the impacts of tide on the downstream water qualities. However, only the time-varying tidal heights during December 2, 2009, and March 26, 2010, were monitored by the deployed data logger at the mouth of estuary. Due to the lack of historical tide record at the seaward boundary, the tide effects on the downstream segments beyond the time period just mentioned were not simulated. In other words, the DYNHYD5 model and water quality model only correctly simulated trends of change of pollutants concentrations at Segments 1 to 7. The water levels of Segments 1 to 7 were not impacted by the tide due to their relatively high river bottom elevations. Therefore, future research is recommended to collect the time-varying tidal heights data at the mouth of estuary to determine the impacts of tide on water qualities at downstream segments of Kelligrews River, closer to Conception Bay.

> Use of a minimal flow for the "freezing" time period in winter.

The measured water level at the Swimming Pool in the winter, especially during the time period from February 3 to 19, 2010, approached zero due to the freezing of surface water. The freezing of surface water hindered the deployed pressure transducer from working properly and minus readings of water levels were obtained during that time period. To solve this, a minimum water level before the freezing of surface water occurred was utilized to replace the negative water level readings as model input, in order to ensure the model worked properly.

As introduced in Chapter 2, the DYNHYD5 model was previously developed as an estuary model and has been mostly applied to simulate the hydrodynamics of large rivers and estuaries. The performance of the model is limited when it is applied to the study area where snow and freezing of surface water occurs in winter. For instance, the model may underestimate the river flow in the summer due to the snow melting.

CHAPTER 6 APPLICATION OF WATER QUALITY MODEL TO THE STUDY AREA

In this Chapter, the Water Quality Analysis Simulation Program (WASP) is applied to the Nut Brook and Kelligrews River watershed for simulation of heavy metal pollution along the river channel. The collection and processing of input data for running the WASP model is introduced. The sensitivity analysis, calibration and verification of the WASP model, and the results analysis are also included in this Chapter.

6.1 WASP Model Input Files Generation

After the running of the hydrodynamic model, the model output file with HYD extension was used as an external linkage for the WASP model. Meanwhile, different types of data were collected and processed for generating input files of the WASP model. As introduced in Chapter 4, the input files were not coded in ASC II format since the release of the WASP 6.0 version. As a result, text editors can not be used to modify the model input files. Instead, a WINDOWS-based preprocessor was utilized to generate the required inputs for the WASP model. The input data was entered in a series of input screens provided by the preprocessor. The preprocessor was used throughout the model sensitivity analysis, calibration and verification. The collection and processing of the model input data are introduced in the following sections, adhering to the sequences of the input list on the WASP screen.

6.1.1 Input parameterization

As discussed in Chapter 4, the data entry form for the input parameterization should be implemented to initiate a project. In this study, the toxicant module in the WASP was utilized in order to simulate the transport and fate of metals in the Nut Brook and Kelligrews River watershed. As introduced in Chapter 3, Iron served as the representative metal of which the concentrations at downstream sampling sites exceeded corresponding guidelines; Zinc served as the representative metal of which the concentrations at downstream sampling sites did not exceed guidelines but indicated potential risks to the aquatic life. For this reason, the concerned metals, including Zinc and Iron, were selected as the trace metals for the water quality simulation during this study.

At the same time, the external hydrodynamic linkage file was prepared and imported to the WASP model. The hydrodynamic linkage file includes information such as segments network, flow rate and direction, and simulation starting time and ending time. The time period from July 25, 2006, to June 22, 2009, was selected for the WASP calibration, while the time period from June 23, 2009 to August 25, 2010 was selected for the WASP verification. In other words, a total of 1064 days was chosen for calibration and 429 days for verification.

The time step option was not used because it is not necessary for the WASP to control the time step when it is linked to a hydrodynamic model (e.g., DYNHYD5). The ratio of water quality time step to hydrodynamic time step was specified as 20 in the DYNHYD5 model. As a consequence, the WASP read in new information from the hydrodynamic linkage after every 20 of the DYNHYD5 time steps.
6.1.2 Model systems

Within the WASP system data screen, the toxicant state variables were simulated and the mass balance option was used for the simulation. The mass of sand, organic solids, silts and fines were assumed to be constant throughout the simulation. A maximum concentration for a simulated toxicant was specified as 999,999 ug/L. As a result, the WASP model will not terminate the simulation until the simulated toxicant concentration exceeds the specified maximum concentration. The boundary and loading scale factors remained unchanged at 1. The boundary and loading scale factors were adjusted during the model sensitivity analysis in order to determine the impact of adjusting model parameters on the model results.

6.1.3 Segmentation

The WASP model segmentation was achieved by linking the external hydrodynamic file created by the running the DYNHYD5 model. All the junctions in the DYNHYD5 model were imported as the segments in the WASP model, which was shown in Table 5.7. The segment numbering in the WASP is the same as the junction numbering in the DYNHYD5, with the exception of model seaward boundary. The junctions in the DYNHYD5 with seaward boundary are mapped as Segment 0 in the WASP. The layout of the WASP segment network used throughout the model sensitivity analysis, calibration, and verification are plotted in Figure 6.1.



Figure 6 1 Plot of WASP segment network

Once the linkage file was imported into the WASP model, the initial segment volumes, velocities, and depths were automatically extracted from the hydrodynamic linkage file, and updated at every WASP time step. The initial WASP segment volumes, velocities, and depths at the segment data screen are shown in Table 6.1.

WASP Segment	Volume	Velocity	Depth
Number	(m ³)	(m/s)	(m)
1	227.25	0.27	0.56
2	595.55	0.20	0.55
3	941.14	0.15	0.57
4	1424.19	0.06	0.60
5	1466.05	0.05	0.62
6	1019.51	0.07	0.67
7	918.72	0.11	0.65
8	4565.15	0.19	0.74
9	19452.62	0.07	0.91
10	11400.70	0.01	1.02

In addition, the initial concentrations of pollutants at the beginning of the model simulation period must be specified for each segment. Therefore, the observed concentrations of pollutants (e.g., Zinc and Iron) on July 25, 2006, at a number of sampling sites were entered as the initial concentrations for Segments 1, 4, 5, 7, and 8, respectively. The initial concentrations of rest segments remained unchanged from the default setting of 0 ug/L due to the lack of sampling data at those segments at the beginning time of model simulation. The initial concentrations of segments were found to have insignificant impacts on the model results because the modeled concentration of pollutants is simulated based on the boundary concentrations and pollutant loading rates after the starting of simulation.

The partition coefficient of each toxicant, which describes the ratio of absorbed metal concentration to the dissolved metal concentration at equilibrium, was also required to calculate the metal transport. The partition coefficient (log K_d in L/kg) for a particular metal depends on the nature of suspended solids or sediment and key geochemical parameters of the water such as pH and concentration of sorbents (Allison & Allison, 2005). Literature reviews (Allison and Allison, 2005; Vezina and Cornett, 1990) have been performed to determine the range and statistical distribution of the partition coefficients of concerned metals, including Zinc and Iron in field studies. The ranges and median values of partition coefficients to suspended matters for the Zinc and Iron are shown in Table 6.2. The median values of partition coefficients were used for this study. Few studies have been conducted to estimate the partition coefficient of Iron between water and suspended solid. Vezina and Cornett (1990) studied the iron transport and

distribution between freshwater and solids, and the partition coefficient for stable Iron was estimated to be ranged from 1600 to 4800 L/Kg, which corresponds to 3.2 to 3.7 in unit of log K_d in L/kg. As a result, a median value of 3.45 was used for estimating the partition of Iron ions in this study. In addition, a constant density (i.e., 0.2 g/L) for the suspended matters was specified in the WASP, by averaging the measured total suspended solids during field trips.

	Zinc	Iron
	(K _d in L/kg)	(K _d in L/kg)
Range	3.5-6.9	3.2-3.7
Median	5.1	3.45

Table 6.2 Partition coefficients to suspended matters for the concerned metals from the literature reviews

6.1.4 Parameter and constants

Within the model parameter and constant screen, the model parameters such as partition coefficients to suspended solids was specified as showed in Table 6.2 and the scale factor were set to 1. The scale factors are used to calibrate the partition coefficients in order to determine their impacts on model results. Other model parameters, including volatilization exchange rate constant, atmospheric chemical concentration, Henry's law constant, and water column/benthic decay rate constant, were not used for the simulation of metals.

6.1.5 Exchange

In the WASP, the user has a choice of up to two exchange fields. The water column dispersion in the model's exchange function was selected to simulate surface water chemical dispersion. The pore water diffusion in the preprocessor, which is used to simulate the exchange of dissolved chemicals in the river bed, was not used in this study due to lack of data for sediment layer. This study used one dimensional water quality modeling, which assumes the chemical concentrations are vertically uniform within the river system. In addition, the scale factor for model exchanges remained unchanged from the default value of 1 and was adjusted during the model calibration.

According to the principle of conservation of mass and Fick's law (Schnoor, 1996), the rate of change of mass in a control volume (e.g., segment in the WASP model) depended on the rate of change of mass caused by the advection, diffusion/dispersion (mixing), and

transformation (degradation). In this study, the decay rate for metals remained unchanged from the default value of 0 per day. The metals are not likely to degrade in the water, but may undergo chemical reactions or biologically mediated redox transformations. However, the total amount of metals in the water system remains unchanged. As a result, the main processes that dominate the transport of metals become the advection and diffusion/dispersion. The transports of chemicals in the rivers are mainly affected by advection, but the transport of chemicals in lakes is often controlled by dispersion. In the one-dimensional model, the advection refers to movement of dissolved or fine particulate material at the current velocity at longitudinal direction. The advective transport of metals is accounted in the WASP model by using the mean concentration of metals and the volumetric flow rate. The transport of metals in the river is also affected by the molecular diffusion and longitudinal dispersion process. In an estuary or coastal water system, the chemical mixing caused by the advection and dispersion processes are much greater than the molecular diffusion process in which the chemical moves due to concentration gradient. This can be reflected by the ranges of values for the dispersion coefficient and the diffusion coefficient, as shown in Table 6.3 (Schnoor, 1996). As a result, the chemical mixing caused by molecular diffusion was not considered during the water quality modelling.

Process	Direction	Typical Range [m ² /s]
Molecular diffusion	Vertical	10 ⁻⁸ to 10 ⁻⁹
	Lateral	10 ⁻⁸ to 10 ⁻⁹
	Longitudinal	10 ⁻⁸ to 10 ⁻⁹
Dispersion	Vertical	10 ⁻³ to 10 ⁻¹
	Lateral	10 ⁻² to 10 ⁰
	Longitudinal	10 ⁻¹ to 10 ⁴

Table 6 3 Range of values for molecular diffusion and dispersion Modified from (Schnoor, 1996)

In this study, the Kelligrews River discharges into Conception Bay and its downstream portion is affected by the tide and influx of saline water from the sea. Meanwhile, a one dimensional hydrodynamic model and a water quality model were used in this study to simulate the transport and fate of chemicals within the river system. Therefore, the longitudinal dispersion was considered as one of the dominant processes governing the exchange of chemicals within the Kelligrews River, and the coefficient served as an important model parameter for the WASP model calibration. Consequently, the longitudinal dispersion function for surface water exchange was defined within the model's exchange function. In the WASP, each exchange function has its own set of exchange segment pairs and a corresponding dispersion time function (USEPA, 2003). As a result, the mixing area and length between adjoining segments and across the open water boundary were specified within the WASP interface. The interfacial mixing area between adjoining segments in the model corresponds to the channel cross-section area connecting the upstream and downstream segments. The channel cross-section area between each pair of segments can be read from the generated output file from the DYNHYD5 model. Likewise, the mixing lengths of dispersion, which represents the distance between the central points of the paired segments, are the same as the channel length. As a result, the mixing length for each segment pair was specified by using the channel length in the DYNHYD5 input file.

In addition, an initial value of the dispersion coefficient for the longitudinal dispersion function must be defined and later adjusted for the model calibration. The estimation of longitudinal dispersion coefficient in rivers was introduced in the WASP manual (Ambrose & Wool, 2009) as follows:

$$E_x = \frac{0.011 \cdot \bar{u}^2 \cdot B^2}{d \cdot u^*} \pm 50\%$$
(6.1a)

$$u^* = \sqrt{g \cdot d \cdot S}$$
 (6.1b)

Where,

 $E_v =$ Longitudinal dispersion coefficient (m²/s),

 \overline{u} = Mean velocity (m/s),

B = Width(m),

d = Depth (hydraulic radius) (m),

 $u^* =$ Shear velocity (m/s),

g = Gravitational acceleration (m/s2), and

S = Channel slope (m/m).

Equation 6.1 only gives an estimated range of the longitudinal dispersion coefficient, but not a specific value for the dispersion coefficient. For this reason, the method for the estimation of the longitudinal dispersion coefficient of rivers, as developed by Fischer (1979), was utilized in this study, as expressed as follows (Schnoor, 1996):

$$E_x = \rho \frac{\overline{u}^2 B^3}{u^* A} = \beta \frac{Q_B^2}{u^* d^3}$$
(6.2a)

$$\beta = 0.5 (u^*/\bar{u})^2$$
(6.2b)

$$u^* = \sqrt{\frac{f}{8}\overline{u}^2}$$
(6.2c)

Where,

 $Q_{R} = river discharge (m^{3}/s),$

A = cross-sectional area (m²), and

 $f = \text{Darcy-Weisbach friction factor} \approx 0.02$ for natural, fully turbulent flow.

As a result, the initial value for longitudinal dispersion coefficient was calculated by Equation 6.2. In the WASP, only one dispersion coefficient with the corresponding time function was used to describe the dispersive exchange of all model segments. For this reason, the longitudinal dispersion coefficients at all segments were averaged and an identical value (i.e., 2.5 m²/s) was applied to all segments along the river. The estimated coefficient for the Kelligrews River was compared with that of other stream and rivers with similar river channel characteristics (e.g., depth, width, slope and shear velocity) reported in the literature (Schnoor, 1996), and the comparison indicated that the estimated value is reasonable for such narrow and shallow river. The dispersive exchange parameters used in the WASP model can be summarized as follows (Table 6.4):

Segment	Mixing	Mixing
Pairs	Area	Length
	(m ²)	(m)
Upstream boundary to 1	0.80	184
1 to 2	1.10	295
2 to 3	3.30	276
3 to 4	3.00	295
4 to 5	4.20	466
5 to 6	3.31	320
6 to 7	2.10	425
7 to 8	1.80	452
8 to 9	35.25	365
9 to 10	115.00	188
10 to downstream boundary	5.40	191

6.1.6 Pollutant loading rate

As introduced in Chapter 3, water quality of the Kelligrews River was significantly impacted by its tributary, the Nut Brook, which was contaminated by the pollutants released from the industrial zone located in the vicinity of Incinerator Road. The pollutants in the Nut Brook were carried through the Nut Gully and discharged into the Kelligrews River. To simplify the modeling system, the pollutant loading from the Nut Brook was considered as a point source of pollution for the Kelligrews River. Accordingly, the pollutant loadings from the outlet of the Nut Gully (Figure 6.2), the portion of the upstream of the Nut Brook and Kelligrews River junction, were used to estimate the pollutant loading rates to the Kelligrews River. However, there is no water quality gauging station located at the outlet of the Nut Gully during the study period, thus the time-series of pollutant concentrations are not available for this study. In this study, a total of 15 instantaneous water quality samples were collected on an intermittent basis during the study period from 2006 to 2010, and most of the samples were collected from June to September of each year because most the sites are inaccessible in the winter.



Figure 6.2 Plot of location of the Outlet of the Nut Gully and upstream and seaward boundaries

The collected water quality samples during 2006 to 2008 were used to determine the intermittent pollutant loading rates during the model calibration. The collected samples from 2008 to 2010 were used to estimate the pollutant loadings for the model verification. In addition, the pollutant loading rates in the WASP model must be specified with an unit of kg/day. As a result, a global conversion factor (-0.0582), which was approximately estimated based on the averaged flow rate at the outlet of Nut Gully during 2009 to 2010 and the pollutant concentrations ($\mu g/L$) were used to calculate pollutant loading rates. The onsite measurement of flow rate along the river channels has been described in Chapter 3. A daily averaged pollutant loading rate for both calibration and verification periods were specified within the WASP (Tables 6.5). In the WASP, if a pollutant loading rate on a specific day is not provided, the value can be determined by linear interpolation based on the loading rates on the neighboring days.

Table 6 5 Pollutants loading rates (Zinc and Iron) in WASP				
Date	Zinc (kg/day)	Iron (kg/day)		
2006/07/25	1.607	11.931		
2006/08/08	1.154	20.729		
2006/08/21	1.524	20.312		
2006/09/05	1.410	19.311		
2007/07/23	1.272	60.994		
2007/08/09	1.523	68.467		
2007/08/28	1.406	138.083		
2007/09/23	1.041	40.565		
2008/11/05	0.198	12.337		
2009/06/23	0.186	23.28		
2009/07/14	0.105	10.476		
2009/08/11	0.129	39.576		
2009/09/15	0.105	49.47		
2009/12/02	0.572	22.273		
2010/03/23	0.182	15.163		

6.1.7 Boundary concentrations

In the WASP, the model boundary concentrations must be specified. In this study, two model boundaries were utilized. The upstream boundary was selected at the headwater of the Kelligrews River, Sandi Pond, which is located upstream from the Nut Brook and Kelligrews River junction. The seaward boundary was selected at the mouth of estuary downstream of segment 10 (Figure 6.2). The selection of upstream boundary assumes that the concentrations of pollutants remain unchanged between the Segment 1 (the Swimming pool) and the Nut Brook and Kelligrews River junction, because rare industrial and human activities occurred along that portion of the river. In addition, as mentioned above, a total of 15 instantaneous water quality samples were collected at the mouth of estuary during 2006 and 2010. However, only 5 samples were collected at the Sandi Pond during the time period from July, 2009 to March, 2010. Due to a lack of historical sampling data for Sandi Pond during 2006 and 2009, water samples falling between July 2009 and March 2010 were used to determine a geometric averaged concentration of pollutants. This assumes that the background concentrations of pollutants at the headwater of the Kelligrews River, Sandi Pond, did not vary significantly during 2006 and 2009 because Sandi Pond is located in a remote area and hardly affected by any human or industrial activities. As a result, the intermittent concentrations of pollutants at the upstream and downstream boundaries during the whole study period were specified within the WASP, along with corresponding sampling dates. Similar to the pollutant loading rate, the time-varying model boundary concentrations

between each of the two specified intermittent boundary concentrations were internally determined within the WASP by using linear interpolation.

The approach of using geometric averaged concentration of pollutants for the WASP model boundary has also been utilized in other WASP studies for simulation of various water quality problems, in the cases lacking a detailed time-series of water quality data. For example, such approach has been used to generate an averaged model boundary concentrations during a certain time period for the simulation of chloride concentration in the Delaware Estuary (DRBC, 2003) and feeal coliform concentration in the Lower Appomattox River, Virginia (Hammond, 2004). The time-varying boundary concentrations of Zine and Iron at model upstream and downstream boundary are presented in Table 6.6.

Date	Concentration of Zine		Concentration of from	
	(ug/L)		(ug/L)	
	Upstream	Downstream	Upstream	Downstream
	boundary	boundary	boundary	boundary
2006/07/25	1.68	20.13	220.8	253
2006/08/08	1.68	17.66	220.8	677
2006/08/21	1.68	16.66	220.8	282
2006/09/05	1.68	28.24	220.8	210
2007/07/23	1.68	37.34	220.8	800
2007/08/09	1.68	33.31	220.8	568
2007/08/28	1.68	23.47	220.8	879.52
2007/09/23	1.68	18.21	220.8	529
2008/11/05	1.68	13.02	220.8	237.3
2009/06/23	1.68	4	220.8	620
2009/07/14	0.9	6	80	490
2009/08/11	0.8	14.2	300	940
2009/09/15	1.7	6.7	310	1280
2009/12/02	18.15	66.57	348.4	515.6
2010/03/23	0.61	4.9	202.63	366.58

Table 6 6 Concentrations of Zinc and Iron for WASP upstr		upstream and downstream boundaries	
Dete	Concentration of Time	Concentration of Iron	

6.1.8 Time step

In the previous DYNHYD5 calibration and verification, the time step of 1 second was used. However, it was noticed that using a small time step for a long time period simulation (e.g., using a time step of 1 second for a simulation time period of 3 year) will result in the early unwanted termination of model simulation. Such model instability was caused by the model limitation on the total number of time steps for execution (number of iterations). Therefore, considering the length of the time period used for the WASP, the time step for the DYNHYD5 was increased to 15 seconds to produce a hydrodynamic linkage file with a 15-second time step. A time step of 15 seconds for the DYNHYD5 model was proved to be suitable and the simulation remained stable throughout the calibration and verification. Meanwhile, the ratio of water quality time step to gor hydrodynamic time step was specified as 20. Consequently, a time step of 300 seconds (0.00347 day in the WASP) was utilized for the WASP calibration and verification.

6.2 Sensitivity Analysis

The sensitivity analysis for the WASP model was performed in order to test the model stability and provide an insight into which model parameters should be adjusted to obtain more reasonable model results. A number of model inputs and parameters were selected for the sensitivity analysis. The model inputs and parameters, including the inflow rate, pollutants loading rate, boundary concentrations, partition coefficient, and dispersion coefficient were studied during the sensitivity analysis. The selected parameters were varied at $\pm 5\%$ and $\pm 15\%$ respectively to determine their impacts on the modeled concentrations of pollutants. For simplicity, the concentration of pollutants in Segment 7, where intermittent water samples have been collected during the study time period, served as the representative downstream segment throughout the model sensitivity, calibration and verification. The major reason for selecting segment 7 as the representative segment is that its location corresponds to the sampling site 7 in the Kelliview Trail where water samples were collected in the stream that flow to the residential area. The change of water quality at this site can directly affect the flora and fauna in the residential area. In addition, the relatively high elevation of Segment 7 eliminates the impacts of tide from the downstream.

The sensitivity analysis was performed by simulating the concentration of Zinc. Consequently, the average percentage changes of concentration of Zinc at Segment 7 due to the variations of model parameters were analyzed and presented in Figure 6.3. The time period used for the model sensitivity analysis remains the same as the model calibration period, starting from July 25, 2006, to June 22, 2009.



Pollutant loading	Boundary concentrations	Dispersion coefficient
Inflow		



The sensitivity analysis of the WASP model was significantly facilitated by adjusting the corresponding scale factors within the model parameter screen. During the model sensitivity analysis, the modeled total concentrations of Zinc due to the changes of model inputs and parameters were compared with the simulated results using the pre-set initial inputs values. The time-varying percent changes in modeled concentrations of Zinc at Segment 7, due to percent changes of model inputs and parameters, are shown in Figures 6.4, 6.5 and 6.6.



Figure 6 4 Change of concentrations of Zinc due to variations of inflow rate (Segment 7)



Figure 6.5 Change of concentrations of Zinc due to variations of pollutant loading rate (Segment 7)



Figure 6 6 Change of concentrations of Zinc due to variations of boundary concentrations (Segment 7)

Through the model sensitivity analysis, the inflow rate was found to have the greatest impact on the modeled concentrations of Zine at downstream segment (Segment 7). As shown in Figure 6.3, the modeled concentrations decreased when the inflow rates were adjusted to 5% and 15%, and increased when the inflows were adjusted to -5% and -15%. It can be concluded that the increased upstream inflow would dilute the concentrations of metals to a lower level. The percent change of modeled concentrations of Zine due to variations of inflow showed a gradually increasing trend when the inflow rates were adjusted to 5% and 15%; by contrast, that showed a general decreasing trend when the inflows rates were adjusted to -5% and -15%. On the other hand, it is found that the modeled concentrations of Zine showed a general decreasing trend throughout the sensitivity time period (Figure 6.4). Thus, it can conclude that the impacts of changing inflow become insignificant in the cases of low concentrations.

The pollutant loading rate was also found to have large impact on the modeled concentrations of Zinc at downstream segment (Segment 7). The percent change of total concentration of Zinc versus percentage change in pollutant loading rate remains approximately stable throughout the period of sensitivity analysis for the downstream segment (Segment 7), as shown in Figure 6.5. As discussed in Chapter 5, the hydrodynamics at Segment 7 and its upstream segments are hardly impacted by the tides from the seaward boundary due to its relatively high elevation. Therefore, it can be concluded that the chemical concentrations at Segment 7 and its upstream segments are mainly impacted by the percent change of upstream boundary concentrations, but not downstream boundary concentration. The percent change of total concentration of Zinc at Segment 7 increased when the boundary concentrations were adjusted to 5% and 15%. and decreased when the boundary concentrations were adjusted to -5% and -15%. Meanwhile, as showed in Figure 6.6, the modeled chemical concentrations showed a general decreasing trend during the sensitivity analysis time period. Therefore, it can be concluded that the impact of changing upstream boundary concentrations on the modeled concentrations at the downstream segment are more significant in the cases of low chemical concentrations.

It is found that the change of the dispersion coefficient hardly affects the modeled concentrations. This is because the Kelligrews River is a narrow and shallow river, thus the dispersive mixing cross-section area as well as mixing length for the longitudinal dispersion are not significant, comparing to large river or lakes. Therefore, the mixing of chemicals between adjoining segments is relatively fast. This can be reflected during the model simulation that the chemical concentrations at the downstream segments changed rapidly according to the change of chemical concentrations at the upstream segments.

The partition coefficient, which is used to represent the ratio of contaminants in the suspended matter phase to that in the water phase, only affects the dissolved chemical concentrations as well as the absorbed chemical concentrations on suspended matters (Allison & Allison, 2005). However, the total concentrations of chemicals are assumed unchanged during the simulation. In other words, the change of the partition coefficient only impacts the distribution of metals between the water column, and suspended matters. In this study, as introduced in Chapter 3, the collected water samples were pre-treated with acid preservative on site to dissolve the absorbed metals into the water. The total

concentrations of metals were actually measured by ICP-MS. For this reason, the partition coefficient was found have insignificant impacts on the model concentrations in this study. However, it has to be noted that the partition coefficient can be useful to investigate the chemical partitions between different phases when the water column and other layers (e.g., sediment) are both simulated by water quality models (Allison & Allison, 2005).

Based on the results of sensitivity analysis, it can be concluded that the transport of pollutants along the river was mainly dominated by the advection process, pollutant loading rates, and boundary concentrations, rather than partition and dispersion processes.

6.3 WASP model calibration

The time period selected for the WASP model calibration was from July 25, 2006, to June 22, 2009, which corresponds to the time period used for the sensitivity analysis. The preparation of input files for the model calibration is similar to that for model sensitivity analysis. The modeled concentrations of Zine and Iron at Segment 7 were compared with the observed instantaneous concentrations during the calibration. The results from sensitivity analysis proved to be useful to determine which model inputs and parameters have the largest impacts on the modeled results. As can be seen from the sensitivity analysis, the modeled concentrations are primarily affected by the model variables, including inflow rate, boundary concentration and pollutant loading rate, rather than internal parameters including the partition and dispersion coefficients. Therefore, the modeled results from the model sensitivity analysis remained unchanged and were used to compare with the observed concentrations. The observed concentrations of Zinc and Iron at segment 7 during the calibration time period were plotted against the modeled concentration, as shown in Figures 6.7 and 6.8.



Date

Figure 6 7 Modeled and observed concentrations of Zinc for WASP calibration



Figure 6 8 Modeled and observed concentrations of Iron for WASP calibration

The modeled concentrations of Zinc and Iron basically fall within the range of observed concentrations and converged on the observed concentrations. The concentrations of Iron were found increased dramatically in August 2007 and reached a peak in September 2007. The increase of modeled concentrations mainly attribute to the increased pollutant loading rate from the Nut Gully during that time period, which can be linked to increased industrial activities or dumping activities at the upstream of the Nut Brook. The observed results and the modeled results during the calibration time period were plotted to obtain a linear regression. A goodness-of-fit test was used to measure how well do the observed concentrations of Zinc and Iron correspond to the modeled concentrations (Figures 6.9 and 6.10). As introduced in Chapter 5, as the R² value approaches 1, the modeled results and the observed results fit the linear regression well. Meanwhile, the observed concentration of Zinc on July 2007 was identified as an outlier and removed during the goodness-of-fit test. The outlier can either attribute to the lab measurement error or incorrect sample grabbing. As a result, goodness-of-fit values (R²=0.55 and R²=0.82) were obtained for the linear regression between the observed and modeled results of Zinc and Iron, respectively.








6.4 WASP model verification

The time period chosen for the WASP model verification was June 23, 2009 through August 25, 2010. The model parameters remained unchanged throughout the verification process. In order to evaluate the model accuracy, the observed concentrations of Zinc and Iron at Segment 7 during the verification period were used to compare with the modeled concentrations, as shown in Figures 6.11 and 6.12. The results indicated that the modeled concentrations basically reflected the trend of the observed concentrations during the model verification time period. Similarly, goodness-of-fit tests were also performed for the linear regressions between the modeled results and observed results for Zinc and Iron. The concentration of Iron on September 2009 was identified as an outlier and removed during the goodness-of-fit test. As a result, relatively satisfying R² values (R²= 0.965 for Zinc and R²=0.904 for Iron) were obtained for the model verification time period, as shown in Figures 6.13 and 6.14.



Figure 6 11 Modeled concentrations of Zinc for WASP verification (Segment 7)



Figure 6 12 Modeled concentrations of Iron for WASP verification (Segment 7)



Figure 6 13 A goodness-of-fit test for modeled concentrations of Zinc during the WASP model verification



Figure 6 14 A goodness-of-fit test for modeled concentrations of Iron during the WASP model verification

The modeled concentrations of Zinc and Iron during the entire simulation time period, including both model calibration and verification time period, were plotted against the observed concentrations, as shown in Figures 6.15 and 6.16. The results indicated that the modeled concentrations of Zinc and Iron reasonably matched with the observed instantaneous concentrations at Segment 7 from July 25, 2006 to August 25, 2010. However, discrepancies existed and the major causes could be attributed to the following reasons: use of estimated weekly averaged inflow as model input for the time period from July 2006 to December 2009, in the cases of lacking historical flow data at the upstream; use of geometric averaged concentrations as the model upstream boundary concentrations for the time period from July 2006 to June 2009, in the cases of lacking a detailed timeseries of water quality data at Sandi Pond; use of limited instantaneous water samples (i.e., 15 sets) collected at outlet of Nut Gully to estimate the intermittent pollutant loadings to the Kelligrews River, in the cases of lacking a detailed pollutant loading rate during the study time period.



Figure 6 15 Modeled and observed concentrations of Zinc for the entire simulation time period (Segment 7)



Figure 6 16 Modeled and observed concentrations of Iron for the entire simulation time period (Segment 7)

At the same time, the model calibration and verification results were combined in order to determine a goodness-of-fit value (R^2) for the linear regression between the modeled and observed results of Zine and Iron during the entire simulation time period. As shown in Figures 6.17 and 6.18, relatively satisfying goodness-of-fit values (R^2 =0.71 for Zine and R^2 =0.76 for Iron) were obtained for the modeled concentrations during the entire simulation time period. As can be seen from Figures 6.17 and 6.18, it can be concluded that the modeled concentrations of Zine are biased on the low side while the modeled concentrations of Iron are biased on the high side. The discrepancy between the modeled and observed results could be caused by a number of uncertainties existing during sample collection and analysis as well as the limited performance of two models.



Figure 6 17 A goodness-of-fit test for the modeled concentrations of Zinc for the entire simulation time period





6.5 Model limitations

The application of the WASP model in this study proved to be effective in simulating the transport of pollutants in the Kelligrews River. However, the performance of the WASP model can be further improved by addressing some modeling limitations. The encountered limitations of the WASP model are summarized as follow:

> Lack of detailed time-series of water quality data at the model boundary

The time-varying model upstream and downstream boundary concentrations must be specified as the WASP model input. The model upstream and downstream boundaries were extended to the headwater of Kelligrews River and the Mouth of estuary, respectively. The arguments for choosing model boundaries have been discussed in Chapter 5. In this study, a total of 15 instantaneous water samples collected at the mouth of estuary during 2006 and 2010 were used to determine the intermittent model downstream boundary concentrations. However, only a total of 5 instantaneous water samples were collected at the headwater of Kelligrews River (Sandi Pond) during July 2009 and March 2010. Due to a lack of historical water quality data for the Sandi Pond, the collected water samples falling between July 2009 and March 2010 were used to determine a geometric averaged concentration of pollutants for the time period between July 2006 and June 2009. This assumes that the concentrations of pollutants at the headwater of Kelligrews River do not vary significantly because the site is located in a remote area and rare human interference occurred around the site. However, using the

geometric averaged concentration of pollutants for the model upstream boundary may compromise the accuracy of model results. Therefore, a detailed time-series of water quality data at the model boundary should be obtained for the better performance of water quality modeling in the future.

> Lack of detailed data for the estimate of pollutant loading rates to the Kelligrews River

The Nut Brook was considered as a point source of pollution to the Kelligrews River since it is the only tributary that flows into the Kelligrews River. As a result, a total of 15 instantaneous water samples collected on an intermittent basis at the outfall of the Nut Gully were used to estimate the time-varying pollutant loading rates to the Kelligrews River between 2006 and 2010, with units of kg/day. To obtain more reliable time-varying pollutants loading rates, future studies should explore the potential of using a basin-scale water hydrology and water quality model in the study area for a time history of the runoff flow rate and water quality.

CHAPTER 7 SUMMARY, CONCLUSIONS, AND

RECOMMENDATIONS

This research presents a comprehensive water quality study at the Nut Brook and Kelligrews River watershed. The water quality at the Nut Brook and Kelligrews River was mainly impacted by the industrial activities adjacent to Incinerator Road. One of the major water quality concerns is that the elevated metal concentrations were found in the Nut Brook as well as Kelligrews River, especially at the sites adjacent to Incinerator Road. The elevated metal concentrations are believed to be attributed to the surface runoff from the abandoned landfill, as well as the active and inactive quarry in the vicinity of Incinerator Road. The surface runoff discharged into the nearby water body led to the violations of corresponding water quality guidelines. To investigate the water quality, intermittent field monitoring and sampling have been conducted since 2006 to monitor the general water quality indicators as well as to collect water, sediment and soil samples for various tests. At the same time, to compensate the limitations existing in sampling and monitoring, water quality modeling was also applied to the study area with the purpose of better characterizing the health of the water body. After performing a detailed literature review of applicable water quality models, a one-dimensional hydrodynamic model and a water quality model, both developed by USEPA and extensively applied for various water quality studies, were utilized for hydrodynamic and water quality simulation of metals in the study area. Zinc and Iron were selected as the representative metals and their concentrations were simulated along the Kelligrews River over the study time period. With the data available and time constraints present, reasonable results were obtained for hydrodynamic and water quality modeling calibration and verification. Overall, the selected DYNHYD5 and WASP models were

proved to be quite effective in the hydrodynamic and water quality simulation of metals within the Nut Brook and Kelligrews River watershed.

7.1 Summary and Conclusions

Over the years, there has been growing concern and significance in studying water quality issues in coastal waters. The coastal waters are extremely important habitats for a wide variety of plant life and animals such as fish, mussels, seaweeds, and other sea life. The coastal waters support valuable biological resources and are meaningful for local recreation and tourism. In addition, the coastal water also served as a physical buffer protecting communities near the coast from storm surges and flooding. Coastal degradation caused by wastewater and stormwater discharges has been an important issue for regional water quality management. In the study area, the coastal water is mainly impacted by the wastewater and surface runoff from the industrial zone located in the vicinity of the Nut Brook. The increases in industrial activities on the Incinerator Road, the expansion of quarry areas, as well as the runoff from the abandoned landfill, have resulted in a gradual deterioration of water quality in the Nut Brook and Kelligrews River watershed. This study aims to provide the most comprehensive study of water qualities in the Nut Brook and the Kelligrews River to date. Study results can be used to determine the effects of industrial activities on water quality and meanwhile to provide valuable information for local authorities in pollution control and watershed management.

7.1.1 Water quality study in the Nut Brook and Kelligrews River watershed

In this study, the water quality problem in the Nut Brook and Kelligrews River watershed was comprehensively studied through field investigation, sampling, monitoring and water quality modeling. The watershed boundary and drainage network were delineated at the beginning of the study, using the DEM data acquired from the City of St. John's. Starting from 2009, 14 sampling sites were selected within the watershed boundary, based on their essentiality in pollution source identification and water quality assessment. Field works were conducted with purposes of collecting water, sediment, and soil samples within the watershed, monitoring the change of water quality along the river channel, and collecting necessary hydraulic data for hydrodynamic and water quality modeling.

The collected water samples were analyzed for various physical-chemical parameters including metals (e.g., Lead, Copper, and Iron), total coliform and fecal coliform, nutrients, and TOC. A number of water quality indicators, including DO, pH, salinity, conductivity, TDS, and turbidity were consistently monitored during each sampling trip to track the water quality changes over time. In addition to the water and sediment samples, soil samples were collected at various depths at the abandoned landfill site for the analysis of PAHs content, due to the concern of its possible impact on the downstream water quality. The results from intermittent water sampling, soil sampling, and water quality monitoring were analyzed and compared with the existing CCME guidelines. Overall, the results from the water sample analysis indicated increased concentrations of many metals compared to background concentrations at several sampling sites in the vicinity of Incinerator Road. The average concentrations of metals, including Copper, Iron and Aluminum, have exceeded the Canadian Water Quality Guidelines for the Protection of Aquatic Life (CCME, 2007) at sites adjacent to Incinerator Road and some did not exceed the guidelines but showed potential risks (e.g., Lead and Zinc). The elevated metal levels at the sites adjacent to Incinerator Road appeared to be attributed to the surface runoff from the abandoned landfill site and quarrying activities.

Meanwhile, a number of PAHs compounds, including Benzo(a)anthracene, Fluoranthene, Naphthalene, Phenanthrene, and Pyrene, were detected at measureable concentrations in the soil and the concentrations showed a decreasing trend as the soil depth increases. The maximum observed concentration of Naphthalene and Phenanthrene were found to be 16.2 and 7.4 times of the existing CCME soil quality guideline, respectively. The presence of PAHs compounds in the soil at the landfill site could pose a potential threat to the nearby fauna, flora and water bodies.

The data collected during the study period gave an indication of contaminant sources and overall water quality in the Nut Brook and Kelligrews River watershed; however, the limited time period and field samples could hardly reflect and especially predict characteristics of the water quality in the watershed. For example, the water samples were mostly collected and analyzed on a monthly basis from June to September of each year. Intensive and prolonged monitoring and sampling efforts required to fully characterize

the "health" of the water body in the study area can be very expensive and timeconsuming.

In order to help address these problems, modeling tools (DYNHYD5 and WASP) were applied in this study to utilize limited sampling data to better interpret and predict water quality responses to the natural and manmade pollution in the Nut Brook and Kelligrews River watershed. The results from this study can be further used to perform total maximum daily load (TMDL) study for the local watershed in the future. Additionally, the model simulation period can be further extended to the present day once the streamflow data and pollutant loading data become publicly available.

^{*} 7.1.2 DYNHYD5 and WASP model application

The DYNHYD5 and WASP models were utilized to examine water quality in this study. In particular, the models were used to interpret and predict the water quality responses in the Kelligrews River due to the pollutant loadings from the Nut Brook tributary. During the application of the DYNHYD5 model, the modeled water levels were calibrated against the observed water levels to achieve the goal of hydrodynamic model parameterization and validation. Prior to model calibration, a number of model input parameters, including inflows, Manning's roughness coefficient and tide height scales, were adjusted at \pm 5% and \pm 15% respectively to determine their impacts on the model results. Through the sensitivity analysis, it was found that the changes of inflow and Manning's roughness coefficient have relatively significant impacts on the modeled water level at the upstream portion. By contrast, the modeled water level at the downstream segments, where the water levels were affected by the tides from Conception Bay, were more impacted by the adjustment of the tide height scales at the model seaward boundary. As concluded from the results of the simulation for a non-tidal river, the upstream boundary concentration for a conservative pollutant will be propagated through all downstream segments. For estuaries and coastal rivers, the upstream concentration is mixed into and diluted by the seawater from downstream seaward boundary. The degree of mixing depended on the relative strengths of the upstream flow, the tidal flow, and the dispersive exchange flow.

The time period from December 3, 2009 to February 2, 2010 was selected for the DYNHYD5 model calibration. The modeled water level at segment 7 was plotted against the observed water levels and reasonable results were obtained after adjusting the model parameters. A goodness-of-fit test was performed to examine the linear regression between the modeled results and the observed results during the model calibration time period, and a satisfying R² value of 0.963 was obtained for the linear regression analysis. The period of February 20 to March 26, 2010 was chosen for the DYNHYD5 model verification, and a goodness-of-fit value of 0.949 was obtained. Overall, a R² of 0.923 was obtained for the entire hydrodynamic simulation period from December 2009 to March 2010. After the calibration and verification, the model was further used to predict the water movement of the Kelligrews River between June 25, 2006 and December 2, 2009. Due to a lack of historical inflow data at the upstream (the Swimming Pool), an empirical approach was applied to estimate the weekly averaged water level, through the

approximated relationship between the weekly averaged precipitation and the weekly averaged water level change at the Swimming Pool. After that, the DYNHYD5 model successfully simulated the water movements in the Kelligrews River from June 2006 to August 2010.

Once the DYNHYD5 correctly simulated the streamflow, the results were further linked to the WASP water quality model to provide the hydrodynamics of the water body (e.g., flow and velocity). Similarly, the modeled results from the WASP model were calibrated and verified against the observed concentrations during the entire study time period from July 2006 to March 2010 in order to ensure that the WASP model could correctly simulate the transport and fate of pollutants along the river channel. Prior to the model calibration, a sensitivity analysis for model input parameters including pollutant loading rates, boundary concentration, and dispersion coefficient was performed to determine which parameters should be modified during the model calibration. The pollutant loading rate, which was estimated based on the intermittent concentrations of pollutants as well as averaged flows at the outlet of Nut Gully, was found to have the most significant impact on the model results. By contrast, the dispersion coefficient was found to have insignificant impacts due to the characteristics of the Kelligrews River (relatively narrow and shallow). The sensitivity analysis proved to be quite useful in providing insight regarding which model parameters should be adjusted during the model calibration for more reasonable model results. The model calibration was also performed within the same time period as the model sensitivity analysis. The concerned metals, Zinc and Iron, were selected as the representative pollutants for the water quality simulation of metals.

A total of 15 concentrations of Zinc and Iron based on grab samples during 2006 and 2010 were used to compare with the modeled concentrations. The goodness-of-fit tests were performed for the linear regression analysis between the modeled and observed results for Zinc and Iron. Relatively satisfying R² values of 0.69 and 0.742 were obtained for Zinc and Iron, respectively. Nevertheless, the comparison between the modeled and observed results also indicated the existing bias which may be caused the limited performance of the models. Overall, it can be concluded that the selected DYNHYD5 and WASP models produced reasonable results in simulating the trends of concerned pollutants levels over the entire study time period.

It is a worth a note that a programming bug existing in the WASP model when connected to the DYNHYDS model was found during this study. The WASP incorrectly read the ratio of water quality time step to DYNHYD5 time step from the hydrodynamic linkage file and thus led to the early termination of the simulation runs. The time step error was introduced in the latest version of the WASP model (WASP version 7.4). The bug was fixed by communicating with the model developers (Robert Ambrose & Tim Wool), and test runs using the data from this study. The correction of the WASP model code contributed to the release of the next WASP version 8.0.

The results from water quality sampling and modeling can provide valuable information for local authorities in pollution control and watershed management. The modeling results can be further used to guide future monitoring and sampling efforts. For example, enhanced sampling frequency and selection of locations should be considered in the area with relatively high concentrations of pollutants during the future sampling and monitoring.

7.1.3 Modeling limitations

With the data available, time and manpower constraints present, relatively reasonable results were obtained for the hydrodynamic and water quality modeling. However, as introduced in Chapters 5 and 6, there are still some modeling limitations that compromised the performance of the modeling. The modeling limitations mainly attributed to the lack of observed data for model input and calibration. For example, a lack of detailed river bathymetry data hindered the development of two-dimensional model for the study area. In addition, the limited sampling and monitoring data at specific sites resulted in the lack of long-term detailed observed data for the water quality model calibration and verification. On the other hand, the statistical methods for the model sensitivity analysis and result analysis could be further improved. For example, the study used One-Factor-at-a-Time method for the sensitivity analysis due to the time and manpower constraints on this study. A factorial method to systemically study the impacts of model parameters is recommended for the future modeling research.

7.2 Recommendations

Based on the field investigation and water quality modeling, a number of recommendations were made to the local authorities for facilitating water pollution control and quality management practices.

1) Environmental management practices for the mine operations phase are recommended for the quarrying at the study area. A site-specific sampling program should be consistently conducted in the vicinity of the quarry site during the time period of guarrying operations, to monitor the quality of collected mine water and seepages from waste rock dumps and tailings management facilities. The water quality in the retention facilities, such as the sedimentation ponds, should also be monitored to check the performance of water management facilities. The river bank adjacent to quarry sites should also be regularly inspected for soil erosion and damage. Furthermore, the use of fresh water should be minimized as much as possible and the recycling of water is recommended during the quarrying operation. In addition to water management, the tailings and waste rock generated from the quarrying should be considered for use as mine backfill, instead of piling them up at the quarry sites. Assessment of the physical and chemical characteristics of the mineral should be conducted to evaluate the suitability of the material for mine backfill. A comprehensive study should be conducted in the near future to develop more effective best management practices and especially to reduce the impacts of quarrying to the nearby water quality.

2) Control of surface runoff from quarry operating by buffer zones as well as effective best management practices for treating wastewater and tailings. As stated previously, the

degraded water quality at the sites in the vicinity of Incinerator Road appeared to be attributed to the surface runoff from the abandoned landfill site, as well as active and inactive quarries adjacent to Incinerator Road. Through the use of buffer zones, the pollutants from surface runoff can be greatly reduced and thus the introduction of pollutants to the streams can be controlled. In practice, the coarse and suspended particles from either quarry or landfill site can be deposited and filtered through the leaf litter and the soil. Meanwhile, a number of pollutants such as metals can be detained and decayed in the buffer zone of soil, or taken up by plants. Furthermore, studies should also be carried to maximize the effectiveness of the buffer zone for local water pollution control, because the degree of effectiveness of buffer zones is attributed largely to the physical properties of the buffer zones (e.g., width and slope), the diversity of pollutants encountered (e.g., organic matters and metals), as well as the proximity of the buff zone. For example, for the non-point source pollution in the study area, buffer zones would ideally extend along tributary streams towards the catchment boundary. Overall, by optimizing the arrangement of the buffer zones, the surface runoff can enter the buff zone as shallow, overland flow in order to be slowed or detained, rather than channelized streamflow.

3) Continuous sampling and monitoring for soil and water quality and post-treatment evaluation are desired. Continuous sampling and monitoring for soil at the landfill site are recommended in the future, as it is a key factor to evaluate the effectiveness of the pollution control and river management actions and their potential impacts to nearby ecological systems. At the same time, a regimented sampling and monitoring program

for water quality is also recommended to ensure the recovery of the water quality within the watershed, as well as to improve the performance of future hydrodynamic and water quality modeling in the study area.

4) Ecological and health risk assessment for the vicinity of the concerned sites along the rivers. Ecological risk assessment should be conducted for the local aquatic species to evaluate the likelihood of adverse ecological effects occurring as a result of exposure to the impacted water quality within the watershed. At the same time, human health risk assessment should also be conducted to provide the nearby residents with an evaluation of their health risk assessment and use of contaminated water resources. The results from ecological and health risk assessment can be used to link industrial activities at the river upstream to their potential effects, and meanwhile provide a basis for comparing different pollution control and watershed management alternatives.

5) Site assessment and enhanced sampling program in the concerned sites (especially the landfill site) to further understand and evaluate the level and scale of the pollution issues. In this study, limited soil samples were collected at the landfill site for persistent organic pollutants analysis, including PAHs and PCB, and the results indicated that a number of PAHs compounds in the soil exceeded the corresponding soil guidelines. The limitations on the quantities and ranges of collected samples compromised a full understanding of the soil pollution level and scale at the landfill site. In addition, the collected sol samples at the landfill were only tested for PAHs and PCB due to the limited budget for this study. Future studies are recommended to investigate the level of other pollutants (e.g., heavy

metals) to evaluate the potential impact of the landfill to the downstream water quality. In the future, more samples should be collected in sediment and surface/ground water in the downstream region.

6) In-situ remediation of the landfill site to restore the natural soil conditions and reduce impacts on water bodies in the downstream areas. As stated previously, the landfill soil has been contaminated by the dumps, as well as remaining residues from the operation of incinerator in the past. Therefore, in-situ remediation is recommended to remove contaminants from the soil, as well as contaminated groundwater if possible. Comparing to ex-situ remediation, the main advantage of in-situ remediation is that it allows the contaminated soil to be treated without being excavated and transported, which would significantly save the remediation cost. Currently, a number of in-situ physical/chemical remediation technologies are available for contaminated soil, such as soil vapor extraction (SVE), enhanced aerobic bioremediation and phytoremediation. The selection of an appropriate remediation technology depends on a number of factors: the size, location, geographical condition, and history of the site; soil characteristic (e.g., structure and pH); the type of contaminants and the degree of pollution (e.g., contaminant concentration and distribution); the fund and technologies available for the target area; the desired final land use; local environmental regulations and stakeholder's concerns. Meanwhile, the cost, benefit and required time of those remediation technologies vary, especially when applied to different sites. Therefore, lab tests and pilot scale experiment for in-situ remediation technology screening and performance evaluation, as well as cost analysis and system design, are much desired before field applications.

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