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MODELLING OF TOXIC CONTAMINANTS

IN

LARGE RIVERS

by

Yuen Ee-Mun, B.A.Sc., M.A.Sc.

A Dissertation
Submitted to the Faculty of Graduate Studies and Research
through the Department of Civil Engineering in Partial
Fulfillment of the requirements for the Degree of
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To my beloved mother
ABSTRACT

In this study, modelling tools for large river systems are developed with the intention that such tools will eventually assist the environmental managers in their efforts to regulate the river water quality. In this endeavour, the St. Marys River was selected for a site specific study. The Upper St. Marys River is simulated by DYNHYD4, a river and estuary model, and by a lake circulation model based on the finite element method (FEM). The Lower St. Marys River is simulated by KETOX, DYNHYD4 and TOXI4. A brief discussion of each of these models is given next.

DYNHYD4 is a time dependent one dimensional model which is calibrated for both the Upper and Lower River. In addition to providing information on surface elevations and velocities, DYNHYD4 gives an indication of the time response hydrodynamic information needed in a dynamic simulation of toxic contaminants by TOXI4. Upon reaching steady state, the model’s results are in agreement with the FEM model.

The FEM model is a rigid lid steady state three dimensional model which was calibrated and verified with available field data. Preliminary runs with a non-linear model indicated that the inertia terms are not important for the Upper River, hence the FEM model neglected these terms. In contrast to DYNHYD4, the FEM model gives detailed circulation information. The model predicted the formation of gyres in the bays of the Upper River under wind conditions. An ice cover option was implemented for the Upper River. Several features of the model were revised and implemented for the microcomputer environment and a users guide has been prepared. As a tool for the user, a colour graphics presentation of the model results was also implemented.

KETOX is a two dimensional steady state river pollutant dispersion model. It includes a solution for the turbulence transport equations (K and E) and the momentum and continuity equations. In addition, the model was modified to include a sub-model component that can model chemical sediment interaction
in the river. Another modification involves the dispersion of excess momentum that occurs in regions of jet-like discharges near the power canals. The model was calibrated and verified for phenol discharged from the Algoma Terminal Basin outfall. There was good agreement between the hydrodynamic results of KETOX and DYNHYD4. KETOX can handle the splitting and combining of flows by the presence of islands or tributaries; however, flows are assumed to be generally unidirectional, and thus KETOX cannot simulate the recirculating flow of the Upper River. KETOX was used to investigate waste load allocations in the river and isoconcentration maps were obtained to determine Limited Use Zones (LUZs) for regulation purposes. As an aid to the user, an interface with colour graphics support is developed to plot the isoconcentration contours. Other aids include a capability to import KETOX results into spreadsheets for viewing and plotting. User guides are available for these model options.

TOXI4 is a time-dependent three-dimensional cell model with toxic chemical kinetics. It was necessary to modify TOXI4 in order to provide for the complex boundary conditions of the Lower River. As in KETOX, the model is calibrated and verified for phenol loads at the Algoma outfall. TOXI4 prediction of phenol levels compared well with both the Ontario MOE measured values and KETOX results. The concept of superposition was applied to set up a time response data base for the simulation of a toxic spill at the Algoma outfall. The assumption that a unit pollutograph can legitimately be used to synthesized the total spill is verified by separate runs using TOXI4. The user can evaluate different spill scenarios with this option.
ACKNOWLEDGMENTS

The material in this study, like ourselves, is clearly a product of the many who have contributed to water quality modelling. Among these modellers, I would like to express my sincere gratitude, respect and thanks to Dr. J. A. McCorquodale, my advisor and teacher. His insightful analysis, extremely wide reaching grasp of scientific and engineering principles and passion for perfection have often sent me stumbling back to my drawing board. However, his guidance and penetrating questions has contributed greatly to my growth and understanding of the skills needed in water quality modelling.

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The Lord has been a source of support and inspiration in overcoming the many trying moments. The patience and support of my parents, sisters and the Reimers, my Canadian family, cannot be overstated. They have proven to be a continual source of motivation and support during my study.

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Chapter 1

INTRODUCTION

1.1. General

A joint effort by Canadian and United States researchers to develop mathematical models for simulating the fate and transport of contaminants in the Upper Great Lakes connecting channels (UGLCC) over a three year period is drawing to an end. The UGLCC study culminated in the development of mathematical models, both mass balance and process oriented models, that will be valuable tools for indicating future research directions for assisting with resource management.

This study focuses on one of the connecting channels, the St. Marys River, which is considered to be a vital navigational channel link between Lake Superior and Lake Nicolet.

The initial study explored the feasibility of using some of the existing models. However, quite often these models have major deficiencies in research needs. Such information usually goes unreported or is buried in the realms of model jargon and simulation output.

In the simulation of hydrodynamics, pollutant transport and dispersion, this study finally settled on four models given below:
(a) the KETOX model which is a 2-D steady state river mixing stream-tube model;
(b) the WASP4 model which is an unsteady 3-D cell model;
(c) a 3-D steady state finite element lake circulation model; and,
(d) DYNHYD4 which is an unsteady 1-D link-node hydrodynamic model.

The model KETOX is very flexible to use and can do a fairly good simulation of contaminant concentrations due to discharges in the Lower River. Several modifications were made to the model, the following summarizes all its available features after the latest modifications:

(a) it is able to handle occurrences of jet like flows due to sudden and rapid changes in bathymetry;
(b) it uses variable grid spacing and its resolution can be changed at will by two controlling input parameters, this allows lateral resolution as low as 1 percent of flow and longitudinal resolution as low as 50 feet (15 metre);
(c) it can handle multiple side outfalls of pollutants;
(d) it provides a solution for the lateral dispersion coefficients across each cross section of a river that is based on the turbulence transport equations (K and E);
(e) it can handle confluences, bends and splitting of flows due to the presence of islands; and

(f) it has toxic chemical-sediment modelling capability (Di Toro et al., 1982, 1984).

Like all models, it has its own limitations. Some of these limitations are:

(a) it uses a forward marching finite difference solution;
(b) it is a steady state 2-D model; and
(c) its hydrodynamic sub-model component is based on a depth averaged velocity solution.

Some additional improvements include built-in post processing of results which allows the user to quickly plot the results through spreadsheet softwares. Otherwise, the user can rely on a program already interfaced to the model to graphically view the isoconcentration maps. The model has been calibrated and verified in the study. It is an ideal tool for waste load allocation study for the purpose of remedial and regulatory actions.

Although the KETOX model has been highlighted in the above discussion, the study also included the WASP4 model from USEPA (Ambrose et al., 1988) which is a widely used water quality model throughout the United States. This model is used in the water quality simulation for the Lower River. It is an unsteady 3-D water quality model that uses cell compartments to discretize the
Lower River. Due to the use of fairly large cells in the model, the model has much less spatial resolution than KETOX in its result. However, the toxic chemical kinetic component of this model contains elements of WASTOX, TOXIWASP and EXAMS II which are all well tested models. The WASP4 model is supported by the Centre for Exposure Assessment Modelling, Environmental Research Laboratory, U.S. EPA, Athens, Georgia. As such, the model has good technical support and is under constant improvement and testing due to the availability of funds.

As for the hydrodynamic simulations, a 3-D steady state model with rigid lid assumption is applied to the Upper St. Marys River. This is a finite element model using triangular simplex elements to discretize the Upper River. It can represent the physical boundary of the Upper River quite accurately. The model provides useful information on the circulation patterns for the Upper River under different flow and wind conditions as well as under ice cover condition. The calibration and verification of this model for the Upper River were completed satisfactorily in this study due to the availability of sufficient field data.

The application of a time dependent 1-D hydrodynamic model (DYNHYD4) to both the Upper and Lower St. Marys River provides information on the lake and river surface elevations. The model also gives information on the average velocities which are, however, fixed in their flow directions by the orientation of the channels used in the discretization. In spite of this, the model can still provide useful information on the flow distribution in both the Upper and Lower River. In the Lower River, the flow
distributions computed by DYNHYD4 are used as estimates to assign flow quantities to the stream tube option available for the WASP4 model.

The application, calibration and effort to verify these models in the simulation work for both the Upper and Lower St. Marys River are discussed in detail in the next few chapters.

1.2. Background of St. Marys River

St. Marys River is part of the Great Lakes – St. Lawrence Seaway transportation system. It is located at latitude N 46° 30' and bounded by longitude W 84° 15' and W 84° 30'. The river provides an important shipping link connecting Lake Superior at Pointe Aux Pins to Lake Nicolet south of Sugar Island. Figure 1.1 gives its geographical location in the Great Lakes system.

The St. Marys Rapids and the Sault St. Marie regulating and canal works, as shown in Fig. 1.2 (also referred to as the Soo Lock), divide the river into an upper and a lower reach herein referred to as:

(i) the Upper St. Marys River, and
(ii) the Lower St. Marys River.

Figure 1.3, a close up view of the study area, shows this physical division into sub-areas which are used in the model study. It also shows the delineating boundaries of the upper and lower reaches of the study area.
The shipping channel in the Upper St. Marys River is dredged to a minimum depth of 28 feet (8.5 metre) for the passage of local and commercial ships. There are two shallow bays, Pointe Aux Pins Bay and Leigh Bay, north of the shipping channel. These bays vary in depth from 3 to 10 feet (1 to 3 metres).

The Lower St. Marys River is a nonuniform natural channel with slightly over half of its width dredged to a minimum depth of 28 feet (8.5 metres) for the passage of ships. The other half of the river width on the Canadian side of the international boundary averages about 20 feet (6 metres).

In addition to commercial shipping, the St. Marys River provides the hydropower (two power canals at the Soo locks) and water supply for the cities of Sault Ste. Marie (Canada and U.S.A.) and the local major steel and paper industries. It also provides for extensive recreational uses such as yacht clubs, swimming, canoeing and fishing. The rich and diversified activities made possible by the river significantly contribute to the growing social wealth and economic prosperity of the local residents of St. Marys River.

1.3. Objective

The first objective of this study is to build hydrodynamic and mass transport models that will simulate the real time circulation patterns and aquatic ecosystem of the freshwater bodies of the Upper and Lower reaches of the St. Marys River.
which are being examined. The hydrodynamic and mass transport models must have the capability of simulating the range of expected flow conditions.

The second objective is to use the resulting information from the first objective to drive water quality models and at a later stage to model the uptake of toxic pollutants into the aquatic food web (not included in this study). Both steady state and time dependent hydrodynamic and convective-diffusion (mixing) models are applied in modelling the St. Marys River. The water quality model must provide an improved understanding of the important water quality interactions in the St. Marys River.

The ultimate objective of this applied modelling study is to predict future water quality impacts resulting from changes in management strategies under an expected (and observed) range of natural conditions. The predictive capability of these site-specific models will allow the environmental managers to screen the myriad of management alternatives when performing preliminary waste load allocation to attain Provincial standards for both conventional and toxic pollutants.

To fully incorporate this last objective, it is also necessary to train management staff in the use of hydrodynamic and water quality modelling techniques. With this in mind, some user-friendly features are incorporated into the computer models to make this task easier.
1.4. Definition of the Problem

The St. Marys River has been subjected to both conventional and toxic pollutants from the surrounding municipalities and industrial sources. In addition, the St. Marys River is also used for shipping and power generation on both the Canadian and United States shorelines. Hence the quality of water in this area is at risk from possible oil spills.

The Ontario Ministry of the Environment (Ontario MOE) has monitored and surveyed the water quality in this area since the early 1960’s. An important baseline water quality investigation was conducted in 1973-1974 by Hamdy, Kinkead and Griffiths (1974). This investigation indicated that the major industrial sources contributing to water quality impairment were the steel and paper industries.

The contaminants of concern are those that are potentially toxic to humans upon ingestion from the drinking water supply, or ingestion from contaminated aquatic foodstuffs, or from food sources that utilize aquatic foodstuffs as a feed. The toxic substances traced to the steel industry were phenols, cyanide, ammonia and heavy metals. Large quantities of suspended solids in the form of wood particles and fibres were traced to the paper industry.

In 1983 the Ontario MOE conducted a water quality survey of both the Upper and Lower St. Marys River and collected further information on the levels of PAH’s (polychlorinated aromatic hydrocarbons) and phenols among other environmental parameters such as pH level, conductivity and water temperature. In 1985,
the Ontario MOE undertook yet another extensive water quality investigation of the area. The 1973-1974 data collection program and both the 1983 and 1985 programs involve intensive, synoptic surveys, long-term trend surveys, and special field and laboratory studies. The purpose of these data collection programs is to compile a large data base of field measurements upon which the development of water quality models for the fate and transport of conventional and toxic contaminants can be calibrated and verified for the St. Marys River. Hence this applied modelling study is a component of the total conceptual framework to better understand and improve the water quality for St. Marys River.

1.5. Motivation

In 1978, Canada and the United States signed a Great Lakes Water Quality Agreement. Some excerpts of the agreement serve to highlight the motivation behind this applied modelling study. The agreement includes:

"reaffirming their intent to prevent further pollution of the Great Lakes Basin ecosystem owing to continuing population growth, resource development and increasing use of water"

and

"reaffirming their determination to restore and enhance water quality in the Great Lakes System."

Among its many provisions and recommendations, the agreement states that
"An early warning . . . shall be established to anticipate future toxic substances problems" including
"development and use of mathematical models to predict consequences of various loading rates of different chemicals."

In the area of research needs, it is stated that
"in particular, research should be conducted to determine:
(a) The significance of effects of persistent toxic substances on human health and aquatic life;
(b) Interactive effects of residues of toxic substances on aquatic life, wildlife, and human health; and
(c) Approaches to calculation of acceptable loading rates for persistent toxic substances, especially those which, in part, are naturally occurring."

It is clear that the model study of the St. Marys River encompasses some of these goals and hence provides the motivation towards the study efforts.

Recently the Great Lakes Water Quality Agreement between Canada and the United States was renewed. With this renewal, the Ontario MOE adopted the Municipal-Industrial Strategy for Abatement (MISA) pilot plan. MISA provides a mechanism for continuous reductions in municipal and industrial water pollution. The explicitly stated goal of the new Canada-U.S. agreement is the virtual elimination of persistent toxics from discharges to waterways.
Under MISA, all major industrial and municipal dischargers to Ontario waterways will be subject to monitoring and regulation which require them to report the concentrations and total amounts of a broad range of contaminants in their effluents. This self-monitoring program will be audited by the Ontario MOE.

Information from the monitoring will then be used to formulate an abatement regulation that will specify allowable concentrations, as well as loadings, of toxic pollutants for each discharger. Hence well calibrated and verified mathematical models can be useful tools at this stage for evaluating the waste load allocation to meet specified discharge limits. The discharge limits will then reflect the contaminant reductions that can be achieved by the dischargers using the best available technology that is economically achievable (BAT-EA).

At the beginning of 1988, the Ontario MOE indicated that it is in a position to proceed further with the St. Marys River modelling studies. This move by the Ontario MOE only reinforces the impetus in the site-specific modelling efforts for the St. Marys River.

1.6. The Approach in General

A preliminary study is made of the physical geometry of the study area in order to decide on the best way to impose the modelling boundaries. In this instance, the control structure at the Soo Locks is chosen to avoid the problem of dynamic hydraulic
boundary conditions. The other model boundaries are chosen to extend to or beyond the limits of the water quality impact zones, backwater or tidal effects.

The resolution of the spatial and temporal scales for the models is decided by the nature of the problem to be analysed. A compromise between the accuracy of important model variables, spatial resolution, numerical stability and reasonable computational time must be resolved.

Next the model network is constructed for the study area. It is necessary to identify sampling stations, points of interest and waste load sources so that the best alignment of the grid network is used. If results generated by the hydrodynamic model are to be stored for use by the water quality model, then both the networks and the time steps must be compatible though not necessarily identical.

With the network constructed, the applied modelling study will proceed through three general stages involving hydrodynamics, mass transport and water quality transformations. There is a final stage involving the modelling of the aquatic food chain mechanism which is not carried out in this study.

A hydrodynamic model is needed to calculate the water circulation and transport characteristics of the river or lake. This stage essentially answers the question of where the water in the river or lake goes. A steady state three dimensional rigid lid model is developed for the Upper St. Marys River. A steady state two dimensional depth averaged model is modified for the Lower St. Marys River. In addition, a time dependent one
dimensional free surface network model (Ambrose et al., 1988), developed by the U.S. Environmental Protection Agency (EPA), is applied to both the Upper and the Lower St. Marys River.

The second stage addresses the question of where the materials (i.e. the pollutants) in the water are routed or transported throughout the river or lake. This question is only addressed for the Lower St. Marys River due to the availability of field data. A steady state convective-diffusion river mixing model using stream function coordinates is applied to the Lower river. The modelling of the Lower River is supplemented by a time dependent three dimensional cell model developed by the U.S. EPA (Ambrose et al. 1988). The second stage is closely linked to the third stage.

The third stage answers the question of how the material in the water and sediment is transformed and what is its fate. Differential equations, based on first order kinetic representations and the law of conservation of mass are derived to describe the rate of change in parameter values as a function of causative factors such as advection, dispersion, inflow (pollutant outfalls), outflow (water export), and sinks and sources. This question is again only addressed for the Lower River and the models used are: (a) a steady state model, KETOX (McCorquodale and Yuen, 1987), and (b) a time dependent model, TOXI4 (Ambrose et al., 1988).

The final stage answers the question of how the concentration level of the pollutant in the water will impact on the water resource, e.g. impacts on the ecological balance.
Usually, the predicted levels are simply compared with water quality criteria adopted as standards to protect the general aquatic community. An example is the adoption of the concept of Limited Use Zone (LUZ), which is essentially an isoconcentration map from the point of discharge, to demarcate the limiting zone of concentration levels from the source. This question is again addressed only to the Lower River.

In terms of modelling, the main focus of the study is actually the third stage. The answers for this stage depend on a combination of laboratory studies and field monitoring by the Ontario MOE. For the modeller, it involves parameter estimation, calibration, testing and verification. The success of this step depends on the skill of the modeller who must combine specialized knowledge with common sense and skepticism in the modelling process.

Model calibration is the first "tuning" of model output to observed data. All the models applied to the Upper and Lower St. Marys River have undergone calibration.

Model verification is testing of the calibrated model using additional field data, i.e. a set of field data not used in the original model calibration, preferably under different external conditions to further examine model validity. This is also carried out for both the Upper and Lower St. Marys River.
Chapter 2

BACKGROUND AND REVIEW OF THE LITERATURE

2.1. Background

The modelling of rivers or lakes is closely related to questions of environmental protection, water supply, and ecology. An analysis and, if possible, a prognosis of these processes is of economic interest.

One of the rudimentary requirements for numerical modelling of rivers and lakes is an understanding of the basic physical processes which must be sufficiently described before formulation into mathematical equations. Generally, use is made of the fundamental conservation laws of mechanics and hydrodynamics. They can be formulated as integral or differential equations. Although the corresponding fundamentals are available, their application to specific situations in natural waters with their non-linear and turbulent behaviour presents some difficulties.

This chapter will review the mathematical equations that exist in the literature and the existing work and successes in the application of numerical modelling techniques to solve these equations. The objective is to demonstrate the advantages and disadvantages of and to gain some insight into the various approaches that one may take.
The review is structured in the following way. It begins by summarizing those systems of fluid equations which are of broad general interest in rivers and lakes. This is reviewed under the heading of mathematical equations and includes a review of the Boussinesq approximation, boundary conditions, linearization of the equations and vertical integration.

Next, the basic numerical models available in the literature (applying these equations at various levels of complexities) are described under hydrodynamic and transport models. The review in this section attempts to look at the different numerical techniques such as finite difference, finite element, method of characteristics and cell methods. Since part of the study deals with the mixing and dispersion of pollutants in rivers, a section entitled convection-diffusion river models is included. It reviews the current knowledge of side discharge of pollutants into a cross flow and how it is diffused by the turbulence.

Finally, a review section on the physico-chemical components of toxic substances is appropriate since one of the main focuses of the study is modelling these contaminants. In this section the review will discuss the special features of toxic substances that separate them from the more conventional pollutants.

2.2 Mathematical Equations

The equations are reviewed first in order to aid in the understanding of the discussion that is to follow on the
numerical models. The physical state of a river or lake can be completely described by seven macroscopic quantities, all of them expressed as function of space and time:

\[ \vec{q} \quad \text{Velocity vector with components } u, v \text{ and } w; \]

\[ p \quad \text{Pressure}; \]

\[ T \quad \text{Temperature}; \]

\[ S \quad \text{Chemical constituent, e.g. salinity}; \]

\[ \rho \quad \text{Density}. \]

### 2.2.1 Governing Dynamic Equations

Seven equations are required for determining these seven variables. They are obtained from the conservation laws of mechanics and thermodynamics (Krauss, 1973; Raudkivi and Callander, 1975).

**Equation of motion (Navier-Stokes):**

For an incompressible fluid with constant viscosity,

\[
(2.1) \quad \rho \left[ \frac{\partial \vec{q}}{\partial t} + (\vec{q} \cdot \nabla) \vec{q} \right] = -\nabla p + \mu \nabla^2 \vec{q} + \rho \vec{g} + \rho \vec{X}
\]

where,

\[ \vec{t} \text{ is the time}; \]

\[ \vec{g} = (0, 0, -g)^T \text{ is the acceleration due to gravity}; \]

\[ \nabla = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}; \]
\[ \nabla^2 = \frac{\partial^2}{\partial x^2} i + \frac{\partial^2}{\partial y^2} j + \frac{\partial^2}{\partial z^2} k; \]

\textit{i, j, k} = \text{unit vectors in the x, y, z directions respectively;}

\( \mu \) \text{ is the viscosity (assumed to be constant); and}

\( \vec{X} \) \text{ is a vector of other body forces (e.g. Coriolis) per unit mass.}

If Coriolis is the only other body force in addition to gravity, then:

\[ \vec{X} = \vec{\xi}q \]

where,

\[ \vec{\xi} = \begin{pmatrix} 0 & 2\Omega \sin \lambda & -2\Omega \cos \lambda \\ -2\Omega \sin \lambda & 0 & 0 \\ 2\Omega \cos \lambda & 0 & 0 \end{pmatrix}; \]

\( \Omega \) \text{ is the angular velocity of the earth; and}

\( \lambda \) \text{ is the latitude.}

The \textbf{equation of heat transfer} (Krauss, 1973; Raudkivi and Callander, 1975) is

\[ \frac{\partial T}{\partial t} + (\vec{q} \cdot \nabla)T + T \nabla \cdot \vec{q} = \beta \nabla^2 T \]
where,

$\beta^T$ is the (molecular) thermo-diffusion coefficient.

The **diffusion equation** for the chemical constituent (Krauss, 1973; Raudkivi and Callander, 1975) is given by

\[
\frac{\partial S}{\partial t} + (\bar{\eta} \cdot \nabla) S + S \nabla \cdot \bar{q} = \beta^S \nabla^2 S
\]

where,

$\beta^S$ is the (molecular) salinity diffusion coefficient.

It is also assumed that the chemical constituents is non-reactive.

The **continuity equation**, obtained from the principle of conservation of mass, is given by (Krauss, 1973; Raudkivi and Callander, 1975),

\[
\frac{\partial \rho}{\partial t} + (\bar{\eta} \cdot \nabla) \rho + \rho \nabla \cdot \bar{q} = 0
\]

The **equation of state**, relating fluid density to both temperature and chemical concentration (Krauss, 1973; Raudkivi and Callander, 1975), may have a general form, like

\[
\rho = F(\rho, T, S)
\]

in which $F$ is an empirical function.
2.2.2 Reynolds Equation

The systems of equations reviewed above include more types of phenomena than are often relevant to the study of natural water bodies, like rivers, lakes and estuaries. A particularly valuable modification (Hinze, 1959), for many such cases, is the application of the Reynolds equation which is described as follows. In many important applications, the Reynolds number associated with most motions in lakes and rivers are large. Therefore, the flow is predominantly turbulent.

If \( q(x,y,z,t) \) is a physical quantity of the fluid, it is split up into a mean and a fluctuating component as given below:

\[
q(x,y,z,t) = q_{\text{mean}}(x,y,z) + q(x,y,z,t)
\]

where the mean component is defined as an averaged value which does not vary with time. The fluctuating component is the random fluctuation of the instantaneous value about the mean value.

The application of Eq. (2.6) to the basic Eqs. (2.1) to (2.5) results in the Reynolds equation in terms of the mean quantities which are of interest in this study. The resulting Reynolds equations in tensor notation for an incompressible fluid with constant viscosity (Hinze, 1959) can be written as,

**Momentum:**

\[
\rho \left( \frac{\partial \vec{u}_i}{\partial t} + \vec{u}_j \frac{\partial \vec{u}_i}{\partial x_j} \right) = -\frac{\partial \vec{p}}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \vec{u}_i}{\partial x_i} - \rho \vec{u}_i \overrightarrow{u} \right) + \vec{F}_i
\]
and,

**Continuity:**

\[
(2.8) \quad \frac{\partial}{\partial x_i} (\bar{u}_i) = 0
\]

in which,

\(\bar{u}_i\) = time mean velocity vector \((i = 1,2,3)\);

\(x_i, x_j\) = coordinates in space \((i \text{ or } j = 1,2,3)\);

\(\rho u_i u_j\) = turbulent stresses, i.e. Reynolds stresses;

\(\bar{p}\) = time mean static pressure; and

\(\bar{F}_i\) = time mean external force (i.e. gravity or Coriolis).

The averaging of the turbulent transport of a scalar quantity, i.e. such as temperature or salinity, for an incompressible fluid is given by (Hinze, 1959):

\[
(2.9) \quad \frac{\partial \bar{\xi}}{\partial t} + \bar{u}_i \frac{\partial \bar{\xi}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( M_{D} \frac{\partial \bar{\xi}}{\partial x_i} - \bar{u}_i \bar{S} \right) + \bar{F}_s
\]

in which,

\(\bar{\xi}\) = time mean scalar quantity per unit mass;

\(\bar{u}_i \bar{S}\) = turbulent correlation for the scalar quantity;

\(M_{D}\) = molecular transport coefficient; and

\(\bar{F}_s\) = time mean driving force or the source.

There remain, however, non-vanishing correlations of the turbulent fluctuations such as the Reynolds stresses in Eq. (2.7) and the correlation between the turbulent fluctuations of the
velocity and the scalar quantity (i.e. temperature or salinity) in Eq. (2.9). These quantities act as additional stresses or diffusion in which their elimination represent the closure problem of turbulence.

Normally, the Boussinesq approximation (Hinze, 1959) is used for parametricizing turbulence by means of eddy viscosity or diffusion coefficients. In most cases the eddy viscosity is determined by calibration of the hydrodynamic model against field data. In doing so, analytical approaches such as the Prandtl's mixing length hypothesis are of some help. Similar calibration process is carried out to determine the diffusion coefficient in which the Richardson number may be of some help.

Recently mathematical models of turbulence have also been increasingly used (Rodi, 1984). Here the eddy viscosity is related to characteristic quantities of the turbulence such as the kinetic energy (K) and the dissipation (E). These are discussed in further detail in Chapter 3. The unknowns K and E are determined by means of additional equations (Lauder and Spalding, 1972). These are given below in tensor notations:

\[
\rho \left( \frac{\partial \bar{K}}{\partial t} + \bar{u}_i \frac{\partial \bar{K}}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left( \nu \frac{\partial \bar{K}}{\partial \bar{x}_i} \right) 
+ \nu_i \left( \frac{\partial \bar{u}_i}{\partial x_i} + \frac{\partial \bar{u}_j}{\partial x_j} \right) \frac{\partial \bar{u}_j}{\partial x_i} - E
\]
and,

\[
(2.11) \quad \rho \left( \frac{\partial E}{\partial t} + \bar{u}_i \frac{\partial E}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left( \nu_t \frac{\partial E}{\partial x_i} \right) 
\]

\[+c_1 \nu_t \frac{E}{K} \left( \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - c_2 \frac{E^2}{K} \]

in which,

\[c_1, c_2, \sigma_k, \sigma_v = \text{empirical constants; and} \]

\[\nu_t = c_\mu \frac{K}{E} = \text{turbulent eddy viscosity.} \]

These empirical constants appear to change very little, even in varying applications.

2.2.3 Specifying Simplification Conditions

In applying the Eqs. (2.1) to (2.6), a number of simplifications can be used for a lake. These simplifications are:

1. The water is incompressible. The density has been taken as constant except in the buoyancy term (the Boussinesq approximation).

2. Vertical accelerations can be neglected.

3. The flow is quasi-hydrostatic, i.e. hydrostatic pressure is assumed.
4. The only external forces are gravity and Coriolis forces. The Coriolis parameter, $f$, is taken as constant.

5. Salinity is taken as constant, i.e. Eqs. (2.3) and (2.5) can be neglected.

6. Temperature is constant or stratification effect is neglected, i.e. Eq. (2.2) can be neglected.

By means of the above simplifications, the following equations are obtained (Pinder and Gray, 1977):

**x-momentum:**

\[
\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} - f \bar{u} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x} + \frac{\partial}{\partial x} \left( \eta \frac{\partial \bar{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \eta \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \eta \frac{\partial \bar{u}}{\partial z} \right)
\]

**y-momentum:**

\[
\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} + \bar{w} \frac{\partial \bar{v}}{\partial z} + f \bar{u} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial y} + \frac{\partial}{\partial x} \left( \eta \frac{\partial \bar{v}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \eta \frac{\partial \bar{v}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \eta \frac{\partial \bar{v}}{\partial z} \right)
\]

**z-momentum:**

\[
\frac{\partial \bar{p}}{\partial z} = -\rho \frac{\partial \bar{g}}{\partial z}
\]
**Continuity:**

\[
(2.15) \quad \frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0
\]

in which,

\(\bar{u}, \bar{v}, \bar{w}\) = time averaged velocity components in the \(x, y, z\) direction;

\(\rho_o\) = variable fluid density;

\(g\) = gravitational acceleration;

\(f = 2\Omega \sin \lambda\) = Coriolis parameter; and

\(\eta_h, \eta_v\) = horizontal and vertical eddy viscosities respectively.

Sometimes a body of water under consideration is so large that the ratio of nonlinear inertial forces to the Coriolis forces (characterized by the Rossby number) in the momentum equations is small enough that the nonlinear inertial terms are relatively unimportant (Liggett, 1975). In such cases, a great simplification can be achieved by neglecting these terms, since the momentum equations then reduce to linear equations. If steady state condition is used, then the time derivatives can be set equal to zero. The following equations then apply:

**x-momentum:**

\[
(2.16) \quad -f \bar{u} = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x} + \frac{\partial}{\partial x} \left( \eta_h \frac{\partial \bar{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \eta_h \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \eta_v \frac{\partial \bar{u}}{\partial z} \right)
\]
**y-momentum:**

\[ f \ddot{u} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \eta \frac{\partial \ddot{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \eta \frac{\partial \ddot{u}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \eta \frac{\partial \ddot{u}}{\partial z} \right) \]

The z-momentum and continuity Eqs. (2.14) and (2.15) remain the same as before.

**2.2.4 Boundary Conditions**

In order to integrate the partial differential Eqs. (2.12) to (2.15), boundary conditions must be prescribed at the physical boundaries of the lake. They represent the fluxes of momentum through any open boundaries (inflows and outflows from tributaries) or through the free surface (precipitation and evaporation) or through the bottom (groundwater infiltration), as well as the kinematic conditions. Normally they are chosen as follows (Ligget, 1975):

**Free Surface:**

\[ \rho \eta \nu \left( \frac{\partial \ddot{u}}{\partial z} \right)_{Surface} = \tau_x \]

\[ \rho \eta \nu \left( \frac{\partial \ddot{v}}{\partial z} \right)_{Surface} = \tau_y \]

\[ \frac{\partial \xi}{\partial t} + \ddot{u} \frac{\partial \xi}{\partial x} + \ddot{v} \frac{\partial \xi}{\partial y} = \ddot{w} \quad \text{on} \ z = \xi \]

\[ p = 0 \quad \text{on} \ z = \xi \]
in which,

\( \tau_x, \tau_y = \) the lake surface stresses due to wind;

\( \bar{u}_x, \bar{v}_x, \bar{w}_x = \) surface velocities in the \( x, y, z \) directions respectively; and

\( \zeta = \) the surface elevation above the original lake surface.

**Bottom:**

\( (2.21a) \quad \rho \eta V \left( \frac{\partial \bar{u}}{\partial z} \right)_{\text{Bottom}} = \tau_{bx} \)

\( (2.21b) \quad \rho \eta V \left( \frac{\partial \bar{u}}{\partial z} \right)_{\text{Bottom}} = \tau_{by} \)

in which,

\( \tau_{bx}, \tau_{by} = \) the lake bottom stresses due to friction.

**Lateral solid boundaries:**

\( (2.22) \quad \bar{u} = \bar{v} = \bar{w} = 0 \)

Sometimes this condition is also used at the lake bottom.

For the surface and bottom stresses, the following empirical relationships are commonly chosen:

\( (2.23a) \quad \tau_x = C_{\text{Drag}} \sqrt{\left( \bar{W}_x^2 + \bar{W}_y^2 \right) \bar{W}_x} \)

\( (2.23b) \quad \tau_y = C_{\text{Drag}} \sqrt{\left( \bar{W}_x^2 + \bar{W}_y^2 \right) \bar{W}_y} \)

in which,

\( C_{\text{Drag}} = \) wind drag coefficient; and

\( \bar{W}_x, \bar{W}_y = \) wind velocities in the \( x \) and \( y \) directions respectively.
\[(2.24a) \quad \tau_{bx} = C_b \sqrt{(\bar{u}_b^2 + \bar{v}_b^2)} \bar{u}_b \]

\[(2.24b) \quad \tau_{by} = C_b \sqrt{(\bar{u}_b^2 + \bar{v}_b^2)} \bar{v}_b \]

in which,

\[C_b = \text{the bottom friction factor; and} \]

\[\bar{u}_b, \bar{v}_b = \text{the bottom velocities in the x,y directions respectively.} \]

Another simplifying approximation, which is often made, if the free surface deviations are assumed small compared to the depth, is called the "rigid lid" approximation. This assumption eliminates all surface waves, long as well as short. It replaces the boundary condition of Eq. (2.19) with,

\[(2.25) \quad \bar{w}_z = 0 \quad \text{on} \quad z = 0 \]

and the boundary condition of Eq. (2.20) is no longer valid. The rigid lid does not act like a solid boundary with respect to friction and shear (Liggett, 1975). Surface elevations can be computed under the rigid lid approximation if the pressures are changed to equivalent water depths. The main advantage of the rigid lid approximation is that it results in a simpler computational process and the ability to use longer time steps in the unsteady lake circulation problem. In the discussion to follow, all the parameters in the equations are taken to refer to the time mean values and the bar notation will be dropped.
2.2.5. Vertical Integration

In shallow water bodies, flow variation through the depth is often less significant. In such cases, vertically integrated equations and variables may adequately describe the situation. In this approach only an estimate of the transport through any cross-section can be obtained. However, the detailed information on the velocity structure is lost. Usually, the water density is assumed constant in the vertical z-direction. This and the assumption of relatively small vertical velocities and accelerations are normally implied by the definition shallow. This also implies that the hydrostatic pressure assumption is used.

The water body can be discretized into a number of vertically stratified layers, with averaged horizontal flows. As a limiting case, a single layer model is obtained when integrating over the whole depth. The use of vertically integrated quantities to predict the dispersion of a tracer in this situation is clearly less satisfactory. This is because of the highly non-uniform velocity profile. However, the total transport may still be reasonably well predicted. In multi-layered models, some improvement on this point can be expected.

For tidal flow, the driving force which is the hydrodynamic pressure, acts over the entire depth, and the vertically integrated values are expected to be representative for the local
velocities, except for those close to the bottom. Finally, any inflows or outflows with a density difference are better simulated in multilayer models. It should also be pointed out that any such space-averaging reduces the computational effort. The dispersion coefficients used in multilayer models are normally determined empirically.

2.3. Review of Hydrodynamic and Transport Models

The basic mathematical equations reviewed in Section 2.2 cannot be solved analytically in a closed form. Therefore, they must be treated by approximation with the help of the discretization methods which have been developed in numerical mathematics. This leads to new problems originating from the computational treatment. Some of these can be dealt with, but a larger portion has not yet been sufficiently studied, particularly in the case of non-linear systems.

Except for simplified models (Shen et al., 1986), there are no detailed hydrodynamic or transport models currently available for the Upper and Lower St. Marys River. However, there are several well tested modelling techniques that can be applied to model the river. These techniques can be classified as: finite difference, method of characteristics, finite element, boundary element and cell methods.

2.3.1 Finite Difference Models

The numerical models have traditionally employed the finite
difference method to solve the governing differential equations. In essence, this method satisfies the governing equations by replacing derivatives by difference approximations.

Some of the earlier efforts in hydrodynamics are the works of Hansen (1956) and Welander (1957). Although both were looking at shallow water circulation and employed vertically averaged equations, two widely different approaches have evolved from their work.

Hansen (1956) outlined the vertically averaged formulation almost as we know it today. In fact, some of the recent models exactly duplicate his work (Laevastu et al., 1974). In his formulation, Hansen did not include the variations in the surface atmospheric pressure or density. However, his formulation does include a horizontal virtual viscosity term with constant viscosity coefficient in the momentum equations. His formulated problem was solved by finite difference on a staggered grid in space and time. This particular scheme with later modifications has proven itself very successful in solving tidal flow-problems.

Roache (1976) in an authoritative book on finite difference for fluid dynamics problems reviewed the importance of satisfying the conservation laws. Roache gives an excellent discussion on the requirements of stability and consistency. A more rigorous treatment of these concepts is also given by Richtmeyer and Morton (1967).

The staggered grid approach has the advantage that it allows
the use of central differences in space and time. This feature is desirable for accuracy and numerical stability. However, one of the problems associated with the staggered grid method is the problem of representing the physical boundaries properly. It requires special treatment at the boundaries to avoid errors and instability. This aspect was not discussed by Hansen (1956) and has remained a major problem in later modelling efforts.

Leendertse (1967) using the same equation as Hansen but without eddy viscosity terms discussed the problems encountered at the boundaries. However, Leendertse was more concerned with the numerical stability and accuracy aspects. He illustrated on the importance of using centred differencing. The treatment of nonlinear terms as usual causes severe problems.

Heaps (1969) modelled the wind surges in the North Sea using staggered grid finite differencing as well. His numerical scheme uses the linearized and integrated dynamical equations transformed in spherical coordinates. Heaps took exceptional care to center the differences in space and he uses an explicit time integration scheme. In his treatment of boundary conditions, Heaps ended up having to consider 22 different types of grid-point configurations.

Reid and Bodine (1968) also developed a finite difference storm surge model based on the space staggered grid of Leendertse. The vertically integrated equations without the convective acceleration terms were adopted for their model. They introduced
a radiation type of boundary condition for the open ocean boundary in their work.

Abbott et al. (1973) developed their models along the same line as Leendertse with the space and time staggered grid. However, they used a special implicit time integration method which has better conservation properties and seems to be more stable. The model package includes graphical display capabilities. They also developed a special feature that allows the model user to change the grid size but not the orientation. However, the model's source code is not available to the public.

Simons (1972) implemented a finite difference model for the Great Lakes. His numerical schemes are based on the vertically integrated equations with eddy viscosity using two space and time staggered grids simultaneously to avoid problems with the convective terms. Simons experimented with several variations on the treatment of bottom friction and convective terms. Since Simons used a high resolution grid to discretize Lake Ontario and his time integration scheme is explicit, his model requires considerable computation time.

Other vertically integrated or storm surge models developed and applied to the Great Lakes are the work of Rao and Murty (1970), Simons (1974, 1975, 1976), Haq et al. (1974) and Sheng (1975). Because these models are two-dimensional, they are relatively easy to program. These models also use relatively little computation time, but they can only yield a first
approximation to the vertically averaged currents. Because the bottom stress is poorly approximated, these models do not give accurate prediction of surface elevation or the three-dimensional currents in a shallow lake such as Lake Erie where the bottom stress is relatively important (Lick, 1976).

Based on the earlier work of Ekman (1905), the approach taken by Welander (1957) is noteworthy because the dependence on the vertical z-coordinate is determined analytically. The is a steady state model that is primarily used to predict wind circulation in lakes (Liggett, 1969). The "rigid lid" assumption is used whereby the water surface is assumed fixed. The other main assumptions in the model are that the effects of horizontal momentum diffusion, nonlinear terms and density stratification are negligible. The vertical eddy viscosity is also assumed constant throughout, and all velocities vanish on the bottom (no-slip).

The solution proceeds by expressing the vertical z-dependence as an infinite Fourier cosine series. Next, the vertically integrated equations are solved by introducing a stream function which identically satisfies the continuity equation. The pressure is eliminated from the momentum equations and one partial differential equation in the stream function results. This equation with the proper boundary conditions is solved using finite differences and the vertically averaged quantities can be derived. From these the velocity distribution
over-depth and vertical velocity can be found. By cross differentiating the momentum equations and adding, it is possible to obtain a Poisson type equation for the pressure from which the surface displacement is inferred. Aside from the already mentioned assumptions which are somewhat restrictive, the stream function solution has to be accurate enough so that the velocities can be obtained numerically.

Unsteady rigid lid models have been used in modelling currents in large lakes by Liggett (1969), Paul and Lick (1974), Bennett (1977) and Schwab et al. (1981). Since the vertical velocity is assumed zero at the undisturbed location of the free surface, it eliminates the motion and time scales associated with the surface gravity waves and allows a much larger numerical time step and reduced computation times.

On the other hand, the free surface models consume a large amount of computer time. The main reason is that the maximum allowable numerical time step is limited by the time it takes the surface gravity wave to travel between two adjacent horizontal grid points - a very severe limitation. Free surface models, in the most elementary forms, are quite general and have been applied extensively to the Great Lakes (Freeman et al., 1972; Kizlauskaus and Katz, 1974; Haq et al., 1974; Sheng, 1975; Schwab et al., 1981).

To reduce the computational time, two-mode free surface models have been developed (Simons 1972, 1974, 1975; Sheng and
Lick, 1977). In these two-mode models, the free surface elevation is treated separately from the internal, three-dimensional flow variables. The free surface elevation and vertically integrated quantities are calculated using vertically integrated equations of motion and the limiting time step for this part of the calculation is that associated with the surface gravity waves. The internal variables are calculated in such a manner that the effect of surface gravity waves are separated out from the three-dimensional equations of motion. Therefore, surface gravity waves no longer limit this part of the calculation and much larger time steps may be used with greatly reduced overall computational times.

Sheng, Lick, Gedney and Molls (1978) give an in-depth discussion of the realistic applications of the rigid lid model and the free surface model to the Great Lakes using actual field data for comparison. Detailed comparisons of the results for the two models indicated that for relatively short time intervals, significant differences between the two models occurred since the seiche motion is eliminated in the rigid-lid model. Long-term time-averaged circulation computed by the two models agree well in periods of strong wind, but differ appreciably in periods of light wind and active seiching.

2.3.2 Method of Characteristics

An outline of the method of characteristics applied to the one-dimensional shallow water equation is given by Ligget et al.
Woolhiser (1967). The advantage of this approach is that the original system of partial differential equations can be written as ordinary differential equations on the characteristics. However, these characteristics are, in general, curved and time dependent, thus making a solution more difficult to interpret. Although the same methodology can be extended to two-dimensional flow there seems to be no incentive for such work as the curvature of the characteristics makes it a difficult book-keeping and interpolation process to obtain a useful solution. Compared with well established finite difference methods, there does not seem to be any advantage in pursuing the method of characteristics for two-dimensional flow.

2.3.3 Finite Element Models

The finite element method has emerged as a relatively powerful method in recent years. In this method, the function satisfying the governing equations and boundary conditions is approximated by piecewise polynomials. Very flexible grid discretization is by virtue of this method. Zienkiewicz (1977) has collected a number of such applications along with some more recent fluid flow problems. A survey of the finite element method in continuum mechanics, with a discussion of the Galerkin expression for a Newtonian fluid, is also given by Connor (1973).

Shallow water circulation has attracted quite a few finite element modellers. Gallagher et al. (1973) analyzed steady wind driven circulation for shallow lakes using the rigid lid
equations. Full advantage of the freedom of varying the grid was not taken in the example given, however, the possibility of using existing general purpose finite element programs was emphasized.

Taylor and Davis (1972) solved the vertically averaged equations for constant density. They used cubic isoparametric elements to discretize their study area. For the time integrations, they compared the effectiveness of using a fourth order predictor-corrector method, the trapezoidal rule, and finite elements in time. Grotkop (1973) treated the same problem using linear finite element in space and time. It was found that the trapezoidal rule was more efficient for their case. Although both the predictor corrector and finite element approaches give more accurate results with the same number of computational elements, the increase in the amount of work discourages their use for larger problems.

A comprehensive report on finite element models for fluid flow is prepared by Norton et al. (1973). Both vertically averaged and two dimensional flow in the vertical plane are discussed in the report.

Others who have applied finite element methods to lake circulation include Cheng (1970, 1972), King et al. (1978) and Chih-lan et al. (1975). Cheng applied a finite element model for Lake Erie, while Chih-lan et al. developed a finite element model for Lake Okeechobee. Pinder and Gray (1977) documented their knowledge and experience in a book on finite element techniques.
for modelling lakes and estuaries. In a similar vein, Connor and Brebbia (1976) also authored a book that discusses finite element techniques in fluid flow. It includes chapters on the simulation of lake hydrodynamics and transport of pollutants using finite element methods. Lynch and Gray (1979) and Kinmark and Gray (1984) had devoted their efforts to developing finite element techniques using nine node elements to solve the wave equation for estuaries and lakes with tidal boundary conditions. Their work was directed towards improving stability and controlling numerical dispersion in their solutions.

Most of the recent researchers have concentrated on refining their finite element techniques to speed up computation time, improving accuracy or reducing numerical dispersion. The mathematical formulations are basically similar to earlier works. However, Laible (1984) attempted to resolve the vertical dimension by the use of higher order shape functions to approximate the natural current profile. Although this approach was attempted previously by Ebeling (1977) using cubic elements. Recently, Ibrahim and McCorquodale (1985) applied the finite element method to Lake St. Clair with notable success. They introduced optimum up-winding finite element schemes to handle the convective terms in their transport model and also developed a bottom slip boundary condition for their hydrodynamic model.
2.3.4 Boundary Element Models

The boundary element or boundary integral method has been used in structural mechanics for some time now. However, Brebbia et al. (1980) used it to solve a simplified lake circulation problem. This method is relatively new in hydrodynamic simulation. The method is mathematically more sophisticated than the finite difference or finite element methods. The method can be used to reduce the input data, the number of unknowns and consequently the computer storage requirements. However, its superiority at the moment is limited to potential flow problems such as Darcy flow in porous media and irrotational flow or flow described by the Poisson equation. The method loses its advantage if depth variation in the lake is significant, or if pollutant transport is an important component in the modelling work.

2.3.5 Cell Models

Several cell or compartmental models (Di Toro et al., 1980,1981) have been developed for the simulation of pollutant transport in rivers, estuaries and lakes. Most of these models are used for aquatic ecological modelling which is intrinsically related with water quality modelling. Lorenzen et al. (1974) reviewed various such models which were used to evaluate the Great Lakes. One class of models is represented by the phytoplankton model developed by Di Toro et al. (1975) for Western Lake Erie. Richardson and Bierman (1976) applied similar models to Saginaw Bay. Others who have applied these type of
models include Canale et al. (1974) to Grand Traverse Bay and Scavia et al. (1976) to Lake Ontario.

The approach used by these models is to divide shallow embayments into segments (cells) that are considered to be well-mixed. Flows among segments are assumed and adjusted until the conformation of observed and calculated distribution of a conservative substance such as chloride is made.

Thomann et al. (1975) applied the same basic methodology to Lake Ontario. The lake was segmented into layers over the depth without subdivision in plan. Thomann also used five layers, each layer being segmented into several cells. It becomes extremely difficult to make initial assumptions for a three-dimensional model of this size. Estimation of the flows is complex since continuity of water mass and conservation of thermal energy must be met simultaneously. However, if one is concerned with horizontal heterogeneity, a hydrodynamic model can be used to calculate the water circulation and transport characteristics of the lake. Based on the results from this model, a water quality-ecological model can route the pollutants throughout the lake and compute their biological consequences. The problem of different time scales and grid compatibility then arises.

Richardson et al. (1977) and Ambrose et al. (1988) of the U.S. EPA (Environmental Protection Agency) as well as researchers at the Manhattan College, New York, have developed and documented a very flexible cell model commonly referred to as WASP4 (Water
Analysis Simulation Program Version 4.12) for rivers, estuaries and large lakes. The WASP4 package includes three components namely DYNHYD4, EUTRO4 and TOXI4. The hydrodynamics can be either specified by the user or read in as input from the one-dimensional hydrodynamic model DYNHYD4. Depending on the problem being studied, the user can use either EUTRO4 and TOXI4 as the kinetics sub-models to link to the main WASP4 model. This will complete the "full" model for simulating the movement and interaction of the pollutant within the water body. EUTRO4 supplies the chemical kinetics for conventional pollutants involving dissolved oxygen, biochemical oxygen demand, nutrients and eutrophication. TOXI4 supplies the chemical kinetics for toxic pollutants involving organic chemicals, metals and sediment. Upon completion of the calculation of toxicant concentrations in space and time for the water body, TOXI4 can be used in conjunction with a Food Chain Model (Connolly and Thomann, 1985) to predict accumulation in the food chain. The Food Chain Model can be considered as a part of the WASP4 system (Ambrose et al., 1988).

2.4 Convection-diffusion River Models

The discharge of industrial and municipal effluents are by and large of the side-discharge type as illustrated by the sketch in Fig. 2.1. The sketch shows that the discharge jet is bent by the river flow. However, near the bank on the same side as the jet, a recirculation zone can form as the river water is
entrained into the expanding jet. Due to the turbulent nature in this zone, a strongly three-dimensional flow field is apparent in the vicinity of the outfall. Beyond this relatively small recirculation zone, the flow field returns to a predominant flow direction. This observation is of great significance to the modelling efforts, since the level of complexities increases rapidly in attempting to model the recirculating flow field. Rodi et al. (1981) categorize the flow regions as near-field and far-field regions.

The near-field region is the region that extends a relatively short distance downstream from the outfall wherein the influence of the jet discharge still affects the flow field. In this region, the generation of turbulence is due partly to the river bed and partly due to the shear layers induced by the jet discharge. Usually the stratification and vertical non-uniformities in this region are eroded rapidly by way of vertical mixing. The governing equations in this region are three dimensional and elliptic in nature. A large computer storage is needed in the computation for the three dimensional flow field. In addition, the elliptic equations require an iterative solution procedure leading to large computing times as well. Due to its highly turbulent nature, the near-field region is difficult to simulate in a numerical model. The complex nature of the flow field in the near-field region makes it difficult to use integral methods which requires profile assumptions and entrainment laws.
Furthermore, integral methods cease to work when the flow loses its jet-type nature in the far-field. Diffusion methods are also not applicable since these approaches require prior knowledge of the velocity field. Diffusion methods are restricted to the simulation of the far-field region.

Shirazi and Davis (1974) and Abdel-Gawad (1986) had used a three dimensional integral model referred to as the PDS model. The model requires specification of shape functions for the lateral and vertical temperature and velocity profiles. Selection of these shape functions enables one to integrate the basic conservation equations over the cross-section of the jet. Abdel-Gawad (1986) also used another near field model referred to as the MIT model. The model was developed by Stolzenbach and Harleman (1971) and like the PDS model is based on the integral approach. In contrast to the PDS model which uses the Gaussian distribution, the MIT model is developed using a "top hat" distribution which is defined in terms of "jet averaged" properties.

Demuren and Rodi (1983) succeeded in modelling the near-field region with a three-dimensional model using the "K-E" turbulence model to determine the turbulent stresses. The so-called "K-E" model employs differential transport equations (K and E equations) for the turbulent momentum transport quantity like the turbulent stresses. It traces the transport, diffusion,
generation and decay of the turbulent energy level "K" and the transport, diffusion, generation and decay of a characteristic length scale, represented by the rate of turbulent energy loss to heat energy, "E". The model performed well for isothermal discharges, however, they did not include the buoyancy terms in their model.

The far-field region begins where the near-field region ends and extends as far downstream as the effluent concentration is detectable. This is a vertically well-mixed region and the turbulence is predominantly generated from the river bed. Under such well-mixed situations when temperature and pollutant concentration vary little over the river depth, it is accurate for practical purposes to use two-dimensional depth-averaged equations (Rodi et al., 1981). Therefore, except in the relatively small recirculation regions, the river flow is predominantly in the main flow direction and turbulent diffusion has a negligible effect in this direction compared with that in the cross-sectional plane. Thus, in most parts of the river, upstream transmission of mass by the turbulent diffusion (i.e. turbulent motion) or by the mean flow (i.e. convective transport) can be neglected. These are the two main mechanisms that govern the distribution of pollutant concentration.

When downstream influences can be predetermined e.g. by using field observations of water levels or by applying backwater programs like HEC-2, the transport equations can be made
parabolic in the main-flow direction (i.e. \(x\)-direction in Fig. 2.1). The solution of the parabolic equations at a certain cross-section does not depend on the solution at cross-sections located downstream nor on the conditions at the outflow-boundary. Therefore, in a numerical scheme, the equations can be integrated by marching from one cross-section to the next, starting with given initial conditions at the cross-section furthest upstream. The forward-marching procedure is extremely economical since all variables have to be stored only at grid nodes in one cross-section.

Since, in a wide river, turbulent transport in the longitudinal direction is negligible compared to that in the transverse direction (Rodi et al., 1981), the transverse mixing of a pollutant that is discharged into a river is the subject of many investigations. Knowledge concerning this transverse mixing coefficient is still very limited. Some researchers have suggested that it is a function of the bulk flow and the channel geometry (Yotsukura and Sayre, 1976; Lau and Krishnappan, 1981). Most of the advective-diffusion equations describing the depth-averaged concentration of a pollutant require prior knowledge of values for the tranverse mixing across the cross-section of the river. This term accounts for the turbulent diffusive transport as well as the transport caused by differential advection. Fisher (1969) derived a relationship for the transverse dispersion coefficient having the form,
\[
(2.26) \quad \frac{E_t}{(hU_*)^2} = \left( \frac{v_x}{U_*} \right) \left( \frac{h}{r_c} \right)
\]

where,

- \(E_t\) is the transverse mixing coefficient;
- \(h\) is the depth of the channel;
- \(v_x\) is the longitudinal velocity;
- \(U_* = \sqrt{ghS_o}\) is the shear velocity;
- \(S_o\) is the energy slope; and
- \(r_c\) is the radius of curvature of the channel centre line.

Data from the Missouri River based on the work of Yotsukura et al. (1970), together with data from flume experiments by Fisher (1969), have shown that this equation predicts the right trend but is not sufficiently close as yet for unrestricted application in the field. A comparison plot of these data is given in a paper by Yotsukura and Sayre (1976).

The studies so far indicate that there is insufficient basis as yet to predict local values for the transverse mixing coefficient. Detailed studies in meandering channels have shown that the transverse mixing coefficient tends to vary periodically in the longitudinal direction. It usually reached a maximum value of about twice the average in the downstream portion of a bend and a minimum of about half the average in the upstream portion.

Due to the inherent problems involved in trying to simulate the process of pollutant diffusion, no single theory can simulate

2.5 Physico-Chemical Characteristics of Toxics

Since this study involves the use of the KETOX and WASP4 models to simulate the movement and fate of toxic substances, a short review of the physical-chemical processes of such substances is appropriate. To better understand the terms used in this study, a knowledge of the types and sources of pollutants is necessary. In their report to the International Joint Commission (IJC), the Great Lakes Water Quality Board (1982), which is the appointed principal advisory to IJC, has given definition guidelines for pollutants under four broad categories:

a. "Conventional" pollutants - a term which includes nutrients, substances which consume oxygen upon decomposition, materials which produce an oily or a sludge deposit on the bottom, and bacteria. Conventional pollutants include phosphorus, nitrogen, chemical oxygen demand, biochemical oxygen demand, oil and grease, volatile solids, and total and fecal coliform.

b. Metals - including mercury, lead, zinc, iron, and cadmium.
c. "Conventional" toxic substances – including phenol, cyanide, ammonia, and chlorine.

d. Persistent organic toxic substances – complex organic chemicals, usually chlorinated, which can persist and can bioaccumulate.

In this review, "conventional" toxic substances are not differentiated from toxic substances. The term toxic substances is used to encompass both substances. The sources of toxicant can be identified in six general categories: municipal and industrial discharges, waste disposal sites, combined sewer overflows, urban land runoff, agricultural land runoff, and in-place pollutants.

There are three important features that separate toxic substances from the more conventional pollutants. Thomann and Mueller (1987) listed these features as:

a. Certain toxicants tend to sorb to particulates in the water column. The contaminated particulates may settle and deposit on the surficial bed sediments and stay there for a long period.

b. Certain toxicants can be concentrated by aquatic organisms and migrate up the food chain.

c. Certain toxicants tend to be toxic at relatively low water concentrations in the ug/L or ng/L level.
The fate and transport of toxic substances in the water body can be affected by several physical-chemical processes. These physical-chemical processes are illustrated pictorially in Fig. 2.2 from Mills et al. (1985). A schematic of the most important processes that will be described in this review is given in Fig. 2.3 taken from Thomann and Mueller (1987). The important physical-chemical phenomena interacting between the water column and the sediment are:

a. Sorption and desorption of the toxicant between dissolved and particulate forms in the water column and sediment.

b. Settling and resuspension mechanisms of sediment-sorbed toxicants between the sediment and the water column.

c. Vertical diffusive exchange between the sediment and the water column such as pore water diffusion and percolation. Also pore water advection due to pore water flows into and out of the sediment bed.

d. Net loss of the toxicant due to biodegradation, volatilization, photolysis, and other chemical and biochemical reactions.

e. Net gain of the toxicant due to chemical and biochemical reactions. This process is complex and quite difficult to identify.
f. Water column transport of the toxicant due to advective flow transport and dispersive mixing and lateral sediment transport in the form of bedload transport of sediment-sorbed toxicants.

g. Net deposition and loss of the toxicant to deep sediments due to sedimentation and compaction over the years.

Not all toxicants require consideration of all of these physio-chemical interactions. Some toxicants are more volatile and less sorbed to solids while the converse is also true. Mills et al. (1982) estimated that for 103 priority organic pollutants, the sorption processes are important for 60 of the chemicals, while volatilization is important for 52 chemicals. Also, since some chemicals sorb to solids, the sediment of the water body becomes particularly significant as a potential long-term storage reservoir of the chemical.

It is also important to have an idea of the time to equilibrium of the transformation mechanism when trying to simulate them in a model. These transformation processes are usually grouped under fast and slow reactions. Fast reactions have characteristic reaction times on the same order as the model time step and are handled with the assumption of local equilibrium. Slow reactions have characteristic reaction times much longer than the model time step. These are usually handled
with the assumption of local first order kinetics using a lumped rate constant that is based on the summation of several process rates.

So far, the review has attempted to give a greater appreciation of the complex and dynamic chemical-sediment interactions that take place in a water body such as a river or a lake. However, a full treatment of the kinetic processes of sorption-desorption, biodegradation, photolysis, hydrolysis, volatilization and oxidation is beyond the scope of this study. These physical-chemical processes are well documented in authoritative sources such as Mills et al. (1982, 1985), Thomann and Mueller (1987) and Ambrose et al. (1988). The review will attempt to give an adequate working knowledge of each of these processes.

**Sorption-desorption** is the movement of chemical between the dissolved phase and a particulate or solid phase. The chemical may be physically associated or chemically bound through attachment to functional groups on the surface of the solid. The process is dependent on such important factors as:

- The characteristics of the chemical - for neutral organics, sorption is related to the hydrophobicity of the chemical.
b. the characteristics of the solid – such as the size and organic carbon content of the solid. For instance the specific surface area and cation exchange capacity of the solids which can be very different for sand, silt or clay.

c. the characteristics of the aqueous solution – the presence of dissolved and colloidal organics such as humic acids as well as the pH and temperature of the aqueous solution.

**Biodegradation** is a decay process in which the chemical is degraded by bacteria and fungi through metabolic activity. The process is sometimes referred to as microbial transformation or biolysis. The presence of large biological processors in natural water means that biodegradation rate is an important loss process of chemical in the aquatic system. Although biodegradation can detoxify or mineralize toxins and defuse potential toxins, they can also activate potential toxins. Two general types of biodegradation are recognized (Thomann and Mueller, 1987). These are:

a. Growth metabolism – this occurs when the organic compound serves as a food source for the bacteria. Microbial adaptation time is from 2 to 50 days. Adaptation time may not be required for some chemicals. After adaptation, biodegradation proceeds at fast first-order rates.
b. Cometabolism - this occurs when the organic compound is not a food source for the bacteria. Adaptation is seldom necessary and the transformation rates are slow compared with growth metabolism.

Photolysis - is the transformation of a chemical due to absorption of light energy. The molecular structure of the chemical is altered by the light energy and as such the molecule undergoes decay. The product of the decay may or may not still be toxic. Mills et al. (1982, 1985) and Delos et al. (1984) provide reviews of the overall mechanism. The photolysis decay rate depends on:

a. The absorption spectrum of the chemical - since the structure of the chemical will only enable it to absorb light from certain wavelength. The level of energy absorbed on the other hand will determine the degree of alteration to its molecular structure.

b. The incoming solar radiation which is dependent on the meteorological conditions and the geographical location of the water body.

c. The subsequent penetration and attenuation of the incoming solar radiation due to different depths in the
water column. The penetration and attenuation will also depend on the presences of suspended solids, phytoplankton, and dissolved organic carbon.

d. The fraction of absorbed photons, referred to as the quantum yield, that will result in a given reaction.

**Hydrolysis.** or reaction with water, is a known major pathway for degradation of many toxic organics. The chemical compound reacts with water and a cleavage of a chemical bond occurs. A new compound with either the hydrogen or hydroxyl bond may be formed. However, the hydrolysis products may not be less toxic than the original compound. The reaction can be catalyzed by hydrogen ions or proceed by consuming hydroxide ions. In natural waters, hydrolysis may also be a biochemical degradation process since hydrolysis can be mediated by enzymes (enzymatic hydrolysis). Handbooks on hydrolysis rates can be obtained from Mills et al. (1982, 1985) and Lyman et al. (1982).

**Volatilization** is the mass exchange of chemical across the air-water interface. The dissolved neutral concentration attempts to equilibrate with the gas phase partial pressure (Ambrose et al., 1988). This exchange can be written mathematically as,
\[
(2.27) \quad \frac{\partial C_w}{\partial t} = -\frac{k_v}{D_{\text{cell}} \left( C_w - \frac{C_a}{H/RT} \right)}
\]

where,

\( C_w \) = dissolved concentration in water, \( \text{ug/L} \);

\( C_a \) = concentration in air, \( \text{ug/L} \);

\( H \) = Henry's Law constant, \( \text{atm/M} \);

\( R \) = gas constant (8.206E-05), \( \text{atm/M-K} \);

\( T \) = water temperature, \( \text{K} \);

\( D_{\text{cell}} \) = depth, \( \text{m} \); and

\( k_v \) = rate constant, \( \text{m/day (conductivity)} \).

This equation infers that equilibrium occurs when the dissolved concentration equals the partial pressure divided by Henry's Law Constant. In most cases, the organic toxicants in the atmosphere are at much lower levels than partial pressures equilibrated with water concentrations. Consequently, the equation reduces to a first-order process with a volatilization rate proportional to the conductivity and surface area divided by volume as follows,

\[
(2.28) \quad K_v = k_v \frac{A_s}{V} \frac{f_D}{D_{\text{cell}}} = k_v \frac{f_D}{D_{\text{cell}}}
\]

where,

\( K_v \) = net volatilization rate constant, \( \text{l/day} \);

\( k_v \) = conductivity of the chemical through the water segment, \( \text{m/day} \);

\( A_s \) = surface area of water segment, \( \text{m}^2 \);

\( V \) = volume of the water segment, \( \text{m}^3 \); and
\( f_D \) = dissolved fraction of the chemical.

For a surface water segment, a dissolved compound can volatize at a rate determined by the two-layer resistance model (Whitman, 1923). The conductivity of the chemical through the water in this case is the reciprocal of the total resistance and is given by,

\[
(2.29) \quad k_v = \left(K_{lp}^{-1} + K_c^{-1}\right)^{-1}
\]

where,

\( K_{lp} \) = liquid phase transfer coefficient, m/day; and

\( K_c \) = gas phase transfer coefficient, m/day.

To use this equation, values for the two transfer coefficients are needed. Both the liquid and gas transfer coefficients can be calculated from semi-empirical relationships by Mackay (1975) and O'Connor (1983). Ambrose et al. (1988) gives an excellent discussion on the use of these empirical relationships in his discussion on volatilization.

**Oxidation** of organic toxicants in aquatic environments can result from the interactions between free radicals and the pollutant. Free radicals can be formed as a result of photochemical reactions. The source of free radicals in natural waters is photolysis of naturally occurring organic molecules (Ambrose et al. 1988). If a water body is turbid or very deep, free radicals are likely to be generated only near the air-water
interface. Consequently, chemical oxidation is only important in the near surface zones of such water bodies. Otherwise, chemical oxidation will be relatively less important.

An important chemical phenomena not mentioned is the effect of the pH level in the natural water body on the toxicant. Toxic organics normally exist at trace levels in the water body and therefore have negligible influence on its pH value. However, the pH level of the water body can significantly influence the toxicant's volatilization, since only neutral species of toxic organics can directly volatize (Mills et al., 1982). The pH level in the natural water body will determine the fraction of organic acid or base which is present in the neutral state. The pH level has a dramatic impact on the metabolic activity of the bacteria on the toxicant. Due to these inter-relationships, there are no general rules available at present to evaluate pH effects.
Chapter 3

THEORETICAL DEVELOPMENTS

3.1 General

Only the hydrodynamics of the Upper St. Marys River was simulated in the study due to the nature of the project arrangement with the Ontario MOE (Ontario Ministry of Environment). However, there are plans to include transport of pollutants modelling at a later time. In the case of the Lower St. Marys River, its water quality and transboundary pollution problems were investigated by hydrodynamic and transport models. The study also included a simulation of chemical sediment interaction for toxic substances using field data from the Ontario MOE.

This chapter is structured into two main parts. The first part discusses the theory behind two hydrodynamic models that were used in the study of the Upper River. The second part discusses the model theory of two models that were used for the Lower St. Marys River.

3.2 Model Theory - Upper St. Marys River

In the process of studying the hydrodynamics of the Upper St. Marys River, two models were used in the simulation, namely:
a. A steady state rigid lid three dimensional 
Finite Element model based on the work of Ibrahim and 

b. A time dependent free surface one dimensional finite 
difference model developed by the US Environment 
Protection Agency (Ambrose et al., 1988) referred to 
as DYNHYD4.

The first model is a finite element model based on the work 
of Ibrahim and McCorquodale (1985). It is a steady state three 
dimensional model with rigid lid and hydrostatic pressure 
assumptions. The model is commonly referred to as the Ekman type 
model. It is mainly designed to study wind induced current 
circulation in lakes. The model builds on the earlier works of 
Ekman (1905), Welander (1957) and Liggett and Hadjitheodorou 
(1969). Some of its improved features include the use of 
upwinding finite element and modifications to allow for bottom 
slip and inflows and outflows at the boundaries. The model can 
accurately represent the lake geometry using triangle elements 
and is ideal for a rapid evaluation of lake circulation dynamics 
under different wind and inflow conditions. Due to its quick 
computation speed, a fine grid discretization is used with this 
model on the Upper St. Marys River.
The second model is a time dependent one dimensional model referred to as DYNHYD4 from US EPA's Center for Exposure and Assessment Modelling (CEAM) at Athens, Georgia. It is a free surface model using link-node network to discretize a river or an estuary. This model can be used to compare the surface elevations as computed in the form of equivalent pressures in the finite element model. However, the main advantage of this model is the fast computation time to give averaged hydrodynamic conditions at each junction of the network for linkage to the transport models.

3.2.1 Finite Element Method

In the analysis of lake circulation problems irregular boundaries must be considered, this makes the finite element method especially attractive. Irregular boundaries can be treated accurately without computational difficulties. Only minimal changes in programme coding or formulation of the method are needed. The finite element formulation for the analysis of wind induced circulation of a shallow homogeneous lake with variable depth is presented here. It is a three dimensional steady state model. The finite element formulation of three dimensional lake and shallow basin circulation analysis have been carried out previously by Liggett and Hadjitheodorou (1969), Gallagher et al. (1973), and Ibrahim and McCorquodale (1985). Therefore the theoretical formulation presented here provides an overview of the theoretical concepts involved. This section is presented to
provide the modeller with sufficient understanding of the model's background in order to apply the model correctly and to its fullest capability while appreciating its limitation.

The approach taken to transform the governing differential equations of momentum and continuity to a point where numerical analysis can be easily applied is similar to the work of Ibrahim and McCorquodale (1985). The governing equations are first linearized by omitting the inertia terms, i.e. assuming small Rossby number. The equations are then further simplified by neglecting the horizontal eddy viscosities and assuming that the vertical eddy viscosity is constant over the depth of the lake. Other assumptions include: homogeneity in the lake (i.e. non-stratification); hydrostatic pressure over the depth for shallow lakes; and the nearly uniform geostrophic wind over the lake since the lake dimensions are small compared to typical weather systems.

With these assumptions, the momentum equations have the form,

\[ (3.1) \quad -fv = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \eta_v \frac{\partial^2 u}{\partial z^2} \]

\[ (3.2) \quad fu = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \eta_v \frac{\partial^2 v}{\partial z^2} \]
z-momentum:

\[ g = -\frac{1}{\rho} \frac{\partial p}{\partial z} \]  \hspace{1cm} (3.3)

and the continuity equation is:

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \]  \hspace{1cm} (3.4)

in which,

- \( x, y \) and \( z \) = Cartesian coordinates system;
- \( u, v \) and \( w \) = velocity components in the \( x, y \) and \( z \) direction;
- \( g \) = gravitational acceleration;
- \( p \) = pressure;
- \( f \) = Coriolis coefficient;
- \( \rho \) = water density; and
- \( \eta_r \) = vertical eddy viscosity.

As boundary condition, it is taken that the vertical velocity is zero on all solid surfaces, so that:

\[ w = 0 \] , on all solid surfaces.

At the bed of the lake, the bottom stresses are assumed to be linearly proportional to the bottom velocity components,
(3.5a) \( s \frac{\partial u}{\partial z} = u_b \)

(3.5b) \( s \frac{\partial v}{\partial z} = v_b \)

where, 

\( s \) = a slip coefficient; and

\( u_b \) and \( v_b \) = bottom velocities in the x and y directions respectively.

For the boundary condition at the free surface, it is assumed that the changes in water surface elevation are small compared to the depth, so that the "rigid lid" assumption is made as given by, at \( z = 0 \), \( w = 0 \). In addition, at the free surface (i.e. at \( z = 0 \)), the boundary condition relating to shear on the lake surface is:

(3.6a) \( \eta_v \frac{\partial u}{\partial z} = \tau_x \)

(3.6b) \( \eta_v \frac{\partial v}{\partial z} = \tau_y \)

in which,

\( \tau_x, \tau_y \) = wind stress functions in the x and y directions respectively.

Since the model is essentially a wind driven lake circulation model, it is important to be able to estimate the wind stresses. A poor estimate of the wind stress will consequently introduce erroneous results in the computed circulation velocities. The
surface stress due to wind is dependent on factors such as the wave height, the length of the fetch and the relative temperatures of the air and water. Schwab and Morton (1984) had reviewed and tested three lake-wind estimation methods for Lake Erie, and had suggested that the method of Phillips and Irbe (1978) seems to give the best correlation. Base on the Phillips and Irbe relations, the surface wind stresses are estimated by,

$\tau_s = \frac{C_{\text{drag}} \rho_a}{\rho} |V_s| V_s$

in which,

$\tau_s$ = the surface wind stress in the prevailing wind direction, $L^2/T^2$;

$V_s$ = wind velocity at 4 metres above the water surface, $L/T$;

$\rho_a$ = density of air, $M/L^3$;

$C_{\text{drag}}$ = a drag coefficient, unitless; and

$C_{\text{drag}} \frac{\rho_a}{\rho} = 3 \times 10^{-6}$ (Jelesnianski, 1967), unitless.

Note: $\tau_x$ and $\tau_y$ are $x$ and $y$ components of $\tau_s$.

The solution proceeds first by writing the equations of motion in non-dimensional form and an exact integration is then carried out in the vertical direction introducing the surface and bottom boundary conditions and resulting in velocity expressions for $u(z)$ and $v(z)$. The details of the integration are given by Welander (1957), Liggett and Hadjitheodorou (1969) and Ibrahim (1986). Then, by integrating the velocity expressions for $u(z)$
and $v(z)$ from the bottom (i.e. $z = -h$) to the surface (i.e. $z = 0$) the mean or depth averaged horizontal velocities $U(x,y)$ and $V(x,y)$ are obtained as follows:

\[
(3.8a) \quad U(x,y) = \frac{1}{h(x,y)} \int_{-h}^{0} u(z) \, dz \\
(3.8b) \quad V(x,y) = \frac{1}{h(x,y)} \int_{-h}^{0} v(z) \, dz
\]

where $h(x,y)$ is the local depth. A stream function which is similar but not identical to the conventional stream function is then defined such that,

\[
(3.9a) \quad U(x,y) = -\frac{1}{h(x,y)} \frac{\partial \psi}{\partial y} \\
(3.9b) \quad V(x,y) = \frac{1}{h(x,y)} \frac{\partial \psi}{\partial x}
\]

in which $\psi$ is the defined stream function.

Then replacing the parameters $U(x,y)$ and $V(x,y)$ of Eqs. (3.8) in terms of stream functions and using the cross differentiation relationship:

\[
(3.10) \quad \frac{\partial^2 p}{\partial x \partial y} = \frac{\partial^2 p}{\partial y \partial x}
\]
It can be shown that an expression similar to the conventional Poisson pressure equation but expressed in terms of stream function is obtained as follows:

\[
(3.11) \quad \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + A(x, y) \frac{\partial \psi}{\partial x} + B(x, y) \frac{\partial \psi}{\partial y} - C(x, y) = 0
\]

in which \( A(x, y) \) and \( B(x, y) \) are known functions of the local depth \( h(x, y) \), its partial derivatives as well as the vertical eddy viscosity; and \( C(x, y) \) in addition to depending on these variables also depends on the wind shear stresses.

The Finite Element Method (FEM) is applied to solve Eq. (3.25) numerically. In the FEM, the approach commonly referred to as the Galerkin's method (Finlayson, 1972; Gallagher et al., 1973; Pinder and Gray, 1977) is used to express an approximate solution as:

\[
(3.12) \quad \int \int_A [\phi_n]^T \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + A(x, y) \frac{\partial \psi}{\partial x} + B(x, y) \frac{\partial \psi}{\partial y} - C(x, y) \right) dA = 0
\]

where,

\( A = \) the domain or region enclosed by the boundary;

\( \phi_n = \) linear shape or basis functions;

\( n = 1, ..., N \);

\( N = \) the number of unknowns not necessarily the number of nodes;

\[
(3.13) \quad \psi = \sum_{i=1}^{N} \psi_i \phi_i
\]
= approximation of the nodal stream function values $\Psi$;
$\Psi$ = nodal stream function value;

$j =\text{nodal number } = 1, \ldots, M; \text{ and}$

$M = \text{the number of nodes in the discretized domain or region.}$

Using two dimensional linear triangular elements as shown in Fig. 3.1, the approximation of the nodal stream function values for each element is,

$$
(3.14) \quad \Psi = [\phi_i, \phi_j, \phi_k] \begin{pmatrix} \psi_i \\ \psi_j \\ \psi_k \end{pmatrix}
$$

in which $i, j, k$ are the nodal index of the triangular element. The linear shape functions for each element are given by,

$$
(3.15a) \quad \phi_i = \frac{1}{2A^s}(a_i + b_i x + c_i y)
$$

$$
(3.15b) \quad \phi_j = \frac{1}{2A^s}(a_j + b_j x + c_j y)
$$

$$
(3.15c) \quad \phi_k = \frac{1}{2A^s}(a_k + b_k x + c_k y)
$$

in which,

$(a, b, c)_i$ = functions of the $x, y, z$ coordinates of node $i$;

$(a, b, c)_j$ = functions of the $x, y, z$ coordinates of node $j$;

$(a, b, c)_k$ = functions of the $x, y, z$ coordinates of node $k$; and
\( A^* \) = elemental area.

The highest order derivative that is allowable in Eq. (3.12) is one greater than the order of continuity in the interpolation or shape function Eqs. (3.14). Since the interpolation equations are of order zero (i.e. first derivative is a constant), derivatives greater than the first order cannot appear in Eq. (3.12). Integration by parts or Green's theorem is applied to Eq. (3.12) to reduce the second order partial derivatives to first order derivatives and at the same time introduce the boundary terms into the resulting equation as follows,

\[
(3.16) \quad - \iint_A \left( \frac{\partial [\phi]^T}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\partial [\phi]^T}{\partial y} \frac{\partial \psi}{\partial y} \right) dA \\
+ \iint_A \left( A(x,y)[\phi]^T \frac{\partial \psi}{\partial x} + B(x,y)[\phi]^T \frac{\partial \psi}{\partial y} \right) dA \\
- \iint_A \left( C(x,y)[\phi]^T \right) dA + \oint_{\Gamma} \left( [\phi]^T \frac{\partial \psi}{\partial x} l_x + [\phi]^T \frac{\partial \psi}{\partial y} l_y \right) d\Gamma = 0
\]

in which,

\( l_x, l_y \) = direction cosines of the normal to the surface, \( \Gamma \);

\( \Gamma \) = the outer surface boundary; and

\( d\Gamma \) = incremental length on the surface boundary.

The last integral term in Eq. (3.16) is a surface integral and it represents the surface flux term. For triangular elements
whose sides are not on the surface boundary, the closure integral along the interelement boundaries or sides would uniformly vanish. At the outer surface boundary of the lake, the boundary condition can be prescribed by specifying stream function values at the boundary nodes. As illustrated in Fig. 3.1, inflow or outflow nodes are handled with appropriate jumps in the prescribed stream function values across the nodes.

Since the nodal stream function are constants, the derivatives of Eq. (3.14) can be written as:

\begin{align}
(3.17a) \quad \frac{\partial \psi}{\partial x} &= \frac{\partial}{\partial x}[\phi](\psi) \\
(3.17b) \quad \frac{\partial \psi}{\partial y} &= \frac{\partial}{\partial y}[\phi](\psi)
\end{align}

Substituting these into Eq. (3.16) and rearranging the terms, it can be shown that,

\begin{equation}
(3.18) \quad [K](\psi) = (F)
\end{equation}

in which,

\begin{equation}
(3.19) \quad [K] = \int \int _A \left( -\frac{\partial [\phi]^T}{\partial x} \frac{\partial [\phi]}{\partial x} - \frac{\partial [\phi]^T}{\partial y} \frac{\partial [\phi]}{\partial y} + A(x,y)[\phi]^T \frac{\partial [\phi]}{\partial y} + B(x,y)[\phi]^T \frac{\partial [\phi]}{\partial x} \right) dA
\end{equation}
and,

\[(3.20) \quad \{F\} = \int \int_A C(x,y)\{\phi\}^T dA\]

The boundary conditions due to the surface integral can be introduced by modifying the rows and columns of the global stiffness matrix \([K]\) corresponding to the prescribed variables and incorporating the prescribed terms in the force vector \(\{F\}\). To simplify the integration of the matrices \([K]\) and \(\{F\}\), the terms \(A(x,y)\), \(B(x,y)\) and \(C(x,y)\) are treated as constants for each element. The resulting matrix \([K]\) after assembling the elements is sparse and nonsymmetric. A specialised matrix inversion subroutine from Gupta and Tanji (1977) is used to solve such large, unsymmetric systems of linear equations.

The solution of Eq. (3.18) gives the nodal stream function values. The pressure gradients and depth averaged velocities \(U(x,y)\) and \(V(x,y)\) at the centroid of each triangular element can then be easily computed from the constant stream function gradient of each element. The horizontal velocities over the depth can then be calculated from the pressure gradients using the analytical solutions as shown previously by Liggett and Hadjitheodorou (1969). To avoid computational singularity at the lake boundaries due to zero depth, a finite small depth of 0.5 m (1.6 feet) was used at the boundaries. The only exceptions are at the inflow and outflow boundaries where the actual depths are used instead.
Further details on the application of the FEM to simulate the hydrodynamics of the Upper St. Marys River will be discussed in Chapter 5. The discretization details and the processes of model calibration and model verification will also be discussed at that time.

3.2.2 DYNHYD4 (USEPA)

This model is an enhancement of the Potomac estuary hydrodynamic model DYNHYD2 (Roesch et al., 1979). It solves the equations describing the propagation of a long wave through a shallow water system (i.e. it assumes that the wave length is significantly greater than the depth). It assumes that the flow is predominantly one-dimensional and that accelerations normal to the direction of flow, channel bottom slopes, coriolis forces and longitudinal density currents are all negligible. Although the model uses the one-dimensional forms of the momentum and continuity equations, its link-node networks allow simplified representation of complex, branching river or estuarine geometry, with some limited lateral resolution. Each link-node channel is assumed to be represented by a constant top width with a variable hydraulic depth (i.e. rectangular shaped channels).

It should be pointed out that the theoretical developments of these governing equations are well documented in US EPA users manuals (Ambrose et al., 1988). Hence, the theoretical description of the model is in Appendix A.
The implementation of the model on both the Upper and the Lower St. Marys River will be discussed in detail in Chapters 5 and 6. At that time the proper discretization to link-node networks will be illustrated as well.

3.3 Model Theory - Lower St. Marys River

The Lower St. Marys River is modelled using the following two models:

a. A steady state depth averaged hydrodynamics and dispersion river model referred to as KETOX (McCorquodale and Yuen, 1987).

b. A time dependent three dimensional compartment model for the transport and fate of toxic pollutants incorporating toxic chemical-sediment dynamics capability for the water column and benthos of ponds, rivers, lakes, reservoir, streams, estuaries, and coastal waters referred to as TOXI4 (Ambrose et al., 1988).

The first model referred to as KETOX is a model that has four sub-models coupled together. It has a depth averaged hydrodynamic sub-model which is coupled to a convection-diffusion (mixing) sub-model that simulates river dispersion of contaminants from single or multiple side discharges of effluent. In addition it has a turbulence transport sub-model that
calculates the variation of the lateral dispersion coefficients at grid locations across each cross-section of the river using the turbulence transport equations (K and E) based on the work of Rastogi and Rodi (1978). Lastly, it has a toxic substances sub-model to simulate the chemical-sediment interaction and transformation of toxic pollutants based on the work of Di Toro et al. (1982, 1984). The Lower St. Marys River is discretized by a fine grid using the KETOX model. One of the built-in advantages of this model is its ability to discretize to a finer grid resolution without major modification.

The second model is a compartment or cell approach model referred to as TOXI4 from US EPA's Center for Exposure and Assessment Modelling (CEAM) at Athens, Georgia. It is a time dependent three-dimensional model using the finite difference method. It also has a steady state modelling capability which is provided as an option to the user. The model assumes that the pollutant introduced into each cell is completely mixed. However, the model incorporates very detailed modelling of the chemical transport and transformation processes. The transport processes allow for equilibrium sorption, ionization, volatilization, bed sedimentation, and settling and resuspension within and across each face of the adjoining cells. In addition, it includes chemical kinetics for photolysis, hydrolysis, biodegradation and oxidation as the toxic substance undergoes transformation. Due to the intensive computation involved in this model, a coarse grid
network is used to discretize the Lower St. Marys River. It should be mentioned at this point that the DYNHYD4 model discussed earlier is used to obtain the hydrodynamic parameters for the Lower St. Marys River that are needed as input parameters for the TOXI4 model.

3.3.1 KETOX

The KETOX model has undergone several major revisions from the original CCIW (Canadian Centre for Inland Water Research, Burlington, Ontario) RIVMIX (Krishnappan and Lau, 1983) transport model. Modifications include the incorporation of the K-E turbulence model to compute the lateral dispersion coefficient, while the present revision includes linkage to a toxic substances sub-model and the dissipation of excess momentum due to jet like discharges in the flow field. Other modifications include developing an interactive micro-computer version of the model and linkage to a graphics support capability which will be discussed further in later chapters.

The mathematical formulation for the depth averaged model KETOX, to be described is developed for the far-field region. Rodi et al. (1981) in their experience with real-life situations had observed that in many rivers the bed roughness will often induce strong vertical mixing so that the depth-averaged approach is sufficiently accurate for practical purposes. Even when there are some three-dimensional effects in the direct vicinity of the
waste-water outfall, the combined turbulence induced by the river, bed roughness and the shear layers of the jet at the outfall will cause sufficient vertical mixing so that a depth averaged model is adequate. However, it is important to remember that the degree of accuracy of the results from the far field model is dependent on an accurate representation of the starting input profiles and initial conditions of the near-field region.

Since the model has four sub-models coupled together, it is only appropriate to discuss the theoretical concepts of each sub-model individually. However, only detailed theoretical formulation will be given for the present modifications, while the previously existing sub-model concepts will be briefly touched on.

3.3.1.1 Hydrodynamic Sub-Model

The steady state depth-averaged equations of motion for a river with variable depth are given by Rodi (1984). However, the computational complexity in solving these equations are avoided by adopting a simplified hydrodynamic model derived by McCorquodale et al. (1983). This hydrodynamic model assumes that the lateral depth profiles and river flow rates are available and can be used to obtain velocity profiles at different sections along the longitudinal flow direction. The model is further enhanced by a modification to include river curvature effects using an analytical approach by Chang (1983).
The model uses the Manning's equation to account for the vertical momentum transfer. To account for the side effects of the river banks, a shape function is incorporated in the model that can be adjusted by calibration. The vertically averaged longitudinal velocity for a wide river is then given by,

\[ U(z) = \chi(z) \frac{h^{2/3} S_o^{1/2}}{n} \sqrt{\frac{r_e}{r_{loc}}} \]  

in which,

\( \chi(z) \) = a shape factor to account for the river bank effects;

\( h \) = an average depth at a specified grid point on the river cross-section;

\( S_o \) = an effective frictional slope;

\( n \) = Manning's roughness factor;

\( r_e \) = radius of curvature of the centre line of the river width;

\( r = r_e - \left( \frac{W}{h} + z \right) \) = a local radius of curvature;

\( z \) = lateral distance of the local grid point from the shore; and

\( W \) = width of the river.

The boundary conditions for Eq. (3.21) are:

at \( z = 0 \), \( U(z = 0) = 0 \), and

at \( z = W \), \( U(z = W) = 0 \).

The relationship proposed by McCorquodale et al. (1983) for the shape factor is,
\begin{equation}
(3.22) \quad \chi(z) = \left( \frac{z - 1}{W/2} + \frac{1}{4} \right)^{n_1}
\end{equation}

in which \( n_1 \) is an empirical exponent to be calibrated. The values for \( n_1 \), the Manning's bed roughness, \( n \), and the river bed slope are adjusted to best fit the available field velocity data.

The continuity equation to be satisfied during this adjustment is given by,

\begin{equation}
(3.23) \quad Q = \int_0^W U(z) h \cdot dz
\end{equation}

During the adjustment for the empirical constants and the bed slope, the continuity Eq. (3.23) is integrated numerically to ensure that mass is conserved from section to section along the river. This simplified model has been proven to be capable of simulating the river hydrodynamics based on its successes in previous applications to the St. Clair River, the Niagara River and the Detroit River.

3.3.1.2 River Pollutant Dispersion Sub-Model

This is a modified model based on the work of Lau and Krishnappan (1981) to solve the transverse mixing of a pollutant discharged into a river which undergoes dispersion. Lau and Krishnappan had adopted the continuity and advective-diffusion equations formulated by Yotsukura and Sayre (1976) in a general orthogonal curvilinear coordinate system in which the x-axis
follows the meander of the river. By using the cumulative discharge to replace the transverse distance coordinate, Yotsukura and Sayre developed the steady state equation for two dimensional mixing which is simplified to include only two terms in the equation. A brief development is included here to derive this equation.

In the far field region, the pollutant has mixed fairly well over the flow depth and the two dimensional steady state continuity and advective-diffusion equations in an orthogonal curvilinear coordinate system can be written as,

Continuity Equation:

\[
\frac{\partial}{\partial x}(m_x hU) + \frac{\partial}{\partial z}(m_x hV) = 0
\]

(3.24)

Advective-diffusion Equation:

\[
m_x hU \frac{\partial C}{\partial x} + m_x hV \frac{\partial C}{\partial z} = \frac{\partial}{\partial z}\left(\frac{m_x h F_z}{m_x} \frac{\partial C}{\partial z}\right)
\]

(3.25)

in which,

\(x\) = longitudinal distance coordinates in the orthogonal curvilinear system;

\(z\) = transverse distance coordinates in the orthogonal curvilinear system;

\(U, V\) = depth averaged velocity components in the \(x, z\) directions;
\( h = \) local flow depth;
\( C = \) depth averaged concentration of the pollutant;
\( E_z = \) turbulent mixing or dispersion coefficient in the \( z \) direction; and
\( m_x, m_z = \) coefficients for the coordinate system.

The transformation of Eq. (3.25) to a more compact and convenient form can be accomplished by introducing the cumulative discharge,

\[
(3.26) \quad q_x = \int_{z=0}^{z=\nu} m_z h U \cdot dz
\]

By integrating the continuity Eq. (3.24) across the river cross-section and combining it with Eq. (3.26) one obtains,

\[
(3.27) \quad m_x h \nu = - \frac{\partial}{\partial x} \int_0^{\nu} m_z h U \cdot dz = - \frac{\partial q_x}{\partial x}
\]

by making use of the Leibnitz's rule to interchange the order of integration and differentiation. Next Eq. (3.27) is substituted into (3.25) to obtain,

\[
(3.28) \quad m_x h \partial \frac{\partial C}{\partial x} - \frac{\partial q_x}{\partial x} \frac{\partial C}{\partial z} = \frac{\partial}{\partial z} \left( m_z h E_z \frac{\partial C}{\partial z} \right)
\]

Using the chain rule for partial derivatives, Yotsukura and Sayre (1976) obtained the following simplified relationship,
(3.29) \[ \frac{\partial C}{\partial x} = \frac{1}{\partial q_e} \left( U h^2 m_x E_x \frac{\partial C}{\partial q_e} \right) \]

A dimensionless stream function which is actually a dimensionless cumulative discharge can be defined as,

(3.30) \[ \omega = \frac{q_e}{Q} \]

in which \( Q \) is the discharge of the river. Substituting Eq. (3.30) into (3.29), one obtains,

(3.31) \[ \frac{\partial C}{\partial x} = \frac{1}{Q^2 \partial \omega} \left( D_x(x, \omega) \frac{\partial C}{\partial \omega} \right) \]

in which,
\[ D_x = (U h^2 m_x E_x) \] a factor of diffusion.

The diffusion factor reflects the local changes in depth, velocity and stream curvature. The boundary conditions can be simply stated as:

At \( \omega = 0 \) on the left bank and \( \omega = 1 \) at the right bank.

**Numerical Solution**

By expanding the right hand side of Eq. (3.31) and rearranging the terms, it can shown that the advective-diffusion equation can be cast in the following form:
\[ (3.32) \quad \frac{\delta C}{\delta x} + J \frac{\delta C}{\delta \omega} = D \frac{\delta^2 C}{\delta \omega^2} \]

in which,

\[ (3.33) \quad J = -\frac{1}{Q^2} \frac{\delta D_z}{\delta \omega} \]

and,

\[ (3.34) \quad D = \frac{1}{Q^2} D_z \]

A variable grid system is used in which the lateral width of the river is discretized by a number of stream lines representing stream tube faces between two adjacent constant stream lines. The river flow \( Q \) is divided by the number of stream tubes used so that the flow within a stream tube remains constant. But the lines of constant stream function values follow the river curvature expanding and contracting where necessary with the river width. For a variable size mesh, Imam (1981) gave the following relationships for approximating the first and second derivatives of a given function "\( F \)" with respect to the stream function coordinates as follows:

\[ (3.35) \quad \frac{\delta F}{\delta \omega} = \left( \frac{\Delta F}{\Delta \omega} \right) = \left( \frac{F_{i+1} - F_i}{z_2} \right) \left( \frac{z_1}{z_1 + z_2} \right) \]

and,
\[ \frac{\partial^2 F}{\partial \omega^2} = \left( \frac{\partial^2 F}{\partial \omega^2} \right)_j = \left( \frac{F_{j+1}z_2 - (z_1 + z_2)F_j + F_{j-1}z_1}{z_1z_2(z_1 + z_2)/2} \right) \]

in which,

\[ z_1 = \Delta \omega \] between nodes \( j \) and \( (j-1) \); and

\[ z_2 = \Delta \omega \] between nodes \( j \) and \( (j+1) \).

From this point onward, the numerical procedure is adopted from Stone and Brian (1963). The finite difference representation of Eq. (3.32) given by McCorquodale et al. (1983) is as follows:

\[ \frac{1}{\Delta x} \left( a_2(C_{i-1,j} - C_{i,j}) + a_3(C_{i+1,j-1} - C_{i,j-1} + C_{i+1,j-1} - C_{i,j+1}) \right) \]

\[ + 2a_1J_{i,j} \left( \frac{z_1(C_{i,j+1} - C_{i,j})}{z_2(z_1 + z_2)} + \frac{z_2(C_{i,j} - C_{i,j-1})}{z_1(z_1 + z_2)} \right) \]

\[ + 2a_1J_{i,j} \left( \frac{z_1(C_{i+1,j+1} - C_{i+1,j})}{z_2(z_1 + z_2)} + \frac{z_2(C_{i+1,j} - C_{i+1,j-1})}{z_1(z_1 + z_2)} \right) \]

\[ = \frac{D_{i,j}}{z_1z_2(z_1 + z_2)} \left( z_1C_{i,j+1} - (z_1 + z_2)C_{i,j} + z_2C_{i,j-1} \right) \]

\[ + \frac{D_{i,j}}{z_1z_2(z_1 + z_2)} \left( z_1C_{i+1,j+1} - (z_1 + z_2)C_{i+1,j} + z_2C_{i+1,j-1} \right) \]

In this scheme the derivatives are approximated using weighting coefficients that are recommended by Stone and Brian (1963). The values of these coefficients are:
(3.38) \[ a_1 = \frac{1}{4} ; \quad a_2 = \frac{2}{3} ; \quad \text{and} \quad a_3 = \frac{1}{6} \]

Rearranging Eq. (3.37) in the manner shown by McCorquodale et al. (1983), the following system of equations forming a tri-diagonal matrix can be obtained:

(3.39) \[ p_i C_{i, j-1} + q_i C_{i, j} + r_i C_{i, j+1} = s_j \]

in which,

\[ p_i = \frac{1}{6 \Delta x} \left( J_{i, i}(z_2/2) + D_{i, i} \right) \frac{1}{z_1(z_1 + z_2)} \]

\[ q_i = \frac{2}{3 \Delta x} + \frac{J_{i, i}}{2} \left( \frac{z_2}{z_1(z_1 + z_2)} - \frac{z_1}{z_2(z_1 + z_2)} \right) + \frac{D_{i, i}}{z_1 z_2} \]

\[ r_i = \frac{1}{6 \Delta x} + \frac{1}{z_1(z_1 + z_2)} \left( J_{i, i}(z_1/2) - D_{i, i} \right) \]

\[ s_j = \left( \frac{1}{6 \Delta x} \left( J_{i, i}(z_2/2) + D_{i, i} \right) \right) C_{i, j-1} \]

\[ + \left( \frac{2}{3 \Delta x} + \frac{2}{z_1(z_1 + z_2)} \left( \frac{z_2}{z_1(z_1 + z_2)} - \frac{z_1}{z_2(z_1 + z_2)} \right) - \frac{D_{i, i}}{z_1 z_2} \right) C_{i, i} \]

\[ + \left( \frac{1}{6 \Delta x} \frac{J_{i, i}(z_1/2) - D_{i, i}}{z_1(z_1 + z_2)} \right) C_{i, j+1} \]

in which \( j = 2, 3, \ldots, (M-1) \) and \( M \) = the number of nodes per cross-section of the river.
The boundary condition at the river inflow section must be known concentration values. This can be the existing ambient concentration of the river and can be determined from field measurements at the inlet of the river. The right and left banks of the river are treated as reflecting boundaries. This implies solid impenetrable boundaries to the pollutants and can be expressed by central differencing on the solid boundary as follows:

Using the reflecting boundary condition of \( \left( \frac{\partial C}{\partial \omega} \right)_{\omega=0} = 0 \) at the boundary, \( j = 1 \), so that, \( C_{1,j-1} = C_{1,j-2} \).

Similarly, for \( \left( \frac{\partial C}{\partial \omega} \right)_{\omega=1} \) at the boundary, \( j = M \), so that, \( C_{1,j-M+1} = C_{1,j-M+1} \).

The values for the coefficients in Eq. (3.39) at the river banks are:

At the bank where the node \( j = 1 \),

\[
q_1 = \frac{2}{3 \Delta x} + \frac{D_1}{\Delta \omega^2}
\]

\[
r_1 = \left( \frac{1}{3 \Delta x} - \frac{D_1}{\Delta \omega^2} \right)
\]

\[
s_1 = \left( \frac{2}{3 \Delta x} - \frac{D_1}{\Delta \omega^2} \right) C_1 + \left( \frac{1}{3 \Delta x} - \frac{D_1}{\Delta \omega^2} \right) C_2
\]
At the bank where the node $j = M$,

$$
\rho_u = \frac{1}{3 \Delta x} + \frac{D_u}{\Delta \omega^2}
$$

$$
q_u = \frac{2}{3 \Delta x} - \frac{D_u}{\Delta \omega^2}
$$

$$
\sigma_u = \left( \frac{2}{3 \Delta x} - \frac{D_u}{\Delta \omega^2} \right) C_u + \left( \frac{1}{3 \Delta x} + \frac{D_u}{\Delta \omega^2} \right) C_{u-1}
$$

At outfall locations, the model treats such sources as mass loading points and does not introduce additional flow into the river system. This is a very good assumption since the flow rate from the outfall points are usually very small compared to the bulk flow rate of the river. Using a mass balance calculation, the model will take the increase in pollutant concentrations at the outfall as,

$$(3.40) \quad \Delta C_j = \frac{C_s Q_s}{Q(z_1 + z_2)/2}$$

in which,

- $\Delta C_j$ = the increase in the concentration;
- $C_s$ = the input concentration discharged by the outfall; and
- $Q_s$ = the flow rate of the outfall.

Finally, the system of equations in (3.39) with the appropriate boundary conditions introduced are solved using a relaxation method. The solution requires a known velocity
component, which is computed by the hydrodynamic sub-model, to be used for the concentration gradient term. It also requires values for the transverse turbulent mixing coefficient which varies laterally across the river cross-section. The turbulent mixing coefficient is obtained by the turbulence transport equations to be discussed next.

3.3.1.3 Turbulence Sub-Model

In a state-of-the-art review of turbulence models and their application in hydraulics, Rodi (1984) concluded that the K-E (K and E equations) model holds the most promise based on its many proven successes when applied to a wide range of engineering problems. In this model, the local state of turbulence is characterized by two parameters: the kinetic energy \( \overline{\varepsilon} \) of the turbulent motion and the rate of its dissipation, \( \varepsilon \). The parameter \( \overline{\varepsilon} \) is a measure of the intensity of the turbulent fluctuations, while the parameter \( \varepsilon \) is closely related to a length scale \( L \) characterizing the turbulent motion. \( L \) is a measure of the size of the energy-containing turbulent eddies.

For open channel flow calculations, the depth averaged version of the K-E equation presented by Rastogi and Rodi (1978) is adopted here. The variation of \( K \) and \( E \) is determined from the following transport equations:
\begin{align}
(3.41) \quad U \frac{\partial K}{\partial x} + V \frac{\partial K}{\partial z} &= \frac{\partial}{\partial x}\left(\frac{\nu_t \partial K}{\sigma_k \partial x}\right) \\
&+ \frac{\partial}{\partial z}\left(\frac{\nu_t \partial K}{\sigma_k \partial z}\right) + P_h + P_{KV} - E
\end{align}

\begin{align}
(3.42) \quad U \frac{\partial E}{\partial x} + V \frac{\partial E}{\partial z} &= \frac{\partial}{\partial x}\left(\frac{\nu_t \partial E}{\sigma_e \partial x}\right) \\
&+ \frac{\partial}{\partial z}\left(\frac{\nu_t \partial E}{\sigma_k \partial z}\right) + c_{1e} \frac{E}{K} P_h + P_{EV} - c_{2e} \frac{E^2}{K}
\end{align}

in which,

\begin{itemize}
\item \(\nu_t\) = turbulent eddy viscosity;
\item \(\sigma_k, \sigma_e\) = empirical diffusion constants;
\item \(c_{1e}, c_{2e}\) = empirical constants;
\item \(P_h = \nu_t \left(2 \left(\frac{\partial U}{\partial x}\right)^2 + 2 \left(\frac{\partial V}{\partial z}\right)^2 + \left(\frac{\partial U}{\partial z} + \frac{\partial V}{\partial x}\right)^2\right)\);
\item \(P_{KV} = c_k \frac{U^2}{h}\);
\item \(P_{EV} = c_{1e} \frac{U^4}{h^2}\);
\item \(c_k = \frac{1}{\sqrt{c_f}}\) = an empirical constant;
\item \(c_f\) = friction coefficient;
\item \(c_e = 3.6c_{2e} \left(\sqrt{c_{u}/c_f^{3/4}}\right)\) = an empirical constant; and
\end{itemize}
\( U_s = \sqrt{c_f (U^2 + V^2)} \) = friction velocity.

All the values for the empirical constants are similar to those used by Rodi (1984). The turbulent mixing or eddy viscosity can be related to the turbulence energy and dissipation parameters \( K \) and \( E \) by dimensional analysis to give the following relationship:

\[
(3.43) \quad \nu_t = c'_\mu \frac{K^2}{E}
\]

The turbulent stress is related to the gradients of the depth averaged velocity components as follows:

\[
(3.44) \quad \tau_{xz} = \nu_t \left( \frac{\partial U}{\partial x} + \frac{\partial V}{\partial z} \right) - \frac{2}{3} K
\]

and the bottom stress is related to the depth averaged velocity components by,

\[
(3.45) \quad \tau_{bx} = c_f \rho U_s \sqrt{U^2 + V^2}
\]

The advantage in the use of stream lines to laterally discretize the river has already been outlined in the previous section. Using a similar approach it can be assumed that the flow is totally confined within the stream lines in the longitudinal \( x \)-direction. Although the effect of longitudinal dispersion is large compared to lateral dispersion, its effect is small relative to the advective transport terms except near the source.
(Rodi et al., 1981). Therefore, the longitudinal dispersion terms can be neglected. With these simplifications, the K-E transport equations become,

\begin{equation}
U \frac{\partial K}{\partial x} = \frac{\partial}{\partial z} \left( \frac{\nu_t \partial K}{\sigma_k \partial z} \right) + P_h + P_{kv} - E
\end{equation}

\begin{equation}
U \frac{\partial E}{\partial x} = \frac{\partial}{\partial z} \left( \frac{\nu_t \partial E}{\sigma_k \partial z} \right) + c_{1e} \frac{E}{K} P_h + P_{ev} - c_{2e} \frac{E^2}{K}
\end{equation}

Each of the K and the E transport equations are now similar to the transport Eq. (3.32) except for the appearance of the source and sink terms. The two equations are again cast into the stream function coordinate system \((x-\omega)\) and solved by the variable grid approach used for the mass transport equation (McCorquodale et al., 1983). The program solves the K equation before the E equation and then calculates the turbulent eddy viscosity. The source and sink terms are decoupled from the solution to permit an analytical solution.

3.3.1.4 Dispersion of Excess Momentum

One of the problems encountered by the model in its application to the Lower St. Marys River is the need to simulate regions of strong jet-like discharges from hydroelectric power canals (in this instance, the Great Lakes Power Corporation Plant and the Edison Sault power plant) in the far field reaches downstream from the outfall location. The original model tends to
smooth out the jet-like nature of the velocity distribution in reaches with excess momentum. In order to correctly simulate these regions of jet-like discharges, the hydrodynamic sub-model of KETOX was revised to incorporate the dissipation and dispersion of the excess momentum introduced into the flow.

Any modification will require a starting estimate of the correct velocity distribution in the cross-section of the river. The approach is to introduce as an upstream boundary condition the actual field measured velocity distribution at cross-sections where jet flows are introduced. Since the measured field data from the US Army Corps of Engineers (1984) are sparsely scattered across the cross-section of the river, a best fit velocity distribution is initially set-up encompassing these sparse velocity data. A numerical integration is then carried out across the river cross-section based on 118 interpolated grid points to properly represent the river bed and the best fitted velocity profile. This numerical integration will enable us to maintain a continuity check by readjusting the interpolated velocity distribution at the cross-section. On completion of this readjustment, an approximate modified velocity distribution is obtained that satisfies continuity of mass.

The next stage is to evaluate the excesses or deficits in the velocities between the unmodified (i.e. the computed velocity profile based on the original sub-model) and the approximate
modified velocity distribution. The velocity differences are obtained for each of the stream nodes across the entire river width. The velocity differences at each stream tube node, which represents the momentum excesses or deficits, are then diffused in the lateral direction as one would diffuse the pollutant concentrations laterally. This can be written mathematically as (Rodi, 1984),

\[
\frac{\partial (\delta U)}{\partial x} = \frac{\partial}{\partial \omega} \left( D_m \frac{\partial (\delta U)}{\partial \omega} \right)
\]

in which,

\(\delta U\) = the excess depth averaged velocity at each node;

\(\omega\) = the longitudinal stream tube coordinate;

\(D_m = \frac{\nu_m U h^2}{Q^2}\) = diffusion factor;

\(\nu_m\) = turbulent transverse mixing or dispersion coefficient;

\(U\) = depth averaged local velocity;

\(h\) = local flow depth; and

\(Q\) = total discharge of the channel.

The McCorquodale et al. (1983) numerical procedure as discussed previously is used to solve Eq. (3.48). In this case, the boundary conditions involved are simply:

\(\text{at } \omega = 0, \quad \delta U = 0, \text{ and}\)

\(\text{at } \omega = 1, \quad \delta U = 0.\)
The only unknown parameter is the turbulent transverse mixing coefficient which is calculated for each node across the cross-section using the K-E turbulence sub-model component in KETOX. Once the dispersed velocity is computed for all the nodes, it is used to readjust the unmodified velocity distribution. This is done either by adding to or subtracting from the unmodified velocity distribution depending on the computed excess or deficiency in momentum (i.e. velocity) at each stream tube node location. On completion of this adjustment, a new excess momentum corrected velocity distribution is obtained. This modification process is illustrated in Fig. 3.2. In order to ensure that continuity in mass is still maintained at the cross-section, a numerical integration is again carried out to readjust the newly obtained excess momentum corrected velocity distribution before obtaining the final modified velocity distribution.

By using stream tube coordinates in the model, the dissipation of the excess momentum is confined within each stream tube. The excess momentum is allowed to convect and dissipate within each stream tube by either expansion or contraction of the stream tube. In transforming to the physical x-y plane, the original stream tube node locations must now be readjusted to absorb the excess or deficiency in the diffused excess momentum.

The program algorithm used to implement this adjustment for the new node locations are summarized mathematically below for
the case of 15 stream function nodes. In this application, nodes 1 and 15 are the two ends of the river cross-section on the shorelines. Figure 3.3 gives the notations used in the node adjustments.

Step 1:
Before adjustment for the new nodes location, the flow area of the entire river cross-section is obtained by numerical integration as follows:

\[ A_r = \sum_{j=1}^{14} \left( \frac{1}{2} (y_{j+1} - y_j)(h_{j+1} + h_j) \right) \]

in which,

- \( j = 1 \) to 14 (i.e. 15 nodes with 14 intermediate panels);
- \( h_j, h_{j+1} \) = local flow depths at nodes \( j \) and \( j+1 \); and
- \( y_j, y_{j+1} \) = lateral distances of the original nodes from the shoreline.

Step 2:
The new excess momentum adjusted velocities at nodes "j" and "j+1" can be related to the flow across panel "j" by the incremental change in the dimensionless stream function value as follows:

\[ \frac{1}{2} (U_{j+1}^m + U_j^m) \Delta A_j = \Delta \omega_j Q \]
in which,

\[ U_{i,i}^m, U_{i,i+1}^m = \text{the excess momentum adjusted velocities at cross-section } i; \]
\[ \Delta \omega_j = \text{unitless stream function value between nodes } j \text{ and } j+1; \]
\[ Q = \text{total river flow}; \text{ and} \]
\[ A_j = \text{cross-sectional area of panel } j \text{ between nodes } j \text{ and } j+1. \]

It should be noted that:

\[
(3.51) \quad \sum_{j=1}^{14} \Delta \omega_j = 1.0
\]

Rearranging Eq. (3.50), one can obtain,

\[
(3.52) \quad A_j = \frac{2(\Delta \omega_j, Q)}{(U_{i,i}^m + U_{i,i+1}^m)}
\]

Step 3:

In order to equate Eq. (3.49) with the sum of the areas in Eq. (3.52) exactly, an area correction coefficient is introduced as follows:

\[
(3.53) \quad C_{\text{area}} = \frac{A_T}{\sum_{j=1}^{14} A_j}
\]

The corrected area for any panel "j" is then given by:

\[
(3.54) \quad A_j^c = C_{\text{area}} A_j
\]

The corrected area of panel "j" can also be related to the adjoining nodal depths as follows:
\begin{equation}
A_i^e \frac{1}{2} (h_{j} + h_{j+1}) (y_{j+1}^m - y_{j}^m)
\end{equation}

in which,

\(y_j^m, y_{j+1}^m\) = the new excess momentum adjusted node locations.

**Step 4:**

Finally, the location of the new node position is obtained by rearranging Eq. (3.55) to obtain:

\begin{equation}
y_{j+1}^m = y_j^m + \left( \frac{2A_i^e}{h_j + h_{j+1}} \right)
\end{equation}

This completes the modification to the model for regions of jet like discharges.

**3.3.1.5 Toxic Substances Sub-Model**

In developing a toxic substances model, it is important to include in the model the physical-chemical components that determine the fate of the toxic substance in the water body. Some of these physical-chemical components are illustrated in Fig. 3.4 and are also described below:

a. sorption-desorption mechanism of the chemical with the suspended particulates in the water column and sediment,

b. loss of the chemical due to mechanisms such as biodegradation, volatilization, chemical and biochemical reactions, and photolysis,
c. transport of the toxicant due to advective flow, transport, dispersion, and mixing, and

d. settling and resuspension of particulates between sediment and water column.

The toxicant is assumed to exist in two basic forms in both the water column and the sediment of the water body. These are:

a. The dissolved form which has the following units and notation,

\[ C_d \left( \frac{M_T}{L^3_w} ; M_T = \text{mass of toxicant} \right) \]

All toxicants passing a 0.45 micron filter can be considered to be in the "dissolved" form.

b. The particulate form which has the following units and notation,

\[ C_p \left( \frac{M_T}{L^3_{w_*}} \right) \]

In this case the toxicant is sorbed onto the particulate matter in the water column or sediment.

The total toxicant concentration, \( C_T \left( \frac{M_T}{L^3_{w_*}} \right) \), is then given by,

\[ C_T = C_p + \Theta C_d \]  
(3.57)

or,

\[ C_T = C_p + C_d \]  
(3.58)
in which,

\[ \theta = \text{porosity, the volume of water per bulk volume, } L^3 / L^3 \]

and,

\[(3.59) \quad C_d = \theta C_d' \]

is the porosity corrected dissolved form of the toxicant. The porosity of the volume must be introduced to maintain a consistent mass balance since the dissolved toxicant concentration is the mass of toxicant per volume of water, while the total toxicant concentration is the mass of toxicant per volume of water plus solids. Therefore, for the water column,

\[ C_d = C_d' \quad (\text{i.e. } \theta \text{ is approximately 1}) \]

since the water volume is equal to the bulk volume. The porosity of the upper strata of the bed sediment is generally in the range 0.7 to 0.8.

Two equations for the toxicant are required, one for the particulate and one for the dissolved form. These equations represent the kinetic interactions of sorption and desorption between the two forms of the chemical. However, for most chemicals these reaction kinetics tend to be "fast", on the order of minutes to hours, compared to the time scales of the other mechanisms of the problem such as bacterial decay and sedimentation rates that have reaction times on the order of days to years.
The "fast" kinetics of sorption-desorption (Thomann and Mueller, 1987) indicate that, for time scales of days to years, there will be a virtually continuous equilibration of the dissolved and particulate forms depending on the local solids concentration. This partitioning between the two components permits the specification of the fraction of dissolved toxicant to the total toxicant, and the fraction of particulate toxicant to the total. The dissolved and particulate toxicant are, therefore, assumed to be always in a "local equilibrium" with each other. A partition coefficient can then be defined as follows:

\[
\pi = \frac{r}{C_d}
\]  

(3.60)

in which,

\(\pi\) = a partition coefficient, \(\left(\frac{M_T}{M_s} + \frac{M_T}{L_w} \right)\); \(M_s\) = mass of solids;

and

\(r\) = toxicant concentration on a per unit dry weight solids basis, \(M_T/M_s\).

A typical unit for \(r\) is (ug tox)/g(dry wt.), in which g(dry wt.) is gram dry weight of solids. Based on Eq. (3.59), the porosity corrected partition coefficient is then,

\[
\pi = \frac{\pi}{\theta} = \frac{r}{C_d}
\]  

(3.61)
in which,

\( \pi = \text{the porosity corrected partition coefficient, } \frac{M_T}{M_s + M_T/L_{w}} \).

The toxicant concentration in the particulate is expressed as a mass of toxicant per bulk volume of solids plus water. Therefore, for a given solids concentration, one can also write,

\[ C_p = \pi C_d m \]  

in which,

\( m = \text{the solids concentration, } \frac{M_s}{L_{w}} \).

Substituting \( r \) from Eq. (3.61) into Eq. (3.62) one can write,

\[ C_p = \pi C_d m \]  

Substituting Eq. (3.63) into Eq. (3.58) gives,

\[ C_T = \pi C_d m + C_d \]

or,

\[ C_d = \frac{C_T}{1 + \pi m} \]  

or,

\[ C_d = f_d C_T \]

in which the fraction of the total toxicant that is dissolved is given by,

\[ f_d = \frac{1}{1 + \pi m} \]
and the fraction of the total toxicant that is particulate is given by,

\[ f_p = \frac{\pi' m}{1 + \pi' m} \]

so that,

\[ C_p = f_p C_T \]

Also it should be noted that the sum of the dissolved and particulate fraction must be unity as follows:

\[ f_p + f_d = 1 \]

The distribution of the toxicant between the dissolved and particulate forms therefore depends on the partition coefficient of the toxicant and the solids concentration. Hence, the assumption of local equilibrium makes it possible to specify the fractions of the total toxicant in the dissolved and particulate forms at all times. This enables attention to be focused mainly on the mass balance equation of the total toxicant.

With the above background on one of the key assumptions, the mass balance for the toxic substance in a river can now be formulated. The river is represented by a sequence of completely mixed volume segments which are segments of stream tubes. Since the KETOX model uses stream function coordinates, the lateral space size discretization is represented by the width of the stream tubes. The longitudinal space size discretization \( \Delta x \) for
the volume segments is again set by KETOX's requirement for numerical stability. Although vertical sediment and interstitial water mixing is still being considered, horizontal and lateral bed motions are assumed to be insignificant, i.e. no bed load. The adjacent downstream segment can receive only a water column input of toxicant as a result of the stream flow (i.e. advective transport) from the upstream segment.

With these key observations, the mass balance for the total toxicant in the water column of a single completely mixed river segment is given by,

\[
V_1 \frac{dC_{T1}}{dt} = -K_1 V_1 C_{T1} - Q_1 C_{T1} - \frac{K_1 V_1}{H_1} (f_{d1} C_{T1} - f_{d2} C_{T2})
- \frac{w_a V_1}{H_1} f_{p1} C_{T1} + \frac{w_r V_1}{H_1} f_{p2} C_{T2} + \nu V_1
\]

in which,

- \(V_1\) = volume of the water column;
- \(C_{T1}\) = (dissolved + particulate) toxicant concentration in water column;
- \(K_1\) = sum of hydrolysis, oxidation, biodegradation, photolysis and volatilization rates in water column;
- \(Q_1\) = flowrate in the water column segment;
- \(K_1\) = water-sediment diffusion exchange coefficient;
- \(H_1\) = depth of the water column;
- \(f_{d1} = \frac{1}{(1 + m_1 \pi_1)}\) = dissolved fraction in water;
\[ f_{d2} = \frac{1}{1 + m_2 \pi_2 / \Theta} \] dissolved fraction in sediment;

\[ f_{p1} = \frac{m_1 \pi_1}{1 + m_1 \pi_1} \] particulate fraction in water;

\[ f_{p2} = \frac{m_2 \pi_2 / \Theta}{1 + m_2 \pi_2 / \Theta} \] particulate fraction in sediment;

\[ m_1 = \text{solids concentration in the water column}; \]
\[ m_2 = \text{solids concentration in the sediment}; \]
\[ w_a = \text{settling velocity}; \]
\[ w_{rs} = \text{resuspension velocity}; \]
\[ \dot{V}_T = Q_1 C_{\tau_0} = \text{mass inflow rate of toxicant}; \text{ and}; \]
\[ C_{\tau_0} = \text{total toxicant concentration from adjoining upstream segment}. \]

The description of each term on the right hand side of Eq. (3.70) is as follows. The first term is an overall loss rate of the dissolved and particulate forms in the water column due to decay mechanisms such as biological degradation, oxidation, photolysis, hydrolysis and volatilization. The second term is the flux of transport out of the river segment under consideration due to flow. The third term is the flux between the sediment and the overlying water layer due to interstitial diffusion of the toxicant's dissolved form. The fourth term is the loss of toxicants absorbed to the particulates which settle to the sediment bed from the water column. The fifth term is the gain in the toxicants in the water column due to particulate resuspension from the sediment bed. The last term is external input of
toxicant into the segment under consideration either by direct loading into the segment or by advective transport with the river flow from the adjoining upstream segment.

Since Eq. (3.70) depends on an interaction with the sediment, a similar mass balance equation for the total toxicant in the active sediment bed layer underlying the water column is given by,

$$V_2 \frac{dC_{T2}}{dt} = -K_2 V_2 C_{T2} + \frac{K_1 V_2}{H_2} (f_{d1} C_{T1} - f_{d2} C_{T2})$$

$$+ \frac{w_s V_2}{H_2} f_{p1} C_{T1} - \frac{w_s V_2}{H_2} f_{p2} C_{T2}$$

in which,

$V_2$ = volume of the sediment column;

$C_{T2}$ = (dissolved + particulate) toxicant concentration in sediment;

$K_2$ = sum of hydrolysis, oxidation, biodegradation, and photolysis; rates in the sediment;

$H_2$ = depth of the sediment column; and

$w_s$ = sedimentation velocity.

All the terms in Eq. (3.71) represent similar mechanisms to those in the water column as described above. These are, in the order from the right, loss due to decay processes in the sediment, diffusive exchange of interstitial dissolved toxicant, gain due to settling, loss due to resuspension, and loss due to net sedimentation.
The analytical solution for the time variable water column and sediment toxicant concentration are given by Di Toro and Paquin (1984). Although the full general solutions for Eqs. (3.70) and (3.71) are available from Di Toro and Paquin, only certain aspects of the solution are implemented into KETOX. The most useful features of the solutions that are incorporated into KETOX are summarized below:

a. The concentrations in the water column and sediment can be evaluated by the analytical solutions which are dependent on two terms given by,

\begin{equation}
(3.72) \quad s_1 = K_1 + \left( w_s f_{p1} + K_L f_d \right) / H_1 + \frac{1}{t_p}
\end{equation}

and,

\begin{equation}
(3.73) \quad s_2 = K_2 + \left( \left( w_{rs} + w_s \right) f_{p2} + K_L f_d \right) / H_2
\end{equation}

in which,

\[ t_p = \frac{V_1}{Q} = \frac{D_{xc}}{U} = \text{detention time of the cell;} \]

\[ U = \text{depth average velocity in the cell; and} \]

\[ D_{xc} = \text{longitudinal length of the cell in the flow direction.} \]

It can be seen that Eq. (3.72) is the sum of three terms, the water column decay rate, the sediment transfer rate coefficients, and the reciprocal of the cell detention.
time. Equation (3.73) is comprised of the sum of sediment decay, sediment resuspension and sedimentation transfer rates.

b. Sediment Capacity Factor. The magnitude of the sediment capacity factor determines the effectiveness of the sediment removal mechanisms (i.e. decay and sedimentation) as chemical sinks. Small values indicate that sediment-related removal mechanisms are insignificant relative to the water column concentration, while large values magnify the sediment effects. The sediment capacity factor is given by,

\[ \beta = \frac{m_2 H_2 f_{p1}}{m_1 H_1 f_{p2}} \]  

(3.74)

c. The ratio of the steady state particulate chemical concentrations in the sediment and water column is given by,

\[ \frac{r_2}{r_1} = \frac{w_z (m_1/m_2) f_{p2} + K_1 (\pi_2/(\pi_1 \Theta)) f_{d2}}{(w_{zs} + w_z) f_{p2} + K_1 f_{d2} + K_2 H_2} \]  

(3.75)

This ratio expresses the degree of chemical contamination of the sediment particles relative to the water column particles. For instance a large value for the ratio indicates that the sediment particles are highly contaminated relative to the water column particles.
d. The "fast" decay rate which represents the rate at which water column and sediment concentrations initially equilibrate is given by,

\[ g_1 = \left( s_1 + s_2 \right) \]

while the "slow" decay rate is given by,

\[ g_2 = \frac{s_2}{(s_1 + s_2)} K_T \]

The apparent total removal rate of the chemical is given by,

\[ K_T = K_1 + \beta \left( r_2 / r_1 \right) \left( K_2 + K_s \right) \]

in which,

\[ K_s = \left( w_s / H_2 \right) \] = sedimentation rate coefficient.

The apparent removal rate parameter controls the steady state water column concentration.

e. The half life of the "fast" and "slow" decay rates are respectively,

\[ t_{\text{half}1} = \frac{0.693}{g_1} \]

\[ t_{\text{half}2} = \frac{0.693}{g_2} \]

For steady state conditions, the time derivatives in Eqs. (3.70) and (3.71) are set to zero and what remains are two simultaneous linear algebraic equations that can be solved
directly for the steady state toxicant concentrations in the water column and the sediment. The steady state solutions are given by,

**Water Column:**

\[(3.81a) \quad C_{T1} = \frac{(W_T/V_1)(AAA)}{(BBB)(AAA)-(CCC)(DDD)}\]

in which,

\[AAA = \left(\frac{w_{rs}}{H_2} f_{p2} + \frac{w_a}{H_2} f_{p2} + \frac{K_L}{H_2} f_{d2} + K_2\right);\]

\[BBB = \left(\frac{Q_1}{V_1} + K_1 + \frac{w_a}{H_1} f_{d1} + \frac{K_L}{H_1} f_{d1}\right);\]

\[CCC = \left(\frac{w_{rs}}{H_1} f_{p2} + \frac{K_L}{H_1} f_{d2}\right);\]

\[DDD = \left(\frac{w_a}{H_2} f_{d1} + \frac{K_L}{H_2} f_{d1}\right).\]

The dissolved and particulate concentrations can be obtained from Eqs. (3.65a) and (3.68) respectively as follows:

\[(3.81b) \quad C_{d1} = f_{d1} C_{T1}\]

\[(3.81c) \quad C_{p1} = f_{p1} C_{T1}\]

It should be noted that \(C_{T1}\) due to loading, dispersion, convection and decay or losses is predicted from the mass transport sub-model of KETOX.
Sediment Column:

\[
C_{T2} = \frac{C_{T1}(w_{s}f_{p1} + K_{l}f_{d1})}{(K_{2}H_{2} + w_{s}f_{p2} + K_{l}f_{d2} + w_{s}f_{p2})}
\]

and similarly one can obtain the dissolved and particulate forms,

\[
(3.82b) \quad C_{d2} = f_{d2}C_{T2}
\]

\[
(3.82c) \quad C_{p2} = f_{p2}C_{T2}
\]

3.3.1.6 Implementation of the Toxic Substances Equations

The toxics sub-model that was developed and linked to the KETOX model allows for a water column overlying an active sediment bed layer in the vertical discretization for the river segment. Each water column and sediment layer is then provided with three solids state variables, which in this case are biotic particles, and fine and coarse abiotic particles. Some modifications to the equations developed so far are necessary in order to incorporate these state variables. It is convenient to interpret the modifications required to incorporate the three state variables using double subscripts; in which \( j = 1 \) indicates biotic particles, \( j = 2 \) is for fine abiotic solids and \( j = 3 \) is for coarse abiotic solids, while the second subscript numerals 1 and 2 denote water column and bed sediment layer respectively.

Then the combined particulate sorbed contaminant fractions for the water column and active bed layer are respectively given by,
\[(3.83a)\quad f_{p1,i} = \frac{\pi_{1,j}m_{1,j}/\theta}{1 + \sum_{j=1}^{3} (\pi_{1,j}m_{1,j}/\theta)} \]

\[(3.83b)\quad f_{p2,i} = \frac{\pi_{2,j}m_{2,j}/\theta}{1 + \sum_{j=1}^{3} (\pi_{2,j}m_{2,j}/\theta)} \]

The combined dissolved fractions for the water column and active bed layer are given by,

\[(3.84a)\quad f_{d1} = \left(1 - \sum_{j=1}^{3} f_{p1,i}\right) \]

\[(3.84b)\quad f_{d2} = \left(1 - \sum_{j=1}^{3} f_{p2,i}\right) \]

The total toxicant concentration in the water column is computed by the river dispersion sub-model of KETOX instead of Eq. (3.81a). However, the total toxicant concentration in the active bed layer is obtained by a modified form of the steady state state solution of Eq. (3.82a) as follows:

\[(3.85)\quad C_{T2} = \frac{C_{T1} \sum_{j=1}^{3} (w_{a,j}f_{p1,i}) + K_L f_{d1}}{\sum_{j=1}^{3} \left(f_{p2,i}(w_{rs,i} + w_{s,i})\right) + K_L f_{d2} + H_2 K_2}

in which,

\(C_{T1}\) = the total toxicant concentration in the water column.
The combined chemical concentration for the particulates in the water column and active bed layer are given by:

\[
C_{P1} = \frac{\sum_{j=1}^{3} f_{P1,i} C_{T1}}{\sum_{j=1}^{3} m_{1,i}}
\]

\[
C_{P2} = \frac{\sum_{j=1}^{3} f_{P2,i} C_{T2}}{\sum_{j=1}^{3} m_{2,i}}
\]

(3.86a) \quad (3.86b)

While the combined chemical concentration in the dissolved phase for the water column and the active bed are given by,

\[
C_{D1} = C_{T1} f_{D1}
\]

\[
C_{D2} = C_{T2} f_{D2}
\]

(3.87a) \quad (3.87b)

The combined sediment capacity factor is given by,

\[
\beta_c = \frac{\sum_{i=1}^{3} (m_{2,i} H_2 f_{P1,i})}{\sum_{i=1}^{3} (m_{1,i} H_1 f_{P2,i})}
\]

(3.88)

The combined ratio of the steady state particulate chemical concentrations in the sediment and water column may be expressed as,
\[
\left( \frac{r_2}{r_1} \right)_c = \left[ \sum_{j=1}^{3} \left( w_{a,j} \left( \frac{m_{1,j}}{m_{2,j}} \right) f_{p_2,j} \right) + K_L f_{D_2} \frac{1}{3 \Theta} \left( \sum_{j=1}^{3} \frac{\pi_{2,j}}{\pi_{1,j}} \right) \right] \\
\div \left[ \sum_{j=1}^{3} \left( (w_{rs,j} + w_{s,j}) f_{p_2,j} \right) + K_L f_{D_2} + K_2 H_2 \right]
\]

The expressions for the combined effects characterizing the water column and sediment decay and transfer fluxes are given by,

\[
S_{1c} = \frac{1}{t_D} \left( \left( \sum_{j=1}^{3} \frac{w_{a,j} f_{p_1,j} \left( + K_L f_{D_1} + \text{Volat}R \right)}{H_1} \right) + K_{1c} \right)
\]

in which, \( \text{VolatR} \) is the volatilization rate coefficient, and,

\[
S_{2c} = K_2 + \left( \sum_{j=1}^{3} \left( (w_{rs,j} + w_{s,j}) f_{p_2,j} \right) + K_L f_{D_2} \right) \frac{1}{H_2}
\]

The combined "fast" decay rate may be expressed as,

\[
g_{1c} = (S_{1c} + S_{2c})
\]

while the combined "slow" decay rate is given by,

\[
g_{2c} = \frac{S_{2c}}{(S_{1c} + S_{2c})} K_{Tc}
\]
in which,

\[ K_{\text{TC}} = K_{1c} + \frac{VolatR}{H_1} + \beta \left( \frac{r_2}{r_1} \right) (K_2 + K_{sc}); \]  

where,

\[ K_{1c} = \text{(photolysis + hydrolysis + biodegradation + oxidation) rates} \]

in the water column; and

\[ K_{sc} = \sum_{i=1}^{3} \left( w_{a,i} f_{p2,i} \right) \left( 1 - f_{p2} \right) H_2 \]  

Finally, the combined half life of the chemical in the water column and sediment can be obtained respectively by the following expressions:

\[ t_{h1/2} = \frac{0.693}{g_{1c}} \]  

and,

\[ t_{h1/2} = \frac{0.693}{g_{2c}} \]

The above equations are used to implement the toxic substances sub-model for KETOX. Further discussion on the application will be covered in later chapters on the toxics simulation.
3.3.2 TOXI4 (USEPA)

The complete TOXI4 system is a water quality program that calculates toxicant concentrations in space and time for ponds, rivers, lakes, reservoir, streams, estuaries, and coastal waters (Ambrose et al., 1988). TOXI4 by itself is a kinetic sub-model which must be linked to the basic and controlling WASP4 sub-model in order to complete the TOXI4 system for simulating the movement and interaction of toxic pollutants (involving organic chemicals, metals, and sediment).

One of the strong features of the model's flexibility is the ability of the user to structure it into one, two, and three dimensional models. A three dimensional model structure for a water body is illustrated in Fig. 3.5. In this sketch, the water column is segmented into an upper surface water cell and a lower subsurface water cell, while the river bed is segmented into a surface and a subsurface sediment layer. It also allows the user to specify time-variable exchange coefficients, advective flows, waste loads and water quality boundary conditions. Finally and most importantly it also permits tailored structuring of the kinetic processes by the user.

It is not the intention here to repeat the theories of this model which are well documented by Di Toro et al. (1983) and Ambrose et al. (1988). The theory of this model is briefly formulated in Appendix B so that in using the model one is aware of the limitations of the results obtained.
Chapter 4

HYDROGRAPHIC CHARACTERISTICS OF ST. MARYS RIVER

4.1. General

It can be seen from Fig. 1.3 that the Upper St. Marys River is made up of a partial lake and river system while the Lower St. Marys River characterizes a river. The most important aspects of the hydrographic characteristic are the flow rate, velocity, geometry, wind effect and ice cover condition.

4.2. Flow and Hydraulic Geometry

Based on the most intuitive notion of dilution, it is clear that one must focus on those times when the flow is "low" when conditions will probably be the most critical. The flows through the control structures at the Soo locks are governed by Plan 1977. Table 4.1 gives the typical flow distribution (McCorquodale and Yuen, 1987) among the structures. A map description of the layout of the control structures is given in Fig. 1.2.

Based on Lake Superior Regulation Plan 1977, log normal plots of the monthly flow frequency curves for St. Marys River are shown in Fig. 4.1 for the period May-November and December-April. The water level at the Upper St. Marys River is regulated between 600.5 and 602.0 feet (183.1 and 183.5 m) IGLD (International Great Lakes Datum) which is the same lake level variations in Lake Superior since these limits are agreed to in
Plan 1977. The LWD (Low Water Datum) is 600.0 feet (182.9 m) IGLD for Lake Superior. According to Plan 1977 the water level downstream of the Soo locks should not exceed 582.9 feet (177.7 m) IGLD, however, the actual maximum recorded is 582.3 feet (177.5 m). Plan 1977 did not specify the minimum water level downstream of the locks. However, this level is influenced by the Lake Huron-Michigan level which varies between 575.4 to 581.0 feet (175.4 to 177.1 m) IGLD.

The width, meander characteristics and bathymetry of the Upper and Lower St. Marys River are best shown by the navigational chart in Fig. 4.2. The depths shown on the navigational chart are measured from the LWD. The depth corrections to these LWD values are given on the chart and are dependent on the month of the year.

Some field measurements of velocities in the area were carried out by the U.S. Army Corps of Engineers (COE, 1984) and the Ontario MOE (1985,1986). This information is compiled in Appendix D.

4.3. Wind Condition

Wind direction and speed have a significant effect on the surface and subsurface flow patterns of lakes and rivers. Usually, velocities increase in the direction of flow if the wind is in the same direction. An opposing wind direction to the flow direction will retard the flow velocities. The exact amount of the wind impacts on the St. Marys River’s velocity and direction depends on water depth, the length and width of the open water:
body over which the wind travels. Therefore it is important to know the prevailing wind speed and direction at the time that the field measurements were conducted since the surface flow pattern can be affected significantly. In order to get some idea of wind conditions in St. Marys River, the long term wind patterns are shown in Fig. 4.3 based on wind speed and direction recorded at the National Weather Service weather station at Sault Ste. Marie, Michigan, airport.

4.4. Ice Cover

A description of the ice conditions along the St. Marys River is provided by the U.S. Army Corps of Engineers (1986), Greene (1983) and Brazel (1971).

Since St. Marys River is used for shipping and power generation, icebreaker assistance is needed each winter. Generally speaking, the freeze over first occurs in Lake Munuscong and Raber Bay. The next site to freeze over is Mosquito Bay. Freeze over is a term used to describe the transitional process upon which the river channel at a certain point has a solid ice cover roughly 5 centimetre thick. January 2 is the mean date of water temperature dropping to 0 °C at Sault Ste. Marie (Greene, 1983).

The U.S. Army Corps of Engineers (1986) conducted ice cover observations for the period 1969-1986 for ice stations located at East Center Pier, Pittsburg Dock and Head of Little Rapids. Using the data they had collected, a statistical analysis was carried
out to establish the probable winter ice regime in the vicinity of the study area. Figures 4.4 and 4.5 show on a weekly basis, the probability of:

(a) no ice cover;
(b) greater than 50% ice cover; and
(c) greater than 80% ice cover.

This study assumes that greater than 80% ice cover can be treated as a complete ice cover situation for the purpose of modelling the fate and transport of contaminants.
Chapter 5

SIMULATION OF THE UPPER ST. MARYS RIVER

5.1. General

The primary factors involved in the flow distribution in the Upper River are gravity, wind, bed friction and the associated pressure forces. One of the causes of water movement in the deep navigational channels of the Upper St. Marys River is the inertial force exerted by the large inflows from Lake Superior through the narrow mouth at Pointe Aux Pins. In the localized shallows of Leigh Bay and Pointe Aux Pins Bay, an appreciable influence on the water circulation is exerted by wind stresses.

The initial objective of the modelling project is to describe the hydrodynamics of this area using mathematical models. Two hydrodynamic models are used in the study of the Upper River. The models used are:

(a) A steady state 3-D rigid lid model using a Galerkin finite element approach; and
(b) A time dependent 1-D free surface model using a link-node network approach.

The application, calibration and verification of each of the model are discussed in detail in this chapter.
5.2. Steady State 3-D Rigid Lid Model

A three dimensional steady state finite element model was applied to this area. The mathematical formulations were based on the three dimensional equations for conservation of mass and momentum. The principal assumptions used and the theoretical background were discussed in Chapter 3.

5.2.1. Finite Element Discretization

The outer boundary of the Upper St. Marys River must be established before the physical discretization of the area into elements is possible. In the case of land boundaries, no problems are posed in the placing of the finite element mesh. However, at the open boundaries upstream and downstream of the Upper River some of the factors dictating the establishment of this boundary include:

(a) the availability of data for the element nodes on the open boundary, which in this instance is the availability of velocity data across the open boundary;

(b) the location of the upstream and downstream boundaries are located reasonably far away from any area of interest such as the slag dump in the Leigh Bay area in order to avoid local disturbances due to instabilities or errors introduced at these boundaries; and

(c) since wind is an essential factor and its effect on the boundary conditions is unknown, the Soo Locks control structure location is a good choice for the downstream
boundary; while the upstream boundary is established at a location of greatest depth which in this instance is at the shipping channel entrance from Lake Superior to minimize uncertainties due to wind effects.

Once the outer boundary is established, the discretization by the finite element mesh can proceed. In carrying out this discretization, an attempt was made to fit the grid within a flow net. Other additional factors considered include:

(a) the rapid depth variations in the shipping channel southward towards the shoreline and northward into the two bays are modeled by placing nodes at pronounced grade changes;

(b) a fine grid of four rows of elements are placed in the shipping channel where flow gradients are expected to be great; and

(c) since triangle elements are used, caution is taken to ensure that no apex angle becomes very small which will result in high aspect ratio or stated more simply triangular elements close to equilateral triangles are used whenever possible.

The use of simplex triangular elements to discretize the Upper St. Marys River is shown in Fig. 5.1. A total of 248 elements and 157 nodes are needed for the finite element mesh.
5.2.2. Ice Cover Simulation

Since the Upper River is covered by ice for almost three months each year, it is appropriate to provide a simulation option for ice cover conditions. For ice cover conditions, the model was modified to account for zero wind shear on the water surface and for the resulting reduced eddy viscosity. The frictional resistance due to the underside of the ice cover must be considered in the model. In addition, the lower flows in the winter months and the ice thickness will reduce the depth of flow in the lake. The ice cover may cause a relatively greater depth reduction in the shallow regions of the system.

A simplified approach is taken to modify the model to incorporate these observations. The simplification treats the ice covered river as an approximate Poisseille flow condition with the hydraulic radius being reduced by half. The vertical eddy viscosity is reduced substantially to a value of 1 cm²/s and zero wind shear is imposed on the model.

5.2.3. Sensitivity, Calibration and Verification

The primary intent here is to see if the steady state finite element model is capable of simulating the main characteristics of the observed circulation patterns in the Upper St. Marys River.

The basic governing equations contain three empirical constants, i.e. the vertical eddy diffusion coefficient, the wind drag coefficient and the bottom slip coefficient, which cannot be
determined from theory alone but must be tuned by means of proper field data set in such a way to obtain the best possible agreement between the model and prototype.

The model was calibrated and verified using current meter data from the following sources:

(i) the U.S. Army Corps of Engineers;
(ii) the Ontario Ministry of the Environment;
(iii) Integrated Exploration Limited; and
(iv) aerial photographs taken of the area.

To facilitate the calibration process, a sensitivity analysis was first carried out to evaluate how the model will respond to the changes in the various system parameters.

5.2.3.1. Sensitivity Analysis

Since the wind effects (drag coefficients), the vertical eddy viscosity and the bottom slip coefficient are the primary calibration parameters, it is appropriate to use these parameters in the sensitivity study. A sensitivity analysis involving a large number of computer runs was made for these coefficients in order to assist with the calibration process.

In this analysis the inflow and outflow through the flow domain were fixed at 81,100 cfs (2,298 m³/s). A uniform wind stress was applied over the entire region with wind speed at 12 mph (19.3 km/h) while the wind directions include both NW (northwest) and ESE (eastsoutheast) winds. One way to assess the
effect of the vertical eddy viscosity, the slip coefficient and the wind stress is to study the velocity distribution for the selected elements in the model at different locations. A total of six elements as shown on Figure 5.1 were selected for this purpose. Among the six elements, elements 25, 125 and 201 are located in the deep region of the shipping channel, elements 164 and 46 are in the shallow region of Leigh Bay and Pointe Aux Pins Bay respectively, and element 98 is near the mid-section where the edge of a gyre is usually observed. The x-axis component of the velocity at the centroid of each element for the lake surface and at 0.2, 0.4, 0.6 and 0.8 of the total depth at each given location were used in the analysis. In addition, the streamline circulation pattern in the model was used to evaluate the model's sensitivity to wind direction and magnitude.

(i) Vertical Eddy Viscosity

In this analysis, the bottom slip coefficient is kept constant at 0.3, while the vertical eddy viscosity is assigned values of 1 cm²/s, 10 cm²/s, 20 cm²/s, 40 cm²/s and 80 cm²/s.

The most dramatic effect on the velocity profile occurs for low values of eddy viscosity and in this example at 1 cm²/s. The velocity profile in Fig. 5.2 (a), (c), (d) and (f) for the deep region of the lake has a double curvature while for the shallow regions as in Fig. 5.2(b) and 5.2(e) it has a parabolic profile. This profile is accentuated quite dramatically by the effect of wind shear at the lake surface. A NW (northwest) wind blowing in the general current direction will cause a tremendous increase in
the near surface velocity as shown in Fig. 5.3 while an opposing ESE (eastsoutheast) wind will tend to severely retard the near surface velocity as shown in Fig. 5.4. The effect this has on the intermediate velocity profile between the near surface and the bed is also quite dramatic. In general large increases in the velocity near the mid-depth of the lake are observed. This is more pronounced in the shallow region than in the deep region.

The velocity profiles for vertical eddy viscosities between 10 cm$^2$/s and 80 cm$^2$/s all have a parabolic profile both in the shallow and deep regions. The influence of wind direction on the near surface velocities is similar to the lower vertical eddy viscosity case but less pronounced. All the velocity profiles in this eddy viscosity range follow a definite trend depending on the wind direction and there is no sudden departure from the norm by any one particular velocity profile.

(ii) **Bottom Slip Coefficient**

The vertical eddy viscosity parameter in this instance is held constant at 10 cm$^2$/s while the bottom slip coefficient is varied in the range 0.1, 0.3, 1.0, 10.0, 50.0, 100.0 and infinity. If the bottom slip coefficient is set at infinity, it is representative of the no slip condition, i.e. when the bottom velocity is zero.
Under no wind over the lake as shown in Fig. 5.5 (b) and (e), the bottom slip coefficient has a very slight effect on the velocity profile in the shallow shore region. In the deep region, (Figs. 5.5 (a), (c), (d) and (f)) the slip coefficient has almost no effect on the velocity profile.

In the case of surface shear due to a NW wind over the lake as in Fig. 5.6, the velocity profiles in both deep and shallow regions are only slightly affected by the slip coefficient.

Although the velocity profiles away from the bed are not sensitive to the bottom slip coefficient, the near bed velocities are significantly affected. Hence, we can conclude that the model is not highly sensitive to variation in the bottom slip coefficient with the exception of velocities near the bed.

(iii) Wind Velocity and Direction

In actual fact the wind drag coefficient can be considered to be a parameter in the sensitivity analysis. However, this parameter is incorporated here (see Eq. (3.7)) in wind shear which is varied with wind velocity from 12 mph (19.3 km/h) to 24 mph (38.6 km/h). The outputs used in the sensitivity study of wind effects included:

(a) the depth-velocity profiles for each of the six selected elements;
(b) the circulation pattern of the velocity vector diagrams for the lake surface and at 2, 4, 6, and 8 tenths of the lake depths under 12 mph (19.3 km/h) and 24 mph
(38.6 km/h) winds in both NW and ESE directions; this is equivalent to varying the drag coefficient by a factor of square root of two;

(c) the streamline pattern giving a clear indication of flow distribution under different wind effects; and

(d) the use of chloropleth maps based on the depth averaged elemental velocity to give an overview of the entire study area. These maps provide useful indications of the dynamic nature of the lake in response to wind direction and magnitude.

The effect of a given constant wind on the velocity profile is most pronounced in the shallow near shore regions. The velocity profiles (Figs. 5.3 (b), (e) and Figs. 5.4 (b), (e)) for elements in Leigh Bay and Pointe Aux Pins Bay illustrate the strong influence of the wind. As mentioned earlier, if the wind direction is in the current direction the velocities are accentuated while an opposing wind tends to retard the flow near the surface.

If the wind direction is towards the shoreline, the surface velocities will be shoreward, but a reverse flow is required to satisfy continuity. This reverse flow is usually against the wind direction and will take the form of underflow or deep water return flow. This mass conservation principle is clearly visible in the circulation pattern of the velocity vector diagrams for mid-depths under both NW and ESE wind in Leigh Bay and Pointe Aux Pins Bay. In the deep region of the shipping channel, the
velocity vector diagrams in Figs. 5.7 and 5.8 indicate that the main river flow direction is dominant except near the surface where the currents respond to the wind shear direction. It is also noted that the near surface flow has a right-hand declination from the prevailing wind direction in all the cases. The velocity vector diagram in Fig. 5.9 is for the no wind case and can be used as a reference for comparison with Figs. 5.7 and 5.8. A collection of velocity vector diagrams for wind directions such as North, East, South, West and Southwest are available in Appendix E to complete the documentation for reference purposes.

The streamline circulation patterns are obtained for the following conditions:

(a) wind directions for North, East, South, West, Northwest (NW), EastSouthEast (ESE) and Southwest (SW);

(b) wind velocities at 12 mph (19.3 km/h) and 24 mph (38.6 km/h);

(c) constant vertical eddy viscosity at 10 cm²/s, constant slip coefficient 0.3 and constant flow of 81,100 cfs (2,298 m³/s); and

(d) an extended study with low flow at 54,000 cfs (1,530 m³/s) and high flow at 126,000 cfs (3,571 m³/s).

With no wind, the flow drives a large anti-clockwise gyre in the Pointe Aux Pins Bay as shown in Fig. 5.10. An almost similar circulation pattern is produced in Fig. 5.11 by a NW wind of 12 mph (19.3 km/h); however, the gyre in this case is slightly
smaller and weaker. A 12 mph (19.3 km/h) wind from either the North or the East as shown in Figs. 5.12 and 5.13 will spread the gyre across the Pointe Aux Pins Bay and into the Leigh Bay. In all these cases the eye of the gyre remains at about the same location. An exception is the ESE wind in Fig. 5.14 which appears to cause two anti-clockwise gyres. The larger gyre is in the Pointe Aux Pins Bay and the smaller one is in the Leigh Bay. The effect of the South, Southwest and West winds (Figs. 5.15, 5.16 and 5.17) is to eliminate the flow driven gyres in the two bays. These streamline results indicate that wind driven recirculation only dominates in the shallow regions such as the Pointe Aux Pins Bay and the Leigh Bay. The deep region of the main shipping channel is dominated by the normal river flow direction.

Figures 5.18 (a) to (h) indicate the extremely dynamic nature of the lake system when driven by wind thus collaborating earlier findings. The maps also indicate that for flows at 81,100 cfs (2,298 m³/s) and 126,000 cfs (3,571 m³/s) the regions of shallow depth such as Pointe Aux Pins Bay and Leigh Bay are almost identical in velocity intensities; except that for the higher flow a greater portion of the flow is in the deep shipping channel causing significant increases in its velocity. This is the case when there is no wind. When the wind speed is at 24 mph (38.4 km/h) in the ESE or the NW directions, noticeable increases of the depth averaged velocities occur in the shallow bay regions.
In order to test the sensitivity to wind speed, the wind speed was increased to 24 mph (38.6 km/h) for all the wind directions (see Figs. 5.19) with the flow kept constant at 81,100 cfs (2,298 m³/s). A comparison of the streamline patterns indicated no significant deviation from the general pattern in the previous results except now the strength of the gyre is greater. Similar conclusions are obtained with the high flow of 126,000 cfs (3,571 m³/s) and as expected the low flow of 54,000 cfs (1,530 m³/s) has the opposite effect of weakening the strength of the circulation. It is therefore concluded that the general circulation pattern is very sensitive to wind direction; increasing wind speed reinforces the gyre pattern.

5.2.3.2. Summary of Findings

The general effect of the vertical eddy viscosity coefficient is to alter the shape of the velocity profile. Decreasing the vertical eddy coefficient from 10 to 1 cm²/s will dramatically change the velocity profile. This effect is amplified if wind shear is present. The effect reduces progressively as the vertical eddy viscosity coefficient increases from 10 cm²/s to 80 cm²/s. The bottom slip coefficient was varied between 0.1 and infinity with only slight effects on the velocity profile.

Finally, the wind magnitude (or drag coefficient) and direction are by far the most influential parameters affecting the velocity profile in the shallow bays. Under the prevailing wind direction, the velocity profile in the shallow regions are
predominantly in the wind direction. However, in order for the mass to be conserved in the model, there is a return flow near the bottom of the shallow bays against the prevailing wind direction towards the deeper water. Since there is a steady flow from west to east through the lake, the velocity profile in the deep shipping channel tends to be less prone to velocity reversal effects.

5.2.3.3. Calibration

The calibration process was initiated by selecting the model parameters for wind (speed and direction) and flow rate (81,100 cfs or 2,298 m³/s) to agree with the U.S. Army Corps of Engineers’ (1984) field data. Since the field measurements by the U.S. Army Corps of Engineers were taken in the month of September, the U.S. National Oceanic and Atmospheric Administration map on the Upper St. Marys River (NOAA - St. Marys River map no.14884, 1980) was used to adjust water level variations from the low water datum in the model.

The Upper St. Marys River was divided into three areas by the U.S. Army Corps of Engineers in their data collection programme. The programme collected information from each area on separate days. Accordingly the simulations were carried out independently for each area using the conditions for the day of measurement.

In the calibration process, the only model parameters that can be tuned are the vertical eddy viscosity, the bottom slip coefficient and the wind drag coefficient. Since the earlier
sensitivity analysis indicated that the slip coefficient does not play a dominant role it was kept constant at the value of 0.3. The effect of the wind drag coefficient (see Eq. 3.7) is incorporated in the wind stresses. The wind speed was held constant for two cases in accordance with the U.S. Army Corps of Engineers' data collection programme which was carried out on separate days with different wind conditions. The two cases were prevailing wind at 12 mph (19.3 km/h) in the NW (northwest) and the ESE (eastsoutheast) direction.

Hence, the only remaining parameter to be tuned in the calibration process is the vertical eddy viscosity. The sensitivity study had indicated that this parameter will affect the velocity profile. Based on the sensitivity analysis, the most suitable value was 10 cm²/s which would allow the model to give velocity profiles fairly representative of the field data.

The initial stage of the calibration concentrated on the direction and magnitude of the flow conditions in the shipping channel. This approach is taken with the assumption that the shipping channel, which is the deepest region in the study area, will be the least responsive to wind conditions. The calibration process initially looks at the two dimensional case. This is accomplished by using the depth averaged velocity comparison between the model and the composite velocity measurement map from the U.S. Army Corps of Engineers. The finite element mesh is overlaid on the U.S. Army Corps of Engineers velocity data map for the composite velocity case. The composite velocity case is
the average of current meter measurements taken at 2, 4 and 8
tenths of the total river depth at each given location below the
lake surface.

The U.S. Army Corps of Engineers' data base is extremely
useful for a quantitative assessment of the current velocities in
various parts of the study area. The depth average velocities and
directions in the main shipping channel are in agreement with the
model as shown in Figs. 5.7 (f), 5.8 (f) and 5.20 (d) for both NW
and ESE wind at 12 mph (19.3 km/h). The circulation pattern in
the Pointe Aux Pins Bay is also well represented for a 12 mph
(19.3 km/h) wind from the NW ( see Fig. 5.7(f) ). The only
exception is the Leigh Bay under a 12 mph (19.3 km/h) ESE wind
which seems to be different from the model. The U.S. Army Corps
of Engineers' current velocities in the Leigh Bay at all depths
in Figs. 5.20 (a) to (d) indicate a strong southeasterly current
against the wind. The U.S. Army Corps of Engineers measured
current velocities at 2, 4 and 8 tenth of the river depth vary
from 2 ft/s (60.9 cm/s) near the surface to 3 ft/s (91.4 cm/s)
near the bed for the entire Leigh Bay. These, when integrated,
violate the mass conservation requirement; there should be a
general decrease in velocities at all depths in the bay to
reflect the actual inflow and return flow to the bay. Hence, the
U.S. Army Corps of Engineers current velocities in the Leigh Bay
must be treated with some reservation until further field data
from other sources can corroborate their measurements.
On the other hand, the model's predicted current velocities and directions in the Leigh Bay do conserve mass, showing clearly a return flow below a depth at six tenths of the total depth all the way to the bed. Figures 5.14 and 5.18(d) indicate a weak gyre in this bay with very low velocities of 0.1 to 0.5 ft/s (3.0 to 15.2 cm/s).

It should be noted that a successfully calibrated model is not automatically verified. It is also important to be able to demonstrate that the selected empirical constants are fairly universal so that further sets of field data from other sources can be simulated as well as the original set.

5.2.3.4. Summary of Findings

The calibration of the model was accomplished by adjusting the same model parameters that were used in the sensitivity analysis. Using both quantitative and qualitative comparisons, the available field information from the U.S. Army Corps of Engineers mentioned above is used to calibrate the model to reproduce as closely as possible the field data information under the wind and flow conditions at the time the data were collected.

The calibrated vertical eddy viscosity was 10 cm²/s; the slip coefficient was 0.3 and the wind drag coefficient was 3.0 x 10⁻⁶. These values were confirmed by comparison of calculated and measured velocities at different depths at various locations in the lake. A few cases are shown in Table 5.1. With the exception of the shallow regions of Leigh Bay and Pointe Aux Pins
Bay where the model gave poor correlations, the model gave a good representation of the velocities in the other regions of the lake.

5.2.3.5. Verification

Similar to the calibration results, the model gives low current velocities in the Leigh Bay and the Pointe Aux Pins Bay regions under no wind condition. These generally low current velocities in the bays are substantiated by the Ontario MOE (Ontario Ministry of the Environment, 1985) measurements which reported no noticeable current velocities at two stations in the Leigh Bay and one station in the Pointe Aux Pins Bay as shown in Table 5.2. The location of these stations is given in Appendix D. The Ontario MOE (1985) used a relative scale of strong, moderate, slight, negligible and none to describe their measurements. It is presumed that the Ontario MOE measurements were taken under light or no wind conditions.

In 1986 the Ontario MOE placed two current meters in Leigh Bay to further confirm the magnitude of the velocities in the bay area. The raw data was examined and compared with the model currents. All the 1986 data was consistent with the 1985 MOE observations and in good agreement with the model as shown in Table 5.3.

A statistical comparison was carried out using the numerical values from Table 5.3. The Student’s t test for paired data is used to determine whether there is a significant difference between the velocities obtained by field measurements and those
computed by the model (Kennedy and Neville, 1976). A 5% level of significance is selected for evaluating the test using two groups of data. Each group of data is drawn from the same location. The results are summarized in Table 5.4. The mean of the differences (i.e. \( \left( \frac{P_i - O_i}{n} \right) \)) are 1.125 for the Leigh Bay and 11.25 for the other regions. The standard deviations of the differences are 2.981 and 7.805 for the Leigh Bay and the other regions respectively. The standard deviations of the mean are 1.4904 and 3.9025 respectively. The Student's t test on the two groups of paired data indicated that there are no significance differences between the paired data at the 5% level of significance. In the Leigh Bay, the value of \( t_{\text{model}} \) is 0.746, while in the other regions \( t_{\text{model}} \) is 2.883. The value of \( t_{\text{table}} \) is 3.182 for both cases since the sample size in each case is four.

A further verification of the predicted circulation pattern is the aerial photographs of the entire Upper Reach area taken under an ESE wind. The model's surface velocities in Fig. 5.8 (a) are compared with the aerial photograph in Fig. 5.21. The comparison shows remarkable agreement in the circulation pattern. Most noticeable of all is the similar strong helical pattern from the surface of the deep shipping channel towards the Leigh Bay under an ESE wind.

5.2.3.6. Summary of Findings

The verification process was accomplished by direct comparison of the model current and circulation pattern with actual field data. Since the field data from the U.S. Army Corps
of Engineers was used for model calibration, it is necessary to use some other source of data to verify the model. The only available data not used in the calibration process are from the Ontario MOE (1985, 1986) and Integrated Exploration (1985), which is an independent consultant group. The procedures and outcomes of the verification process are tabulated in Table 5.5.

The field data needed for a quantitative verification is rather scarce because most of the available data are qualitative in nature. Therefore, it is recommended that further verification of the model is still needed when new data are available. All of the data sources used in the Table 5.5 are given in Appendix D for future reference.

5.2.4. Steady State Rigid Lid Model Results

The hydrodynamic model can be used to simulate a number of different uniform and steady surface wind stress conditions. The wind magnitude and direction can be chosen to be representative of certain storms whose effects on the circulation patterns are of interest. The long-term fluctuations in the lake level can be represented by adjusting the inflow or the outflow and the water elevations in the model. The model results are presented for two seasonal conditions:

(a) when there is no ice cover over the lake, and

(b) when there is a complete ice cover.
5.2.4.1. With No Ice Cover Results

Figure 5.7(f) shows the depth averaged velocity vectors with the prevailing NW (northwest) wind of 12 mph (19.3 km/h) and a river flow of 81,100 cfs (2,298 m³/s). The corresponding stream flow pattern is shown in Fig. 5.11. A weak counter clockwise gyre is predicted in the Pointe Aux Pins Bay. The U.S. Army Corps of Engineers' current meter data also indicate a gyre in this region.

The predicted circulation pattern for a 12 mph (19.3 km/h) north wind is shown in Fig. 5.12. The previously mentioned gyre has increased in size and strength under this wind.

Figure 5.13 shows the predicted circulation pattern for an east wind. This simulation indicated a further increase in the size of the gyre; in this case the gyre affects both Pointe Aux Pins Bay and Leigh Bay.

Figure 5.14 shows the circulation pattern under a ESE wind. Two weak gyres appear in this case, one in Leigh Bay and one in Pointe Aux Pins Bay.

The gyres virtually disappear under a south wind as shown in Fig. 5.15. A large fraction of the main channel flow is advected into the Pointe Aux Pins Bay and Leigh Bay under this wind condition. This would result in the flushing of these bays during these wind episodes.

Figure 5.16 shows the circulation for a SW (southwest) wind which produces somewhat similar conditions to a South wind.

Figure 5.17 shows that the flow pattern for a West wind is similar to the south and southwest cases.
Figure 5.10 shows the circulation pattern under calm conditions on the lake. A weak counterclockwise gyre is predicted in Pointe Aux Pins Bay under calm conditions. In general, the wind direction has a very significant impact on the circulation patterns in the shallow regions where gyres are produced. The magnitude of the wind will correspondingly increase or decrease the strength of the circulation current velocities. The dynamic nature of the model under different wind conditions are clearly illustrated by the chloropleth maps (Figs 5.18 (a) to (h)).

5.2.4.2. With Ice Cover Results

The case of complete ice cover is simulated. Since no calibration or verification is possible for this case, use of the ice cover results should be limited only to qualitative observations. The velocity vectors under an ice cover are shown in Fig. 5.22. No gyres are predicted while the highest current velocities remain in the main shipping channel. In the shallow region of Pointe Aux Pins Bay and Leigh Bay, the current velocities are extremely low due to the increased frictional resistance to flow in the shallow depths. These observations are clearly illustrated in the chloropleth map in Fig. 5.23. The streamline circulation pattern under ice cover in Fig. 5.24 also shows no gyre and extremely low flow in the shallow regions.
5.3. USEPA DYNHYD4 - Unsteady 1-D Free Surface Model

The EPA DYNHYD4 is a one dimensional time dependent hydrodynamic model. It is one of the large class of "link-node" models whose main advantage lies in its flexibility of application to a relatively complex study area using a network of one dimensional channels.

The flow in a link or channel is computed by using the one dimensional momentum and continuity equations together with the Manning's formula for flow in open channels. The water surface elevations at the nodes at each end of the link is computed at each time step. Much of the attraction of the link-node method is its ability to combine in one program a quasi-two-dimensional flow in an open water such as a bay, and a network of one dimensional channels in a channelized portion of the same water body.

5.3.1. Finite Difference Discretization

The Upper St. Marys River can be easily discretized by a network of junctions and one-dimensional channels or links. The main shipping channel and both the Leigh and Pointe Aux Pins Bays are discretized as one dimensional segments even though the flow in the individual bays might have important two-dimensional aspects. The distribution of nodes (i.e. junctions) in the bays can define the equivalent of a two-dimensional grid, although the program is not truly two-dimensional because the flow is confined to links between nodes.
Such a link-node network is illustrated in Fig. 5.25 and 5.26 for the Upper St. Marys River. If the two networks of junctions and channels are superimposed on top of each other, it can be easily observed that the channel numberings are given between two junction numbers connecting the ends of the channel. A total of 51 junctions and 81 channels are used to discretize the Upper St. Marys River with an open downstream boundary at the Soo Lock control structures and an open upstream boundary where Lake Superior enters the study area. Since seasonal flow data are available from the U.S. Army Corps of Engineers, the nodes at the open boundary upstream (i.e. Lake Superior entrance) are prescribed with inflow as a boundary condition. The downstream open boundary is prescribed with a reference surface elevation (e.g. zero) reflecting a non-dynamic water level at the control structure location.

5.3.2. Calibration and Verification

Due to the lack of field data, it was decided that the model would be calibrated to agree with the long term average elevations documented by the U.S. Army Corps of Engineers which are shown in Fig. 5.27. However, it should be pointed out that a good agreement in the water surface elevations does not imply that the velocities are automatically calibrated. It can be seen from Fig. 5.27 that the difference between the upstream elevation at Lake Superior and the downstream location of the Soo Locks (the St. Marys Falls) is 0.16 feet (about 5.0 cm). Since the inflow is kept constant at 81,100 cfs (2,298 m³/s), the primary calibration parameter is the Manning’s roughness coefficient. The
value of the Manning’s roughness coefficient is highly variable depending on such factors as bed roughness, vegetation, channel irregularities in cross-section or shape, obstructions and depths. The value typically varies between 0.01 to greater than 0.08 (Ambrose et al., 1988).

In calibrating DYNHYD4 for the Upper St. Marys River, it is noted that changing the roughness coefficient in one channel can affect both the upstream and downstream channels. Several computer runs were carried out varying the roughness coefficient systematically in order to calibrate the model. A value of 0.04 in the main shipping channel and a value of 0.02 along the shoreline gave the best agreement in the elevation gradient. At the downstream region just before the Soo Locks on the Canadian side, a value of 0.01 was found to be necessary to bring the river profile inline with the U.S. Army Corps of Engineers data.

On completion of the calibration process using the Upper St. Marys River water level profile (Fig. 5.27), the next step is calibration of the velocities. The composite velocities maps from the U.S. Army Corps of Engineers’ field data, which are averages of velocities taken at 2, 4 and 8 tenths of the river depths below the water surface, were used for this purpose. The velocities in the main shipping channel agreed with the field data. Only qualitative findings were possible for the two shallow bay areas. The velocities in the bay areas were low which agreed with the previous model. A comparison of the velocities is given in Table 5.6. A Student’s t test for paired data is applied to the DYNHYD4 results and the corresponding field measurement values. The statistical test indicated that there are no significant
differences between the field data and the DYNHYD4 values at the 5% level of significance for both the Leigh Bay and the shipping channel.

The verification of the model was not carried out because of the lack of field data for the shipping channel. Due to the one dimensional nature of the model, the flow directions of the channels are predetermined by the modeller. This can be approximated reasonably well for the main shipping channel since we know its predominant flow direction. However, the same approximation cannot be carried out for the bay regions where circulation gyres can form. Although additional data for verification purpose are available for the bay regions, a proper verification is not possible for the bay regions.

5.3.3. Summary of Findings

After imposing constant inflow at the upstream open boundary and constant surface elevation at the downstream open boundary, the Upper St. Marys River was calibrated by adjustment of the Mannings roughness coefficient for no wind. Good agreement was obtained for the Upper River water surface profiles in the calibration process.

In the calibration of the velocities, the U.S. Army Corps of Engineers' composite current velocity data were compared with the model's values. Qualitative agreement in the magnitude of the velocities were obtained for both the Leigh Bay and the Pointe Aux Pins Bay regions. Since the flow directions were imposed by the orientation of the channel directions, it is not possible to make conclusive comments on recirculation patterns. However, in
the main shipping channel, good agreement along the entire channel was obtained for the model. The channel directional orientations in this case were appropriately aligned with the expected main flow direction.

The verification of the model is not possible since no separate sets of velocity data are available for the shipping channel. Although there are some verification data for the bay regions, the flow directions of the bay regions are predetermined by the orientations of the channels. Hence a meaningful comparison is not feasible since this is a one dimensional model.

5.3.4. USEPA DYNHYD4 Model Results

Since surface elevations and velocities are computed by the model at the junctions and channels respectively, the results are presented graphically in the same fashion. Figure 5.28 shows the surface elevations in centimetres at each node or junction. It can be seen that the drop in the surface gradient starting at Lake Superior to the Soo Locks is almost exactly 5 centimetres on the U.S. side of the Soo Locks as well as at the Canadian side of the Power Canal.

The velocities in centimetres per second are given in Fig. 5.29. It can be seen that the main shipping channel velocities range between 23 cm/s (0.8 ft/s) and 47 cm/s (1.5 ft/s). In the Leigh Bay area, velocities are about 13 cm/s (0.4 ft/s) which are generally the same as the values obtained by the previous model.
Chapter 6

SIMULATION OF THE LOWER ST. MARYS RIVER

6.1. General

The flow in the Lower St. Marys River is strongly influenced by the large inertial forces exerted by the St. Marys Rapids and the hydro-electric power canals on both the Canadian side (Great Lakes Power Corporation Plant) and the U.S. side (U.S. Govt. Hydro-electric Plant) of the river. The Lower River is a nonuniform natural channel with slightly over half of its width dredged to a minimum depth of 28 feet (8.5 metres) for the passage of ships mainly on the U.S. side of the river. However, very high velocities occur along the Canadian half of the river up to the Lake George channel north of Sugar Island. The curvature of the Canadian shoreline causes secondary flows to traverse across to the U.S. shoreline in the Lake George channel due to centrifugal forces.

The velocity field data on the Lower River is available from the U.S. Army Corps of Engineers (1984). The data also indicate the presence of some dead zones and re-circulation zones in the river due to natural or man-made protuberances from the shoreline.

In contrast to the Upper St. Marys River, the modelling objectives for the Lower St. Marys River include the simulation of both the hydrodynamics and the pollutant transport problems.
For the hydrodynamics, the depth averaged model by McCorquodale et al. (1983) is used to drive the KETOX model, while the unsteady 1-D DYNHYD4 is used to drive the WASP4 model. For the pollutant transport study, both the KETOX and the WASP4 (TOXI4 component) models are applied to the Lower River to simulate point source discharges on the Canadian side. The pollutant selected in this study is phenol. The simulation efforts concentrated on field data available for phenol in 1974 and 1983. The 1974 field data is used to calibrate the models while the 1983 field data is used for verification of the models.

The application and coupling of these models including the calibration and verification aspects will be covered in detail in the sections to follow in this chapter.

6.2. KETOX - Steady State 2-D Dispersion Model

The Lower River is simulated by KETOX (McCorquodale and Yuen 1987) which is a model that has a steady state depth averaged hydrodynamic sub-model coupled to a convection-diffusion (mixing) sub-model. KETOX has evolved from the earlier modified K-E model which had performed well in successful applications to the St. Clair River, the Detroit River and the Niagara River.

The objectives of the simulation are to be able to predict the fate as well as the impact of toxic chemicals in the Lower River system. This not only involves the simulation of the exposure levels of the chemical in the water column but also the bed sediments as well as the bioaccumulation of the chemical in the biota.
Due to the availability of field measurement data, the pollutant selected as the most reliable one for model calibration is phenol. Besides being a toxic chemical, phenol is known to taint fish flesh and it is one of the 129 most commonly discharged priority pollutants in the USEPA list of priority pollutants (Mills et al., 1982).

The model requires information on the sources of phenol discharges to the Lower River. The Ontario MOE (Ministry of the Environment, 1974) has reported that the discharges from the Algoma Steel Corp. Ltd. and Abitibi-Price Paper Mill into a common terminal basin just downstream of the Great Lakes Power Corporation Plant have contributed to the high phenol levels in the Lower River. Frequent equipment breakdowns in the coke oven by-product plant of Algoma Steel is largely responsible for the elevated levels of phenolic compounds.

The Ontario MOE (1974) has collected both loading and ambient concentration data for phenol at various stations along the river in the years 1973-74 and 1983. Figure 6.1 summarizes the 1973-74 ambient phenol concentrations documented by the Ontario MOE as presented by Hamdy, Kinkead and Griffiths (1974). Figure 6.2 shows the estimated variation in phenol loading to the terminal basin of the Algoma outfall. The phenol loads for 1973-74 are summarized in Table 6.1. The loading data as supplied by the Ontario MOE (1985) for the year 1983 is given in Table 6.2. A map of the Lower St. Marys River showing the locations of
these industrial waste discharges as well as the municipal 
intakes and outfalls on both the Canadian and U.S. shore is given 
in Fig. 6.3.

6.2.1. Finite Difference Discretization

The Lower St. Marys River is discretized into a system of 
reaches as shown in Fig. 6.4 in order to handle the occurrence of 
splitting of flows by the presence of islands, the confluence of 
flow at the end of islands and the occurrence of natural river 
curvature in the study area. The upstream boundary is chosen to 
extend further upstream beyond the pollutant source at the Soo 
Locks. The upstream boundary is then prescribed with the ambient 
phenol concentrations which are about 2.3 ug/L in 1974 and 0.3 
ug/L in 1983. The downstream boundaries extend across two 
channels, one north of the Sugar Island into the Lake George 
channel and the other channel west of Sugar Island into Lake 
Nicolet.

A total of 18 reaches are used to model the Lower St. Marys 
River as shown in Fig. 6.4. The splitting of flows occurs from 
Reach 1 into 2 and 3, Reach 2 into 4 and 5, Reach 3 into 6 and 7, 
and Reach 19 into 13 and 14. The confluence of flows occurs at 
Reaches 8, 9, 11 and 16. The power canals are assumed to produce 
a uniform mixing of their initial contaminant distribution. The 
downstream part of Reach 4 contains the terminal basin diffuser 
from Algoma Steel.
In preparing for the forward marching numerical scheme, each reach is further discretized by the modeller into cross-sections. The distance between cross-sections is determined by the modeller, which in this case is selected as 2000 feet (609.6 metres) apart. With this spacing, the user then generates as many cross-sections as is necessary to fit each entire reach. If necessary, this grid spacing can be further subdivided by setting parameters within KETOX; this may be required to achieve numerical stability. A total of 15 nodes are assigned to each cross-section in the lateral direction. The nodes lie on the boundary of assigned stream tubes. The physical spacing of the nodes is computed internally by the program which does a numerical integration of the flow across the cross-section. However, the magnitude of the 15 stream tube values are assigned initially by the user for the model. It should also be pointed out that in computing the lateral node spacings, the model requires information on 40 river depth values to be specified by the user for each of the cross-section. The 40 depths are further linearly interpolated by the program into 118 depths before numerical integration for the flow proceeds.

6.2.2. Calibration

There are two aspects to the calibration of the KETOX model. The first aspect is the calibration of the velocity distribution for the hydrodynamic sub-model, while the second is the calibration of the dispersion level for the pollutant.
The hydrodynamic component of KETOX was calibrated using U.S. Army Corps of Engineers' (COE, 1984) field data based on current meter measurements and drogue surveys. In computing the velocity distribution, the model uses a shape function with river specific parameters which can be set to best reproduce the observed lateral velocity distribution. The calibration parameters previously obtained for the St. Clair River studies (McCorquodale and Ibrahim, 1985) were used as first approximations for the St. Marys River. Some of these parameters include the Manning’s bed roughness, the river bed slope and an empirical exponent (n1) to adjust the shape factor that accounts for the river bank effects. The radius of curvature parameter was adjusted in a series of computer runs based on a flow of 104,000 cfs (2,945 m³/s). These parameters were then used to predict the river velocity distribution which was then compared with the observed COE (1984) velocities. A fully developed lateral velocity distribution was used initially. It was found that the St. Clair River parameters were acceptable for the St. Marys River except in zones of highly complex flow and in recirculation zones.

It was noted that the recirculation zones, which are mainly due to hydroelectric power discharges, were excluded from the main stream flow. Some predictions of the fully developed velocity profiles and the corresponding COE measured values across the Lower River are shown in Figs. 6.5 (a) to (g). Based on the fully developed option, it can be seen that reasonable agreement between the measured and the predicted velocities is
obtained in Reaches 12 and 13. However, the velocity distributions in Reaches 8 to 11 are strongly affected by hydropower discharges. The model tended to smooth the jet-like nature of the velocity distribution in these Reaches.

The momentum equations in the model were solved in the parabolic form using a forward marching solution algorithm (McCorquodale et al., 1983; Rodi, 1984). The consequence of this simplification is that zones of recirculation phenomenon are not properly simulated. In order to represent the zones of recirculation phenomenon, the hydrodynamic sub-model of KETOX was revised to incorporate the dissipation and dispersion of the excess momentum from the hydropower discharges (Rodi, 1984). The numerical solution is performed in the stream function coordinate system, thus ensuring that mass is conserved. A transformation is provided to convert from stream function to physical coordinates. The details of this revision to the hydrodynamic sub-model of KETOX is described in Chapter 3. In the previously mentioned set of Figs. 6.5 (a) to (g) are plotted the excess momentum corrected velocity profiles for comparison with the COE measured values. A significant improvement over the original velocity prediction is noted, especially near the power tail-races. This revision provides sufficient flexibility so that the modeller can simulate simple confluences which have different average velocities.

The contaminant dispersion sub-model of KETOX was calibrated using the 1974 Ontario MOE (Hamdy et al., 1974) information on phenol loadings, ambient and other sample measurements along the river including some transects across the river samples. Since
the dispersion sub-model is based on the work of Rodi et al. (1978) and Rodi (1984), the calibration constants suggested by Rodi were used as first approximations for KETOX. Then the phenol loading data and field observations presented by Hamdy et al. (1973-74) were used to adjust Rodi’s constants. The adjusted calibration constants that produce the best results for the Lower St. Marys River by KETOX as well as those used by Rodi are tabulated in Table 6.3 for comparison. The meaning of each of these empirical constants is dealt with previously in Chapter 3 except for "n" which is Manning’s roughness coefficient and "k" which is Karman’s constant.

A comparison of the measured and predicted phenol concentrations at selected locations along the river is given in Fig. 6.6. At each selected location two values are given, one on the Canadian shoreline and the other on the U.S. shoreline. In order to obtain these comparisons, a series of computer runs were made with KETOX to represent the variation in the loading and thus to establish the upper and the lower bounds (standard error) on the predictions. Using the 1970-1974 loading data for phenol and a ±35% variation in the outfall discharges, randomly selected combinations of total load and discharge were simulated.

A statistical analysis using the normal distribution test (Kennedy and Neville, 1976) on the significance of the differences between the Ontario MOE measured values in Fig. 6.6 and the predicted values by KETOX is given in Table 6.4. Using the 5% level of significance, the test indicated no significance differences between the values obtained by KETOX and the Ontario
MOE measured values for all the locations on the Canadian shoreline. On the U.S. shoreline, all the tested locations indicated no significance differences at the 5% level of significance except for two locations. At location SMD-5.3W on the U.S. shoreline southwest of Sugar Island, the test indicated no significance difference at the 1% level of significance (i.e. 99% confidence limit band) instead of the 5% level. At location SMD-5E on the U.S. shoreline north of Sugar Island, the test indicated a significance difference between the measured and predicted values. It should be noted that these comparisons have neglected the possible errors in the predicted concentrations.

A series of comparison plots are also given in Figs. 6.7 (a) to (k) for different locations based on 1974 phenol loadings and an average flow of 81,100 cfs (2,298 m³/s). It can be seen that excellent correlations of the predicted values and the measured values by the Ontario MOE (1974) are obtained indicating good calibration of the KETOX model. A second series of comparison plots at similar locations to the previous case are given in Figs. 6.8 (a) to (k) to illustrate the effect of a high flow of 126,000 cfs (3,571 m³/s) on the 1974 ambient concentration. These comparison plots indicate the combined effect of the higher dilution and greater advective transport.

Finally, the simulated concentrations were expressed as relative concentration and compared with the Ontario MOE (1974) measurements in Fig. 6.9 along the Canadian shoreline. The plot shows very good agreement between the predicted values and the clusters of measured values for 1974 which is expected since the
model is calibrated with these data. The statistical analysis involves plotting the 95% confidence limits for the mean estimated value of the dimensionless concentration parameter (Kennedy and Neville, 1976). The plot shows that most of the calibration data falls within the 95% confidence band which is obtained using the Ontario MOE field data. Hence the values computed by the model is statistically shown to agree with the field data.

6.2.3. Verification

Since both the depth averaged current velocity measurements and drogue surveys data from the U.S. Army Corps of Engineers were used to calibrate the hydrodynamic sub-model, this component of the model cannot be considered to be verified at the moment. However, so far the model has performed well but the model verification will be possible only if new field data are available in the near future.

The 1983 Ontario MOE field measurements were next utilized to validate the calibrated model. The degree of verification is illustrated in Fig. 6.9 which is a dimensionless plot of the measured and predicted phenol concentrations along the Canadian shoreline starting from the Terminal Basin outfall location for the years 1974 and 1983. Since the 1974 data was used for calibration, the comparison for verification should be the plots of the 1983 group of data points. An acceptable agreement is evident. The statistical analysis for these data is described below.
A series of comparison plots for different locations with transects across the river are given in Figs. 6.10 (a) to (d) based on the 1983 Ontario MOE field measurements. It is noted that the samples from the Ontario MOE have random fluctuations over a mean concentration value. Looking at the mean value it is clear that only satisfactory correlation between predicted and measured values are given by these plots. At present no explanation can be given for the random background noise in the collected samples. The loading is random and the background is also random and a relatively large fraction of the total load. An estimate of the 1974 random loading pattern of Fig. 6.2 at the Algoma Terminal Basin gives a mean value of 255 kg/d (or a pipe concentration of 709 ug/L) and a root-mean-square (rms) value of 62.3 kg/d (or a pipe concentration of 173 ug/L). This indicates that the random loading pattern fluctuates approximately 25% about the mean value. The rms value gives some indication of the large deviations that may randomly occur in the loadings.

The normal distribution test is used to determine whether there are any significance differences between the 1983 Ontario MOE measured values and the values predicted by KETOX. The results are tabulated in Table 6.5 for a 5% level of significance. The results indicate that there are no significant differences between the two sets of data at all locations on or near the Canadian shoreline; the only significant differences were for two stations on the U.S. shoreline. One of the stations is in Reach 10 and the other is in Reach 12. It is also noted that two other stations on the U.S. shoreline, one in Reach 12
and another in Reach 19 passed the test at the 1% level of significance instead of the 5% level used for all the stations tested.

6.2.4. Summary of KETOX Results

The hydrodynamic sub-model of KETOX was calibrated using the U.S. Army Corps of Engineers current and drogue surveys data. At this stage of the study, the model is performing quite well and can be used to simulate different flow conditions. A further modification to the model is included to allow for the simulation of possible ice-cover conditions. Since the river is covered with ice for almost three months each year, the flow in the Lower River is reduced during this period due to the ice thickness and possibly ice jams further downstream caused by the natural pile up of broken ice. Also the frictional resistance to river flow is increased due to the roughness of the underside of the ice cover. A rather simplified approach to simulate ice cover is to reduce the hydraulic radius by half thus approximating the Poiseuille flow condition. Although the method is not totally correct, it does provide a simple means to assess ice cover conditions.

The dispersion sub-model was calibrated using the 1974 Ontario MOE phenol loadings and ambient measurements. The model was subsequently verified with the 1983 Ontario MOE phenol data on loadings and transect samples from the river. It is evident that acceptable accuracy in the prediction of phenol levels in the Lower St. Marys River is achieved by the model. Further
verification is needed for the model for contaminants that are more hydrophobic than phenol; field data are now being assembled by the Ontario MOE for this testing.

6.3. USEPA DYNHYD4 — Unsteady 1-D Free Surface Model

In the KETOX model the hydrodynamics information of the Lower St. Marys River is computed within KETOX itself and internally coupled to the other components. A similar approach is used here where the hydrodynamic information computed by DYNHYD4 is used to drive the TOXI4 model. The proper distribution of flow quantities is needed as input information for the cell segments of TOXI4. The cell segments are arranged to coincide with the junction network of DYNHYD4. In order to ensure that TOXI4 will give good results, the computed flow distributions from DYNHYD4 must be fairly representative of the actual flow conditions for the Lower River since advective transport of the pollutant is an important factor in the simulation.

6.3.1. Finite Difference Discretization

Most of the concepts on the discretization process for DYNHYD4 have been discussed in Chapter 5 for the Upper St. Marys River. In contrast to the previous case, the physical characteristic of the Lower St. Marys River is that of a river with minimal bay areas. Since the river bathymetry is essentially comprised of a deep shipping channel (28 feet or 8.5 metres) and a shallower channel on the Canadian side (20 feet or 6.1 metres), the junction network will be two rows of nodes running along the
flow direction of the channel as shown in Fig. 6.11. The resulting channel or link network is given in Fig. 6.12 with the ends of each channel connected by two corresponding junctions. A total of 30 junctions and 38 channels are used to discretize the Lower St. Marys River.

The nodes along the upstream open boundaries located at the Soo Locks are prescribed with inflow values in accordance with available flow distribution at the Locks as described in Chapter 4. The nodes along the open downstream boundaries are prescribed as fixed surface elevations chosen as 0.0 m in this case. There are four inflow locations at the upstream boundary and similarly four outflow locations at the downstream boundary.

6.3.2. Calibration and Verification

Since the main source of field data available is from the U.S. Army Corps of Engineers (COE, 1984), the calibration process was carried out for the 1983 flow distribution conditions at the upstream Soo Locks location. As in the previous calibration process for the Upper St. Marys River, the only primary calibration parameter that need to be varied is the Manning's roughness coefficient since the upstream inflows were kept constant at 100,000 cfs (2,832 m³/s).

The composite velocities which are depth average values of the U.S. Army Corps of Engineers' current meter measurements taken at 2, 4 and 8 tenth of the river depth (below the water
surface) at each location are used to calibrate the model. The junction network is overlaid on the U.S. Army Corps of Engineers' data map as shown in Fig. 6.13 for this calibration process.

The calibrated velocities for the entire network of the Lower St. Marys River is shown in Fig. 6.14, while the computed surface elevations are shown in Fig. 6.15. It can be seen that the correlation between the calibrated velocities in Fig. 6.14 and the measured values in Fig. 6.13 is quite good. This comparison of the velocities in the calibration of DYNHYD4 is also tabulated in Table 6.6. A statistical analysis using the Student's t test for the paired data (n = 11) between the U.S. Army Corps of Engineers' current meter velocities and the computed velocities by DYNHYD4 was carried out. The mean value for the difference is 0.1291. The standard deviation of the difference is 0.28801, while the standard deviation of the mean is 0.0868. With a degree of freedom of 10, the value of $t_{\text{table}}$ is 2.228 at the 5% level of significance (Kennedy and Neville, 1976). The value of $t_{\text{model}}$ is 1.287 indicating that there is no significant difference between the paired data at the 5% level of significance. A visual inspection of the computed flow pattern indicates fair agreement with available field data with no abnormalities.

The verification of the model presents a problem, since only data on surface velocities based on drogue measurements were available from the U.S. Army Corp of Engineers. However, these data are useful in giving general quantitative verification of the regions of high and low flows in the study area. A comparison
of the drogue surveys with the model results indicate good general agreement of velocities, however, further verification of the model is necessary when additional field data is available. The drogues survey data is documented in Appendix D for future reference.

A statistical comparison between the velocities of KETOX and DYNHYD4 using the Student’s t test for paired data was carried out with the results shown in Table 6.7. Using a 1% level of significance and 10 degrees of freedom (n = 11), the test indicated that there was no significance difference between the velocities obtained by KETOX and DYNHYD4.

6.3.3. Summary of DYNHYD4 Results

For the hydrodynamic component, the calibration results are good for the 1983 flow conditions. It is not possible to make conclusive verification of the model due to insufficient field data. However, so far the computed results give no indication of abnormal flow patterns that would shake our faith in the results.

After calibration and limited verification of the model based on the 1983 flow conditions, DYNHYD4 was also used to compute the flow conditions for 1974 based on the flow distribution at the Soo Locks in 1974. It is assumed that the calibration parameters based on the 1983 values for DYNHYD4 will apply equally as well for the 1974 flow conditions. The resulting computed velocities and surface elevations for the 1974 flow
conditions are shown for the networks in Figs. 6.16 and 6.17. No verification for the 1974 flows is possible since there are no field data available.

6.4. USEPA TOXI4 – Unsteady 3-D Transport Model

The second simulation model chosen to compute the dynamic pollutant migration of the Lower St. Marys River was TOXI4 which is a kinetic transport sub-model of the main WASP4 model. TOXI4 is able to handle all the required physical and chemical processes for the study such as sediment transport, sorption, volatilization, hydrolysis, bacterial degradation, oxidation, and photolysis. The model originated from the flexible Water Analysis Simulation Program (WASP) developed by Di Toro et al. (1983) which is structured for site-specific applications. Large portions of the basic WASP code have been thoroughly tested in other applications (O’Connor et al., 1983; Thomann et al., 1979).

6.4.1. Finite Difference Discretization

The Lower St. Marys River is segmented vertically into two layers with an upper water column and a lower benthic or active bed layer. The horizontal plane of the river is discretized into a network of 30 cells with two rows (in some reaches three rows) of cells across the river width that extend along the entire study area of the river. Underlying these water column cells are another 30 cells used to discretize the river bed. A schematic
diagram of the three dimensional discretization is given in Fig. 6.18, while the corresponding cell representation in the horizontal plane of the Lower River is shown in Fig 6.19.

Since the hydrodynamic information from DYNHYD4 is needed for the cells in TOXI4, the cell segmentation is arranged to closely coincide with the junction network of DYNHYD4. A total of 4 inflow locations make up the open upstream boundary. At each inflow boundary location, a water column cell and a bed layer cell are needed. Similarly, there are also 4 outflow locations at the open downstream boundary. Again two cells, a water column cell and a bed layer cell, are placed at each of the outflow locations.

The Algoma diffuser discharging from the Algoma main trunk sewer is the main point source and is located in water column segment number 1 on the Canadian shoreline of the model. An initial phenol concentration representing the background level is assigned to all the cells before the simulation begins. The background phenol concentration level is based on information provided by the Ontario MOE. In order to maintain a constant ambient phenol level at the inflow boundaries, the upstream boundary is prescribed with a time independent ambient phenol level.

The flow quantities for each cell are assigned based on the values computed from DYNHYD4. Since the phenol loading rate and the flow distribution were different for 1974 and 1983, it is necessary to set up the input data in TOXI4 for both the 1974 and 1983 conditions.
6.4.2. Calibration and Verification

The calibration of the TOXI4 model was carried out for the 1974 phenol loading rate and flow distribution conditions (Ontario MOE 1974). The river flow used was 81,100 cfs (2,298 m³/s) and the phenol load was 252 kg/d at the Algoma terminal basin. The parameters that can be adjusted in the calibration process are mainly the lateral and longitudinal diffusion coefficients. The lateral diffusion coefficients were based on the values computed by KETOX and generally averaging about 0.4 m²/s (4.3 ft²/s). While the longitudinal diffusion coefficient used for the model averages at 4.0 m²/s. The values for each cell were adjusted from these average values in the calibration process. Currently TOXI4 only allows for a maximum of 10 different values.

For the purpose of comparison, the predicted phenol levels from TOXI4 were superimposed on the plots in Figs. 6.7 (a) to (j). The calibrated results agree reasonably well with the Ontario MOE (1974) measurements and the KETOX results for cells located along the Canadian and U.S. shorelines. However, the model under-predicts the phenol levels at the mid-section of the river for most locations. As expected the model is not able to predict the peak concentration at the outfall. This is due to uniform mixing assumption for the relatively large water cells.

Using the calibrated parameters for 1974, the TOXI4 model was then ran using the 1983 phenol loading rate and flow distribution conditions. The river flow used was 100,000 cfs (2,832 m³/s) and the phenol load at the Algoma terminal basin was
reduced to 101 kg/d (or a concentration of 280 ug/L). The results from TOXI4 were superimposed on plots for the 1983 Ontario MOE field data in Figs. 6.10 (b) to (d). These plots show reasonably good agreement on both the Canadian and U.S. shorelines with the expected fair predictions for cells located at the middle of the river. Hence a verification of the TOXI4 model is achieved here, however further verification is still recommended when more field data becomes available.

6.4.3. Summary of TOXI4 Results

Due to the limitation of TOXI4 to 60 cells for a model, the size of some of the cells can be quite large. Hence the spatial resolution of the model at some locations is extremely coarse. Therefore it was found necessary to place more cells along the Canadian shoreline in order to have reasonable prediction of the highest phenol concentrations.

Although comparison of cells along the Canadian and U.S. shorelines indicates good results on the predicted phenol levels, the prediction for the larger cells located at the middle of the river is generally not as good. This can be attributed to the nature of this type of cell approach model which uses the complete mixing assumption for each cell. The concentration of the pollutant in cells with relatively large cell volumes is usually smoothed out by the model.
Chapter 7

MODEL APPLICATIONS

7.1. General

The final aspect of this study is to demonstrate the use of the model as a tool for predicting future water quality impacts resulting from changes in management strategies. The predictive capability of these models provides a means for the environmental managers to easily screen the many management alternatives.

For instance, the model can be used to predict the relative differences in water quality to be expected from wastewater management changes. This includes such options as consolidating individual wastewater treatment plants into a regional facility, relocating existing wastewater discharges, or incrementally reducing wastewater loads. The effects of nonpoint source load reductions can also be evaluated.

7.2. Post-Processing and Graphics Visual Aids

When it is necessary to screen a number of management alternatives, it is important for the environment managers to quickly extract specific results from the huge data base generated by the models and at the same time graphically display these extracted results to assist in making decisions. This is especially relevant in the case of a spill of a toxic pollutant. In such situations a preliminary evaluation of the impact can be
carried out quickly and a decision can be made on the best remedial action. This feature can be made available to the environment manager by building post-processing capabilities into the models.

Post processing capabilities have been developed for both the Upper and Lower River models. Colour graphics are used extensively as visual aids to highlight regions of concern. Figure 7.1 shows photographs taken of the monitor illustrating the graphical supports. It is also possible to use zoom features to enlarge a particular location for details. These graphic programs are written to automatically interface with the models and can be displayed on either the CGA (medium resolution - Colour Graphics Adapter) or the EGA (high resolution) monitors. The software compilers used to develop these programs are Borland Turbo-Pascal™, Microsoft QuickBasic™ and Microsoft™ FORTRAN Optimizing Compiler (Version 4.01).

In addition to the above capabilities, the user may also import an ASCII text/number file (i.e. KEmodel.WAT), created by the model at the end of a simulation run, into spreadsheet softwares such as LOTUS 123™, LOTUS Symphony™ or SuperCalc4™. Then the user can easily view graphically any cross-section of the Lower River for any reach, either by using automated macros or by entering the appropriate commands through the spreadsheet menus. The velocity profile, depth profile, water column and bed column concentration profiles can be plotted by this spreadsheet approach. An illustration of this application is given in Table 7.1, while the corresponding plots are shown in Fig. 7.2.
7.3. Limited Use Zones (LUZ) for Phenol

In this section it will be shown that the model can be used to investigate the Limited Use Zone (LUZ) for pollutants for different loading scenarios. The reason for a Limited Use Zone investigation is:

(a) to prevent the problem of transboundary pollution so that Agreement objectives between Canada and the United States will be met; and

(b) to prevent impacts on other water users including municipalities, fisheries and recreational interests.

Phenol has been selected to show the application of the model to a Limited Use Zone study for different loading scenarios at the Algoma diffuser. The KETOX model was calibrated and verified as discussed in Chapter 6. The following scenarios were investigated:

(a) average summer river flow (87,000 cfs or 2,464 m³/s) with an in-pipe initial concentration $C_0$ of 280 ug/L at the Algoma diffuser;

(b) average summer river flow with an in-pipe $C_0$ of 50 ug/L at the Algoma diffuser;

(c) extreme low flow (54,000 cfs or 1,529 m³/s) with $C_0$ of 280 ug/L at the Algoma diffuser;

(d) extreme low flow with $C_0$ of 50 ug/L at the Algoma diffuser;
(e) average winter flow (77,000 cfs or 2,180 m$^3$/s) with complete ice cover and $C_0$ of 280 ug/L at the Algoma diffuser; and

(f) average winter flow with ice cover and $C_0$ of 50 ug/L at the Algoma diffuser.

The Algoma diffuser discharge was fixed at 4.2 m$^3$/s (147 cfs). The measured background level for phenol at the terminal basin is approximately 0.3 ug/L. The provincial water quality objective for phenol levels outside of the Limited Use Zone is less than 1 ug/L. For steady state loading, isoconcentration maps can be developed with longitudinal resolution of the order of 50 ft (15 m) and lateral resolution as low as 1 percent of the flow in the reach. This permits a reasonably accurate Limited Use Zone to be defined so that various loading scenarios can be compared and evaluated.

Figure 7.3 is a plot showing the results for a typical summer variation in the maximum phenol concentration along the Canadian shoreline when the initial phenol concentrations at the Algoma diffuser are 50 ug/L and 280 ug/L. The end of the near field zone of the Algoma diffuser is treated as the origin for the longitudinal axis. The longitudinal axis represents distances along the Canadian shoreline. The corresponding LUZs for the outfall concentrations of 50 ug/L and 280 ug/L under an average summer flow of 87,000 cfs (2,464 m$^3$/s) are shown in Fig. 7.4. It is noted that the 280 ug/L outfall concentration results in a LUZ that extends along the Canadian shoreline from the Algoma
terminal basin to the easterly Sewage Treatment Plant (STP) in Lake George channel north of the Sugar Island. However when the outfall discharge concentration is decreased to 50 ug/L, the length and the lateral extend of the LUZ is shortened drastically to the near field zone of the diffuser (approximately less than 1,500 feet or 457 metres). It is also observed that the LUZ is confined to the Canadian side with no transboundary pollution problem in either case.

Figure 7.5 shows typical winter variation of the maximum phenol concentration that will occur along the Canadian shoreline for initial concentrations of 50 ug/L and 280 ug/L at the Algoma diffuser. The average winter flow is taken as 77,000 cfs (2,180 m³/s) with ice cover. The corresponding LUZs are shown in Fig. 7.6 for outfall concentrations of 50 ug/L and 280 ug/L. Similar to the earlier findings, the 280 ug/L outfall concentration will result in a LUZ that extends past the easterly STP at the Lake George channel north of Sugar Island. In the case of the reduced, 50 ug/L, outfall concentration, the LUZ extends approximately 915 metres (3,000 feet) downstream from the diffuser location.

Finally, the model was also run for the extremely low flow condition of 54,000 cfs (1,529 m³/s). The phenol concentrations along the shoreline are shown in Fig. 7.7 for outfall concentrations of 50 ug/L and 280 ug/L. This represents the worst case scenario for the dilution of the Algoma discharge. The corresponding LUZs plots are shown in Fig. 7.8. The LUZs are quite similar to the winter condition results discussed above.
However, the LUZ for the 280 ug/L case crosses the international boundary upstream of Sugar Island before entering the Lake George channel.

A graphics post-processor has been prepared to assist in the interpretation of the output from the KETOX model. The graphic processor can produce the isoconcentration map as shown in Fig. 7.9 in which the concentration intervals to be plotted can be easily controlled by the user. This will reduce considerably the efforts needed to produce the LUZ maps each time a new scenario is investigated.

7.4. Use of the Model in Load Allocation

Several specific examples of observed and possible loading scenarios have been analyzed as a further illustration of the use of the models. In a draft report to the Ontario MOE, McCorquodale and Yuen (1988) have applied the KETOX model to load allocation at the Algoma Diffuser. The selected contaminants are: phenols, ether solubles, suspended solids (SS), ammonia and cyanide. Loads representing existing conditions for these parameters are available from: UGLCCS (Upper Great Lakes Connecting Channel Study, 1986), MISA (Municipal Industrial Strategy for Abatement, 1986) and Industry Self Monitoring (1986). Table 7.2 summarizes the 1986 loads at the Algoma Diffuser. The guidelines allow for a relatively small LUZ of the order of 1000 ft (300 m) or less in which the concentration level guidelines in Table 7.3 must be met.
Several loads were introduced at the Algoma Diffuser in the Terminal Basin. Figure 7.10 shows a sample of data selected from these runs for phenol in the form of the maximum concentration versus distance downstream of the diffuser. The background concentration for phenol was taken as 0.1 ug/L in the study. It is noted that, for all practical purposes, the maximum concentration can be assumed to occur at or near the Canadian side of the Lower River. The in-pipe initial phenol concentrations at the Algoma outfall were set at 63 and 278 ug/L while the average diffuser discharge was set at 147 cfs (4.2 m³/s). These concentrations represent respectively loads of 22.7 and 100 kg/d; the former corresponding to a possible objective and the latter to the existing loading (MISA, Industry Self Monitoring and UGLCCS 1986).

Figure 7.10 also shows that the 1 ug/L limit for phenol is exceeded by the outfall load of 100 kg/d for a distance of more than 10,000 feet (3,050 metres) along the Canadian shoreline from the diffuser. However, the LUZ criterion is met under average summer flow at 1,000 feet (305 metres) downstream from the diffuser for the 20 kg/d outfall load. At the minimum river flow of 54,000 cfs (1,529 m³/s), the guidelines are met at a distance of 1,500 feet (457 metre) downstream of the Terminal Basin outfall. Finally, Fig 7.10 shows that a load of 22.7 kg/d yields a LUZ well within the Canadian zone of the River even under low flow conditions.
Table 7.4 summarizes the loads for the other selected chemicals in order to achieve a LUZ of 1,000 feet (305 metre). Also shown in the same table are the LUZ distances for the 1986 loads.

7.5. Application to Spill of Toxic Substances

This application is developed to use the TOXI4 model results to produce a response function for a selected river site, i.e. similar to a unit hydrograph or pollutograph, due to a unit spill of a toxic pollutant at a given point source. In this case the point source is the Algoma Terminal Basin and the pollutant is phenol.

A spreadsheet is used to set up this application using LOTUS Symphony™. The TOXI4 model is first run for a unit load (1 kg) over 0.25 hour duration to produce a unit response function for the eight locations on the Canadian shoreline. Similar response functions are also produced on the U.S. shoreline. Figure 7.11 illustrates a unit spill load function at the Algoma diffuser. The corresponding unit pollutograph response at a typical location downstream of the diffuser is shown in Fig. 7.12.

The results from TOXI4 are used to set up the unit response function for each of the locations (eight on the Canadian side and eight on the U.S. side) in the spreadsheet. Using the same concept that is used to obtain a synthesized hydrograph based on unit hydrographs, a synthesized pollutograph is obtained for each location.
As an illustration, a hypothetical spill load function and its associated pollutograph are shown in Figs. 7.13 and 7.14 respectively. These plots are for a typical location on the Canadian shoreline. The corresponding impact of the spill on the U.S. shoreline is shown in Fig. 7.15. Each of the sixteen locations on the Canadian and U.S. shorelines will have its own pollutograph. To assist the user, the application is written using spreadsheet macros to automate the calculations. A user menu is programmed into the spreadsheet to guide the user in the changing of the load function and the plotting of the response for each of the sixteen locations. A dilution factor is also allowed which is simply proportional to the river flow. The effects of the dilution factor will be computed within the spreadsheet when the user changes the default river flow in the spreadsheet.

This application assumes that there is a linear response to the increase in the load function and an inverse response to an increase in flow values. This approach avoids the efforts needed for the tedious input data preparation and the long computation time needed to run TOXI4 for each spill scenario. It is also possible to extend this technique to multiple point sources.

7.6. Microcomputer Applications

Affordable microcomputers such as the IBM AT/XT™ or compatibles are readily accessible to all potential users of the models in this study. This is the reason for developing the models in the microcomputer environment. However, to minimize the
trade off in terms of speed and memory relative to the mainframe machines, it is advisable to use add on features such as math co-processors and multi-tasking, i.e. the ability to run several applications at the same time using Microsoft Windows/386™ which is based on the 80386 microprocessors technology. These add on features will enhance the microcomputer speed and versatility.

In the area of visual graphics presentation of results, microcomputers have a definite hardware and speed advantage over the mainframe machines since interactive graphics can be employed by the user to immediately display the results and organize his next action. The availability of EGA (Enhanced Graphics Adapter) and VGA (Video Graphics Array) displays significantly improves the resolution of a graphical presentation to the point where acceptable accuracy in determining the objectives on limiting boundary of influence is possible. Such options are not available on many mainframe machines.

Hence these models are developed for specific minimal microcomputer hardware requirements. Such requirements are documented in the users manuals that accompany each of the models. In order to take advantage of what is available now in the microcomputer technology, it is expected that the user will have the minimal hardwares (i.e. math co-processor, 10 megabytes hard disk and CGA or EGA option) to enhance the model's usefulness to the user's applications.
Chapter 8

CONCLUSIONS AND RECOMMENDATIONS

8.1. General Overview

A modelling framework has been demonstrated for the Upper and Lower St. Marys River in this study. This modelling framework encompasses both the numerical simulation of river and lake hydrodynamics as well as the simulation of the fate and transport of toxic contaminants. Although the St. Marys River is used in the study, an effort was made to generalise the models for application to other large river system with similar characteristics. The models help to explain the complex relationship between the hydrodynamic responses and the transport of contaminants in large rivers. The external factors include the wind effect, the river flow, the gravitational effect, the Coriolis effect and the existing topography of the area. The availability of modelling tools, allows one to predict the river or lake response to certain external factors.

The calibration and verification of the models for the St. Marys River were made possible with the field data available from the following sources:

(i) the U.S. Army Corps of Engineers;
(ii) the Ontario Ministry of the Environment;
(iii) Integrated Exploration Limited; and
(iv) aerial photographs taken of the study area.
8.2. Upper St. Marys River - Specific Conclusions

The Upper River is intermediate between a lake and river system. The hydrodynamics of the area were simulated using two models:

(i) a three dimensional steady state model with the rigid lid assumption using the Finite Element Method;
(ii) time dependent one dimensional finite difference network model, DYNHYD4, that can be applied to rivers or estuaries.

The finite element model neglects the inertia terms; the justification for this is substantiated by a preliminary investigation using a model that includes the inertia effects. It was found that the effect was negligible. With the linearized model, a much shorter computation time is needed by the model. By using a very high grid resolution, the model provides detailed information on the 3-D steady state velocity field. This is valuable to the understanding of other processes such as sediment transport, biological activity and transport of pollutants. The model indicates that the Upper River is highly responsive to wind speed and direction. Its dynamic behaviour is important in the shallow bays where gyres form. Some of the contaminants (e.g. PAHs) in the Bays are associated with the movement of fine-grained sediment particles; it is expected that the gyres will play a significant role in the transport of contaminants from the area of the slag dump to Leigh Bay and Point Aux Pins Bay. The model has indicated that up to two strong gyres can be formed simultaneously.
Combined with existing field data on current measurements in this area, the calibrated model provides a better understanding of the cause and effect relationship between the wind and the circulation patterns in the Upper River. This will eventually lead to the construction of more detailed fate models for management purposes. In addition, the model may provide new insights into the hydrodynamics of the Upper River for those who are involved in collecting field data for the area.

DYNHYD4 is a dynamic one dimensional model (USEPA 1988) that can provide information on the water levels in the Upper River. In calibrating the model to reproduce the water elevations as reported by the U.S. Army Corps of Engineers (1984), DYNHYD4 was allowed to reach steady state conditions. DYNHYD4 performed satisfactorily in the simulation of the velocities in the shipping channel; however, its performance in the shallow bays was only acceptable in comparison with the measured velocities. A comparison of DYNHYD4's steady state mean velocity results with the finite element model results indicated good agreement. DYNHYD4 can be used to estimate the time response or "spin-up" time of the Upper and Lower St. Marys River for different flow and wind conditions.

DYNHYD4 can be linked to TOXI4 (USEPA 1988) at a later stage when loading data are available for the dynamic simulation of toxic contaminants for the Upper River. Since the model is of the link-node type, its discretization network can easily be made compatible with the TOXI4 cell segmentation. In addition, TOXI4 is structured to allow for easy transfer of flow quantities
computed by DYNHYD4. However, a large computer storage of intermediate information is necessary for a dynamic simulation by TOXI4 if many cells are used in the discretization of the study area.

8.3. Lower St. Marys River - Specific Conclusions

The hydrodynamics and the transport of toxic contaminants in the Lower St. Marys River were simulated by the following models:

(a) KETOX;
(b) DYNHYD4; and
(c) TOXI4.

The KETOX model is interactive; the user may modify flows, depths and ice conditions at run time. KETOX can easily simulate rivers with many divided channels and confluences. In addition, the model has toxic chemical-sediment modelling capability. This feature of the model is used in the waste load allocation study in Chapter 7. The capability of the KETOX model to provide a refined grid of the study area and its ability to compute the lateral dispersion coefficients were found to be useful features. The KETOX model provides solutions for the lateral dispersion coefficients at each selected cross section of the river based on the turbulence transport equations (K and E). The lateral dispersion coefficients computed by KETOX were also used by TOXI4. An important advantage of KETOX over TOXI4 is its built-in hydrodynamic sub-model which avoids the tedious process of transferring hydrodynamic information for the dispersion modelling. The main disadvantages of KETOX are (i) that it is a
steady state model; and (ii) it is designed to model nearly unidirectional flows and cannot simulate recirculating flows such as those in the bays of the Upper St. Marys River.

KETOX was used to simulate the transport and dispersion of phenol which was being discharged into the Algoma Terminal Basin. The field data indicated that the high longitudinal convection in the river relative to its lateral dispersion results in the pollutant plume being confined to the Canadian shoreline. KETOX performed very well and was later used to evaluate the LUZ for the line source at the Algoma diffuser in the Terminal Basin for regulation purposes.

DYNHYD4 was applied to the Lower River to compute the flow distribution for the TOXI4 model. DYNHYD4 enables us to evaluate the water levels and the velocities in the river when subject to seasonal flow rates. The water levels as computed by DYNHYD4 may be used as estimates for water level adjustments in KETOX for simulating different seasonal scenarios. The steady state mean velocities computed by DYNHYD4 compared favourably with the values from the hydrodynamic sub-model of KETOX.

TOXI4 was used to predict phenol concentrations in the Lower River with a line source located at the Algoma diffuser in the Terminal Basin. TOXI4 had to be modified to include the more complex boundary conditions. It was also necessary to place cells carrying about 8% of the river flow along the Canadian shoreline in order to reproduce observed concentrations on the shoreline. Although TOXI4 results were satisfactory on the Canadian and U.S. shoreline, the predicted concentration levels for cells at the
centre of the river were lower than the measured levels. A possible explanation for this is the assumption of complete mixing in the TOXI4 cells. Since the cells located at the centre of the river have relatively large volumes, they tend to have lower concentrations than those measured along the shore.

Since TOXI4 is an unsteady model, it was used to generate a database for the construction of pollutographs due to spills of toxic contaminants. To do this, TOXI4 was used to simulate the advection and dispersion of phenol in the Lower River due to a unit load of phenol at the Algoma Terminal Basin. The time series responses from the cells on both the Canadian and U.S. shoreline are then assembled into a spreadsheet program, Lotus Symphony™. The spreadsheet is then used to reconstruct pollutographs due to different spill scenarios. The recomputation and reconstruction of the pollutographs, as well as the final graphing of the results, are automated using menu driven macros. The approach of superpositioning to build up a total pollutograph from a unit hydrograph is correct if the process response is linear. This was verified by separate runs of TOXI4.

8.4. Recommendations

The recommendations for this study are summarized below.

(a) The variability of field data which is always present in any sampling effort makes it necessary to obtain more field data for better model verification.

(b) The field data collected must be reliable and they should cover the wide range of conditions that may occur naturally for the study area. If the models can be verified for a wide
range of conditions, then the models can be applied with some confidence to simulate different scenarios in the study area.

(c) Since the plume from the Algoma diffuser is mainly confined to the Canadian side of the Lower River, future sampling efforts should be concentrated near the Canadian shoreline. This will assist in further verification of the concentration profiles predicted by the models which have steep concentration gradients near the Canadian shore.

(d) It is usually difficult to obtain information on the physical-chemical properties of the toxic pollutants. An information database can be established to gather more information on the toxicant’s partition coefficient for bed sediment, the effect of toxicant concentration on partitioning, the effect of sediment grain size on partitioning. Other information include sediment concentrations, resuspension and settling velocities of sediments and sedimentation rate of the bed. It is also useful to compile typical ranges of suspended solids concentration and data on atmospheric sources and emission rates in the study area.

(e) The verification of the models includes the definition of a fairly objective verification strategy based on statistics which will give a quantitative measure of the quality of the models. Hence it is recommended that some agreement on which statistical diagnostic tool be established for model
evaluation. This will help in the model application since an objective statement of model credibility can be made for the decision maker.

(f) This study did not succeed in the fully dynamic short term simulation of the Lower River using TOXI4. This type of simulation requires coupling of the unsteady hydrodynamic information from DYNHYD4 to the TOXI4 model. One of the problems is the need for large computer storage of the intermediate hydrodynamic information. The time step of the two models must be made to be compatible and is restricted by the small time step used for TOXI4. It is recommended that faster machines with bigger storage be acquired in order to resolve these limitations.

(g) Although the KETOX model used in this study yielded satisfactory results, there is a need to extend the model to include unsteady state options. With the unsteady option, KETOX can be used for dynamic short term simulation of the Lower River.

(h) Some problems were encountered when the TOXI4 model was used to model small study areas like the Lower St. Marys River. Due to the assumption of complete mixing in each cell, the TOXI4 model can only predict cell average results. In order to achieve better spatial resolution, the toxics sub-model of KETOX can be used to supplement the TOXI4 model.

(i) Due to the long computational time and stability requirements, it is not recommended the cell sizes for the existing small cells be reduced in the model beyond that
already used in this study. A possible alternative is to replace the larger cells with more, smaller cells if better spatial resolution is desired. However, this requires recompiling the WASP4 source code to increase the size of the arrays in the program beyond the existing provision for 60 cells. Based on previous experience, the number of cells should not be increased to beyond 80 to 90. The executable task image of WASP4 may exceed 600K (kilobytes) of RAM (random access memory). Since most microcomputers have only 640K of RAM, of which 40K is reserved for DOS (disk operating system), the user may not be able to load the enlarged WASP4 program.

(j) Further improvements on the existing software for user applications are required. An area of possible future improvement is the inclusion of multiple sources for the spills of toxic chemicals. The advantage of using an analytical Instantaneous Unit Pollutograph (IUP) may be developed. This will give more flexibility to the existing application in the simulation of toxic spill scenarios.

(k) Other applications that may be developed in the future include the use of load probability functions to evaluate the risk of non-compliance in waste load allocation planning.

(l) A dynamic model such as TOXI4 must be used for simulating the decontamination process of in place pollutant in the bed layer of the river. In such cases the bed may act as a sink or source.
APPENDIX A

USEPA DYNHYD4 MODEL THEORY
Overview

This model is an enhancement of the Potomac estuary hydrodynamic model DYNHYD2 (Roesch et al., 1979). It should be pointed out that the theoretical developments of these governing equations are well documented in US EPA users manuals (Ambrose et al., 1988). The purpose of including an overview of the theoretical formulation of the model here is to provide a brief explanation of the theory so that one may be aware of the model's capability and limitations. This will to some degree avoid the tendency of the modeller to extrapolate results from the model without knowing its limitation. It is not the intention to repeat the theory of this model but to give some limited understanding of the model's theoretical background to aid the modeller in applying it to investigative work.

Equation of Motion

The equation of motion in one dimension can be written as:

\[
\frac{\partial U}{\partial t} = -U \frac{\partial U}{\partial x} + a_k + a_f + a_w.
\]

where,

\( U \) = the velocity along the channel axis;

\( x \) = the distance along the channel axis;

\( t \) = the time;

\( \frac{\partial U}{\partial t} \) = the local inertia term;
\[
U \frac{\partial U}{\partial x} = \text{the convective inertia term;}
\]
\[
a_g = \text{the gravitational acceleration term;}
\]
\[
a_f = \text{the frictional resistance term; and}
\]
\[
a_w = \text{the wind stress term.}
\]

**GRAVITATIONAL ACCELERATION.** This term is due to the slope of the water surface along the longitudinal axis as shown in Fig. A.1 and is given by,

\[
(A.2) \quad a_g = -g \cdot \sin S
\]

where, \( g \) is gravitational acceleration, and \( S \) is the slope of the water surface. Since the water surface slope is relatively small then taking the sine of the slope (\( S \)) is approximately equal to the value \( S \) so that,

\[
(A.3) \quad a_g = -g \frac{\partial H}{\partial x}
\]

where, \( H \) is the water surface elevation (i.e. water depth above an arbitrary datum).

**FRICIONAL RESISTANCE.** This term is generally related to the Manning equation for steady uniform flow. The Manning's equation (in S.I. units) is given by,

\[
(A.4) \quad U = \frac{R^{2/3}}{n} \sqrt{\frac{\partial H}{\partial x}}
\]
where, $R$ is the hydraulic radius of the channel, and $n$ is the Manning’s roughness coefficient. Since the gravitational acceleration must balance the frictional resistance in a channel for steady uniform flow, as illustrated in Fig. A.2 we can write,

\[(A.5) \quad a_f = a_g = -g \frac{\partial H}{\partial x}\]

It is approximately true that over short time intervals the flow is relatively steady and uniform, so that combining Eqs. (A.4) and (A.5) we get,

\[(A.6) \quad a_f = -\frac{g n^2}{R^{4/3}} \cdot U \cdot |U|\]

where, the square of the velocity, $U$, has been replaced by $U$ times the absolute value of $U$ so friction will always oppose the direction of flow.

**WIND STRESS.** Finally, the wind acceleration term can be obtained from the shear stress relationship between the air and water boundary. At the water surface, the wind stress is given by,

\[(A.7) \quad \tau_w = C_d \rho_a U^2\]

so that the force acting on the water surface area is given by,

\[(A.8) \quad F_w = \tau_w \cdot A_s\]
where,

\( \tau_w \) = the shear stress at the air-water boundary;

\( C_d \) = the drag coefficient (assumed constant at 0.0026);

\( \rho_a \) = the air density;

\( W \) = the wind speed at 10 meter above the moving water surface; and

\( A_s \) = the water surface area.

Combining Eqs. (A.7) and (A.8), the force on the water surface,

(A.9) \[ F_w = C_d A_s \rho_a W^2 \]

This shearing force on the top face of the water surface, as shown schematically in Fig. A.3, causes a volume of water to accelerate in the wind direction so that we can write,

(A.10) \[ \alpha_w = \frac{F_w}{V_w \rho_w} \]

where,

\( \alpha_w \) = the wind acceleration term;

\( V_w \) = the volume of water; and

\( \rho_w \) = the density of water.

Since the wetted perimeter of a wide channel is approximately equal to the channel width (i.e. depth to width ratio is very small), the hydraulic radius for a wide channel can be taken as,
(A.11) \[ R = \frac{V_w}{A_x} \]

Substituting Eqs. (A.9) and (A.11) into (A.10) we get,

(A.12) \[ a_w = \frac{C_d \rho_a}{R \rho_w} V^2 \]

where, \( \frac{\rho_a}{\rho_w} = 1.165 \times 10^{-3} \).

This is the magnitude of wind acceleration in the wind direction. However, the component of acceleration along the channel axis is given by,

(A.13) \[ a_{w,t} = \frac{C_d \rho_a}{R \rho_w} V^2 \cos \psi \]

where, \( \psi \) = the angle between the channel and wind direction.

This is because both the water and the wind have velocity components that contain both magnitude and direction. This is illustrated in Fig. A.4 for a channel.

**Equation of Continuity**

The continuity equation in one dimension is given by,

(A.14) \[ \frac{\partial A}{\partial t} = -\frac{\partial Q}{\partial x} \]
where A is the channel cross-sectional area, and Q is the flow in the channel. In the case of rectangular channels with constant width B, then this equation becomes,

\[(A.15) \quad \frac{\partial H}{\partial t} = -\frac{1}{B} \frac{\partial Q}{\partial x}\]

where the derivatives have the following physical meaning,

\[\frac{\partial H}{\partial t} = \text{the rate of change in water surface elevation with time; and}\]

\[\frac{1}{B} \frac{\partial Q}{\partial x} = \text{the rate of change in water volume with distance per unit width.}\]

**Implementation of the Equations**

In order to apply the link-node numerical computation, both the differential Eqs. (A.1) and (A.15) must be written in finite difference form. The finite difference of the equation of motion is,

\[(A.16) \quad \frac{U_i^{t+1} - U_i}{\Delta t} = -U_i \frac{\Delta U_i}{\Delta x_i} - g \frac{\Delta H_i}{\Delta x_i} - \frac{g n_i^2}{R_i^{4/3}} U_i |U_i|\]

\[+ \frac{C_d \rho_a}{R_i \rho_w} \frac{V_i^2}{2} \cos \psi_i\]
where,

\( U'_i \) = the velocity in channel \( i \) at time \( t \);

\( \Delta x_i \) = the channel length;

\( \Delta t \) = the time step;

\( i \) = channel or link number;

\( \frac{\Delta U_i}{\Delta x_i} \) = velocity gradient in channel \( i \); and

\( \frac{\Delta H_i}{\Delta x_i} \) = water surface gradient in channel \( i \).

All values on the right hand side of Eq. (A.16) are values at the previous time step, that is at:

\[ (t - \Delta t) \]

In Eq. (A.16), the water surface gradient can be calculated from the heads at the two junctions of a channel. However, the velocity gradient cannot be computed from the velocities at the upstream and downstream channels because branching in the network may occur. Instead, an expression for the velocity gradient can be derived from the continuity Eq. (A.14) for the channel by replacing \( Q \) in the equation by \((UA)\) so that,

\( (A.17) \quad \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = -U \frac{\partial A}{\partial x} - A \frac{\partial U}{\partial x} \)

Rearranging the terms in the equation will give the velocity gradient as,
\[ \frac{\partial U}{\partial x} = \frac{1}{A} \frac{\partial A}{\partial t} \frac{U \, \partial A}{A \, \partial x} \]

If \( B \) is the channel width, then the incremental change in the area as the water surface moves a small distance is,

\[ \partial A = B \Delta H \]

Also by using the approximate hydraulic radius relationship \( R = \frac{A}{B} \), we can replace \( A \) by \( BR \). Substituting these relationships in Eq. (A.18) and finite differencing the resulting equation gives,

\[ \frac{\Delta U_i}{\Delta x_i} = -\frac{1}{R_i} \frac{\Delta H_i}{\Delta t} \frac{U_i \Delta H_i}{R_i \Delta x_i} \]

The water surface gradient with respect to distance term is taken as the average water surface elevation change between the junctions at each end of channel \( i \) during the time step \( t \).

The final form of the equation of motion can now be written by combining Eqs. (A.19) and (A.16) and rearranging the terms as,

\[ U_i' = U_i + \Delta t \left[ \frac{U_i \Delta H_i}{R_i \Delta t} + \left( \frac{U_i^2}{R_i} - g \right) \frac{\Delta H_i}{\Delta x_i} \right] \]

\[ -\frac{g R_i^2}{R_i^{4/3}} U_i \left| U_i \right| + \frac{C_a \rho_a}{R_i \rho_w} \left| W_i \right|^2 \cos \psi_i \]
This is the explicit finite difference equation of motion applied to channel \( i \) at time \( t \).

The equation of continuity (A.15) in finite difference form is given by,

\[
(A.21) \quad \frac{H_i^j - H_j}{\Delta t} = \frac{\Delta Q_j}{B_j \Delta x_j}
\]

where \( j \) is the junction or node number. The following relationships may be defined for a junction:

- \( \Delta Q_j \): the summation of all flows entering and leaving the junction
- \( B_j, \Delta x_j \): the surface area \( A_j^z \) of the junction

Substituting these variables into Eq. (A.21) and rearranging will give the explicit finite difference form of the continuity equation applied at each junction \( j \):

\[
(A.22) \quad H_i^j = H_i - \frac{\sum Q_j}{A_i^f}
\]

At this point of the theoretical formulation, there exists one equation for each channel and one equation for each junction in the computational network. Given the input parameters describing the network configuration and geometry, initial values for channel velocities and junction heads, boundary conditions for downstream heads, and forcing functions for inflow and wind stress, Eqs. (A.20) and (A.22) are solved using a modified
Runge-Kutta procedure. The stability requirement is based on the Courant-Friedrichs-Lewy (C.F.L) condition. The details of the programming procedures is given by Ambrose et al. (1988).

The implementation of the model on both the Upper and the Lower St. Marys River is covered in detail in Chapters 5 and 6. The site-specific discretization to link-node networks is illustrated in these chapters.
GRAVITY

Acceleration of Gravity = \( g \)

\[ a_{g,l} = -g \cdot \sin S \approx -g \cdot S \]

Figure A.1 Gravitational Acceleration Component (Ambrose et al., 1988).
FRICIONAL RESISTANCE

For Steady Uniform Flow

Manning Equation: \[ U = \frac{1.485 R^{2/3}}{n} \sqrt{\frac{\partial H}{\partial X}} \]

\[ \frac{\partial}{\partial X} \]

\[ \alpha_f \rightarrow \alpha_g \]

\[ \alpha_f = \alpha_g = -g \frac{\partial H}{\partial X} \]

Over Short Time Interval

\[ q_f = \frac{g n^2}{2.208 R^{4/3}} \cdot U \cdot |U| \]

Figure A.2 Frictional Resistance Component (Ambrose et al., 1988).
WIND STRESS

A. Magnitude

\[ \tau_w = C_d \rho_a \, W^2 \]
\[ F_w = \tau_w \cdot A_s \]
\[ a_w = F_w / (\mathcal{V}_w \cdot \rho_w) \]

\[ a_w = \frac{C_d}{R} \frac{\rho_a}{\rho_w} \, W^2 \]

\[ C_d = 0.0026 \]
\[ \rho_a / \rho_w = 1.165 \times 10^{-3} \]

Figure A.3  Wind Stresses Component (Ambrose et al., 1988).
WIND STRESS

B. Direction

\[ \bar{W} \]
Magnitude = \( W \)
Direction = \( \alpha \)

Channel Direction = \( \theta \)
Wind Direction = \( \alpha \)
Relative Angle = \( \psi \)

\[ a_{w,l} = a_w \cdot \cos \psi \]

Figure A.4  Effects of Wind Direction (Ambrose et al., 1988).
APPENDIX B

USEPA TOXI4 - MODEL THEORY
General Overview

TOXI4 is an important component of WASP4 (Water Quality Analysis Simulation Program 4) that calculates toxicant concentrations in space and time for ponds, rivers, lakes, reservoir, streams, estuaries, and coastal waters (Ambrose et al., 1988). It is not the intention here to repeat the theories of this model which are well documented by Di Toro et al. (1983) and Ambrose et al. (1988). The theory of this model is briefly formulated here so that in using the model one is aware of the limitations of the results obtained from this model. This understanding is important to the modeller who is using the model to apply to investigative work.

The Mass Balance Equation

The equations solved are based on the principle of conservation of mass. This principle requires that the mass of each water quality constituent entering and leaving the water body, which can be taken as the control volume, through direct and diffuse loading, advective and dispersive transport, and transformation processes which can be physical, chemical and biological must be accounted for in one way or another. Based on the schematic sketch of the coordinate system for a water body in Fig. B.1, the mass balance equation for an infinitesimally small fluid volume can be written as:
\[
\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(U_x C) - \frac{\partial}{\partial y}(U_y C) - \frac{\partial}{\partial z}(U_z C)
\]

**Advective transport terms**

\[
+ \frac{\partial}{\partial x}(E_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(E_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(E_z \frac{\partial C}{\partial z})
\]

**Diffusion or dispersion transport terms**

\[
( S_L + S_B ) + S_K
\]

**Loading terms** \hspace{1cm} **Transformation term**

where,

- \( C \) = concentration of the water quality constituent, mg/L;
- \( t \) = time, days;
- \( U_x, U_y, U_z \) = advective velocities in the x, y, z directions, m/day;
- \( E_x, E_y, E_z \) = diffusion coefficients in the x, y, z directions, m²/day;
- \( S_L \) = direct and diffuse loading rate, g/m³/day;
- \( S_B \) = boundary loading rate, g/m³/day and;
- \( S_K \) = total kinetic transformation rate, (+/-) source/sink, g/m³/day.

This equation represents the three major classes of water quality processes, i.e. the transport terms, the loading terms, and the transformation terms. It is now just a matter of writing the finite difference approximations for each term in Eq. (B.1). Based on the finite difference form of the initial control volume, the entire problem can be formulated by incorporating the adjoining segments into a larger model network taking care to specify proper transport, loading, and transformation parameters.
However, for the sake of brevity and clarity, a finite difference form of the one dimensional mass balance equation will be used to illustrate the formulation. This one dimensional model can be obtained by integrating over the y and z directions if we assume vertical and lateral homogeneity within the control volume. A one dimensional mass balance equation can be written as,

\[
\frac{\partial}{\partial t}(AC) = \frac{\partial}{\partial x} \left( -U_x AC + E_x A \frac{\partial C}{\partial x} \right) + A \left( S_I + S_B \right) + A \frac{S_T}{S_F}
\]

where \(A\) is the cross-sectional area in square metres.

**Implementation of the Mass Balance Equation**

The application of finite difference approximation to the one dimensional advection-diffusion Eq. (B.2) will derived next. First the equation is re-written as below:

\[
\frac{\partial}{\partial t}(AC) = -\frac{\partial}{\partial x}(QC) + \frac{\partial}{\partial x} \left( E_x A \frac{\partial C}{\partial x} \right) + A S_T
\]

where,

- \(S_T = \text{total source/sink rate} = (S_I + S_B + S_K)\), \(g/m^3 \cdot \text{day}\); and
- \(Q = \text{volumetric flow} = A U_x\), \(m^3/\text{day}\).

Consider the finite difference approximation of a spatial derivative of concentration evaluated at a point:
At a point \( x_0 \),
\[ \left( \frac{\partial C}{\partial x} \right)_{x_0} \]

If the derivatives of \( C \) are single-valued, finite, continuous functions of \( x \), as shown in Fig. B.2(a). Then using Taylor's series expansion about a point and dropping terms containing the third and higher powers, it can be shown that the following relationships can be derived:

a. **Central difference:**

\[ (B.4) \quad \left( \frac{\partial C}{\partial x} \right)_{x_0} = \frac{C_{x_0+\Delta x} - C_{x_0-\Delta x}}{2\Delta x} \]

b. **Forward difference:**

\[ (B.5) \quad \left( \frac{\partial C}{\partial x} \right)_{x_0} = \frac{C_{x_0+\Delta x} - C_{x_0}}{\Delta x} \]

c. **Backward difference:**

\[ (B.6) \quad \left( \frac{\partial C}{\partial x} \right)_{x_0} = \frac{C_{x_0} - C_{x_0-\Delta x}}{\Delta x} \]

Substituting the central difference approximation for the spatial derivatives into the,

a. **advection term gives:**

\[ (B.7) \quad \left( \frac{\partial}{\partial x} (QC) \right)_{x_0} = \frac{Q_{x_0+\Delta x}C_{x_0+\Delta x} - Q_{x_0-\Delta x}C_{x_0-\Delta x}}{2\Delta x} \]
b. dispersion or diffusion term gives:

\[ (B.8) \left( \frac{\partial}{\partial x} \left( E_A \frac{\partial C}{\partial x} \right) \right)_x = \frac{(E_A)_{x+\Delta x} \cdot \left( \frac{\partial C}{\partial x} \right)_{x+\Delta x} - (E_A)_{x-\Delta x} \cdot \left( \frac{\partial C}{\partial x} \right)_{x-\Delta x}}{2\Delta x} \]

\[ = \frac{(E_A)_{x+\Delta x} C_{x+2\Delta x} - C_x}{2\Delta x \cdot 2\Delta x} - \frac{(E_A)_{x-\Delta x} C_{x-2\Delta x} - C_x}{2\Delta x \cdot 2\Delta x} \]

When applying the central difference approximations to segment j as shown in Fig. B.2(b), the mass balance equation can be written as:

\[ (B.9) \frac{\partial}{\partial x}(A_j C_j) = -\frac{Q_{i,j,i-1}}{l_j} C_{j,i-1} + \frac{Q_{i-1,j}}{l_j} C_{j,i-1} \]

\[ + \frac{(E_A)_{j,i-1}}{l_j \cdot l_{j-1,j}} (C_{j,i-1} - C_j) - \frac{(E_A)_{j-1,i}}{l_j \cdot l_{j-1,j}} (C_j - C_{j-1}) \]

\[ + A_j \cdot S_j \]

Multiplying Eq. (B.9) by the length of segment j gives:

\[ (B.10) \frac{\partial}{\partial t}(V_j C_j) = -Q_{i,j,i-1} C_{j,i-1} + Q_{j-1,i} C_{j-1,i} \]

\[ + R_{i,j,i-1} (C_{j-1} - C_j) - R_{j-1,i} (C_j - C_{j-1}) \]

\[ + V_j S_j \]
where,
\[ V_j = \text{volume of segment } j = A_j l_j, \ m^3; \]
\[ R = \text{dispersive flow} = \frac{E A}{L_c}, \ m^3/\text{day}; \text{ and} \]
\[ L_c = \text{characteristic length}, \ m. \]

The concentration values at the upstream and downstream interface of segment \( j \) may be expressed in terms of segment concentration as:

\[ (B.11) \quad C_{i,j-1} = \theta C_{i,j} + (1 - \theta) C_{i-1,j}, \]
\[ (B.12) \quad C_{i,j+1} = \theta C_{i,j} + (1 - \theta) C_{i,j+1}, \]

in which,
\[ \theta = \text{a numerical weighting factor (advection factor) between 0 and 1.} \]

A central difference approximation for the advective term is obtained if the advection factor is 0.5, while a backward difference approximation scheme is obtained if the advection factor is zero.

Extending Eq. (B.10) to the multi-dimensional case which is used by TOXI4 for segment \( j \) with adjoining segments "i" where segment interfaces are denoted by "ij". The full TOXI4 equation becomes:

\[ (B.13) \quad \frac{\partial}{\partial t}(V_j C_i) = -\sum_i Q_{ij} C_{ij} + \sum_i R_{ij}(C_i - C_{ij}) + \sum L V_j S_{Lj} + \sum B V_j S_{Bj} + \sum V_j S_{kJ}. \]
in which,
\( Q_{ij} \) = flow entering or leaving segment \( j \), \( m^3/\text{day} \);
\( L \) = notation for direct or distributed loading terms;
\( B \) = notation for boundary loading terms; and
\( k \) = notation for kinetic transformation terms.

The sign convention for the flow is positive if the it is leaving segment \( j \), and negative if it is entering segment \( j \). TOXI4 uses Eq. (B.13) to compute the mass derivatives for every segment "j" during each time step "t" from the initial to the final time of simulation. If the initial concentrations and volumes are known at time \( t \), the new masses at the next time step are computed using the one-step Euler's method given by:

\[
(V_j C_j)_{i+\Delta t} = (V_j C_j)_i + \frac{\partial (V_j C_j)}{\partial t} \Delta t
\]

where,
\( \Delta t \) = the time step, days.

The time step used is typically between 15 minutes and a half day. With the newly computed masses from Eq. (B.14), the new concentrations are obtained by dividing by the new volumes as follows:

\[
C_{j,i+\Delta t} = \frac{(V_j C_j)_{i+\Delta t}}{V_{j,i+\Delta t}}
\]
The new volumes are computed by TOXI4 internally using either the specified time variable flow fields or computed using the principle of continuity.

**Numerical Dispersion**

The finite difference approximation used for the derivatives will introduce artificial mixing commonly referred to as numerical dispersion. The numerical dispersion caused by each approximation scheme is summarized below:

a. Backward difference approximation of the derivative in the flow term:

Derivative approximated \( \leftrightarrow \frac{\partial C}{\partial x} \)

\[ E_{\text{num}} = \frac{U \Delta x}{2} \]

in which,

\( E_{\text{num}} \) = numerical dispersion;

\( U \) = velocity; and

\( \Delta x \) = length of the segment.

b. Forward difference approximation of the derivative term in the Euler scheme:

Derivative approximated \( \leftrightarrow \frac{\partial C}{\partial t} \)

\[ E_{\text{num}} = \frac{U^2 \Delta t}{2} \]

in which,
\[ \Delta t = \text{time step.} \]

c. Total numerical dispersion:

\[ E_{\text{num}} = \frac{U \Delta x}{2} - \frac{U^2 \Delta t}{2} \]

Note that if \( \Delta t = \frac{\Delta x}{U} \), then \( E_{\text{num}} = 0 \).

**Stability Requirement**

If the reactions are first-order, then the numerical stability requirement is given by:

\[
(B.16) \quad \Delta t \leq \min \left( \frac{V_i}{\sum Q_{ij} + \sum R_{ij} + K_i V_i} \right)
\]

where,

\[ R = \frac{E A}{l} = \text{the bulk exchange coefficient}; \text{ and} \]

\[ E = \text{the dispersion or diffusion coefficient}. \]

If the reactions are non-linear then this stability requirement is only a guide. A trial and error process of increasing the size of the time step can be carried out to determine the optimum value of the time step.

**Summary of Model Equations**

Equation (B.13) in its present form does not give credit to the fact that it is incorporating the complete chemical- sediment
dynamics in the water column. The equation can be expanded to show how the transport of dissolved and particulate matter in the water column and benthos is incorporated into the equation as follows:

\[
\frac{\Delta (V_j C_j)}{\Delta t} = \sum_i (-Q_{ij} C_{ij}) + \sum_i (-Q_{pij} C_{ij} f_{pij})
\]

water column and pore water advection

\[+ \sum_i \sum_k (-w_{sij} A_{ij} C_j f_{sij})\]
solids transport

\[+ \sum_i (R_{ij} A_{ij} C_j) + \sum_i (R_{piij} f_{pij} C_j n_j - f_{pdj} C_j n_j)\]
water column and pore water dispersion

\[+ \sum_{L} V_{Li} + \sum_{N} V_{Ni} + \sum_{B} (Q_{pi} C_{Bj})\]
point, nonpoint, and boundary loads

\[+ \sum_i \sum_k (V_j S_{Kij})\]
kinetic transformations

where:

\(j\) = segment index;

\(i\) = adjacent segment index;

\(s\) = solids transport field index;

\(L\) = point source index;

\(N\) = nonpoint source index;

\(B\) = boundary source index;

\(k\) = kinetic transformation index;
c = chemical index;

\( t = \) time, day;

\( V_i = \) volume of segment j, \( \text{m}^3 \);

\( C_j = \) concentration of the water quality constituent in segment j, \( \text{m}^3 \);

\( E_j = \) evaporation rate from segment j, \( \text{m/day} \);

\( P_j = \) precipitation rate into segment j, \( \text{m/day} \);

\( A_j = \) surface area of segment j, \( \text{m}^2 \);

\( Q_{ij} = \) advective flow between segments i and j, \( \text{m}^3 \)

\(+\) when flow is leaving segment j, and

\(-\) when flow is entering segment j;

\( Q_{p,ij} = \) pore water flow between segments i and j, \( \text{m}^3/\text{day} \)

\(+\) when flow is leaving segment j, and

\(-\) when flow is entering segment j;

\( C_{ij} = \) constituent concentration advected between i and j, \( \text{g/m}^3 \)

\( = \theta C_j + (1 - \theta) C_i \) when entering j, and

\( = \theta C_i + (1 - \theta) C_j \) when leaving j;

\( \theta = \) numerical weighting factor (advection factor), 0 to 0.5;

\( W_{s,ij} = \) solids transport velocity between segments i and j, \( \text{m/day} \)

\(+\) when leaving segment j, and

\(-\) when entering segment j;

\( f_{D,i} = \) dissolved fraction of chemical in segment j;

\( f_{S,i} = \) fraction of chemical sorbed to solid type, s, in segment j;

\( R_{ij} = \) dispersive flow between segments i and j, \( \text{m}^3/\text{day} \)

\( = \frac{E_j A_{ij}}{L_{eij}} \);
\[ E_{ij} = \text{dispersion coefficient segments between } i \text{ and } j, \ m^2/\text{day}; \]
\[ A_{ij} = \text{cross-sectional area between segments } i \text{ and } j, \ m^2/\text{day}; \]
\[ L_{cij} = \text{characteristic mixing length between segments } i \text{ and } j, \ m; \]
\[ R_{pji} = \text{pore water diffusive exchange flow, } m^3/\text{day}; \]
\[ = \frac{E_{ij} A_{ij} n_{ij}}{L_{cij} t_{ij}}; \]
\[ t_{ij} = \text{average tortuosity of segments } i \text{ and } j, \ m_{\text{water}}/m; \]
\[ n_{ij} = \text{average porosity of segments } i \text{ and } j, \ m^3_{\text{water}}/m^3; \]
\[ W_{ij} = \text{point source loads into segment } j, \ g/\text{day}; \]
\[ W_{nj} = \text{nonpoint loads into segment } j, \ g/\text{day}; \]
\[ Q_{ij} = \text{boundary inflows to segment } j, \ m^3/\text{day}; \]
\[ C_{bij} = \text{boundary concentrations for segment } j, \ g/m^3; \text{ and} \]
\[ S_{kci} = \text{kinetic transformation } k \text{ for chemical } c \text{ in segment } j, \ g/m^3 \cdot \text{day}. \]

The parameters specified for the water columnm are water column advection and dispersion across the interfaces connecting adjoining segments. The parameters specified for the benthic segments are pore water advection and diffusion. In addition, the adjacent water column and benthic segments may be joined by pore water advection and diffusion parameters and by solids transport parameters such as scouring and deposition at the water-bed boundary.
MODEL NETWORK

Figure B.1 Schematic of Cartesian Coordinate System for 3-D Discretization of a Study Area into Cells (Ambrose et al., 1988).
Figure B.2(a) Finite Difference Index Notation about a Point $x_0$.

Figure B.2(b) Central Differencing Scheme at a Point $j$ (Ambrose et al., 1988).
APPENDIX C

SPILL SIMULATION USERS GUIDE
Overview.

The spill simulation application uses a spreadsheet to compute the synthesized pollutograph. The unit pollutograph is for a spill duration of 0.25 hour. In order to simulate a spill function, the user must sub-divide the given spill function into 0.25 hour intervals and represent each interval as a constant spill loading. These loadings are to be entered into the spreadsheet.

The user can change the spill load values and the default river flow in the appropriate spreadsheet cells. By changing the flow, the user is introducing a dilution factor into the simulation. The dilution factor is computed as inversely proportional to the flow. This is automatically calculated by the spreadsheet. The user must press the "F8" function key to update any modifications on the spreadsheet. The user can check whether modifications to the spreadsheet have been updated by the "Calc" message displayed at the bottom right corner of the screen. If the "Calc" message is not displayed, it means that the spreadsheet calculations have been updated.

In addition, the user can activate the menu option in the spreadsheet by pressing the "Alt-m" keys combination. Using the menu driven option, the user can plot the load function and plot the synthesized pollutographs for each of the eight locations on the river.
To use this application, it is necessary to have access to the LOTUS Symphony™ software. Although the application is demonstrated with this software, it can be readily modified for Borland's Quattro™ or LOTUS 123™. Some modifications to the program macros in the spreadsheet are necessary.

A Guide to Getting Started.

The following general steps can be used as a guide:

Step 1
Change to the directory containing Symphony files on the hard disk and copy the files "SpillCan.wrk" and "SpillUS.wrk" from the single diskette provided for the spill application. If Symphony is already configured to place all its ".wrk" files in a sub-directory, the two files may be copied to the sub-directory.

* Note:
SpillCan.wrk - file containing the 8 cell locations on the Canadian shore.
SpillUS.wrk - file with the 8 cell locations on the U.S. shore.

Step 2
Get into the Symphony spreadsheet mode, normally by typing "access" or "symphony". Then load either of the files, SpillCan.wrk or SpillUS.wrk, by the "F9-FILE-RETRIEVE" keys sequence. An example of the spreadsheet loaded into Symphony is shown in Fig. C.1.
Step 3
Press the "Alt-m" key combination to activate the menu driven option. Use the help description on the second line at the top of the screen for guidance. Each of the items on the menu can be selected by typing the first alphabet of the item or by using the left-right arrow keys on the keyboard. For instance, to quit from the menu driven option, type the letter "Q" or "q". Finally, the user can quit from Symphony by the "F9-EXIT-YES" key sequence.

A listing of the spreadsheet macros used to program the menu driven option is given in Fig. C.2. The user may modify these macros if necessary to add new features.

System Requirements

- LOTUS Symphony™ version 1.0 or later
- 640 kilobytes RAM
- recommended minimum 3 megabytes space on harddisk to load Symphony the spill files
- IBM or MS DOS version 3.0 or later
The quality of this microfiche is heavily dependent upon the quality of the thesis submitted for microfilming.

Please refer to the National Library of Canada target (sheet 1, frame 2) entitled:

NOTICE
Figure C.1 Layout of the Spill Application Spreadsheet.
Figure C.2  Listing of the Symphony's Macros for the Spill Application Menu Option.
APPENDIX D

CURRENT METER AND DROGUE SURVEY DATA
Overview.

The field data compiled in this appendix are from the following sources:

(a) Integrated Explorations – Environmental Research Consultants (1985);

(b) Ontario MOE (1985); and

(c) U.S. Army Corps of Engineers (1984).
INTEGRATED EXPLORATION
ST. MARY'S RIVER CLAM BIOMONITORING

FIELD NOTES FOR 1985

I.E. REPORT # PJ8504
NOVEMBER, 1985
Table D.1
WATER QUALITY PARAMETERS DURING DEPLOYMENT (Dec. 3/85)

Stations are listed in the order of their deployment.

<table>
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<th>Station Number</th>
<th>Depth (m)</th>
<th>Conductivity (umho)</th>
<th>Temperature (°C)</th>
<th>Oxygen (mg/L)</th>
<th>pH</th>
<th>Current (cm/s)</th>
</tr>
</thead>
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<td>top  mid</td>
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<td>10.2* 10.2*</td>
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* Indicates saturated oxygen levels.
Table D.2

WATER QUALITY PARAMETERS DURING RECOVERY (Oct 24/67)

Stations are listed in the order of their recovery.

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<th>Conductivity (umho)</th>
<th>Temperature (°C)</th>
<th>Oxygen (mg/L)</th>
<th>pH</th>
<th>Current (cm/s)</th>
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<td>top</td>
<td>mid</td>
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<td>12</td>
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</table>

* Indicates saturated oxygen levels.
Figure D.2  Location of the Stations in Tables D.1 and D.2.
Table D.3

SEPTEMBER 1983 ST. MARY'S RIVER SURVEY - FIELD OBSERVATIONS AND SEDIMENT DESCRIPTIONS

<table>
<thead>
<tr>
<th>Station</th>
<th>Date</th>
<th>Current Velocity</th>
<th>Depth (m)</th>
<th>Temp. (°C)</th>
<th>Sediment Appearance</th>
<th>pH</th>
<th>Eh (mv)</th>
<th>Sediment Odour</th>
<th>Presence (X) of Oily/Phenolic Sheen</th>
<th>Macrophytes</th>
</tr>
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<tbody>
<tr>
<td>127-950</td>
<td>02.10.85</td>
<td>slight</td>
<td>6.0</td>
<td>11.9</td>
<td>dark brown silt over sand with iron and coal particulates</td>
<td>-173</td>
<td>none</td>
<td>x</td>
<td>-</td>
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<tr>
<td>SMU1.0-2130</td>
<td>01.10.85</td>
<td>negligible</td>
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<td>13.2</td>
<td>black silt (0.5-3 cm) over woodchips and sand</td>
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<td>x (abundant)</td>
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<td>SMU1.0-1650</td>
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<td>slight</td>
<td>5.0</td>
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<td>dark brown silt over sand, gravel</td>
<td>-150</td>
<td>oily (slight)</td>
<td>x (abundant)</td>
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<tr>
<td>121-1300</td>
<td>01.10.85</td>
<td>moderate</td>
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<td>12.7</td>
<td>light brown silt (0.5-5 mm) over coarse sand</td>
<td>-277</td>
<td>none</td>
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<td>122-1580</td>
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<td>12.2</td>
<td>silt over fine and coarse sand</td>
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<td>organic</td>
<td>x (slight)</td>
<td>thick Chara with Elodea</td>
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<td>123-1530</td>
<td>09.10.85</td>
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<td>2.5</td>
<td>12.3</td>
<td>some silt over coarse sand and stones over compact clay</td>
<td>-133</td>
<td>none</td>
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<tr>
<td>124</td>
<td>04.10.85</td>
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<td>11.7</td>
<td>coarse silt over gravel</td>
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<td>none</td>
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<td>Potamogeton sp. / Chara</td>
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<td>SMU2.3-1300</td>
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<td>brown silty sand</td>
<td>-160</td>
<td>slight organic</td>
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<td>11.3</td>
<td>uneven rolling bottom, grey-brown silty sand and clay</td>
<td>-40</td>
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<td></td>
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<td>Isoetes</td>
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<td>slight organic</td>
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<td>Eh (mv)</td>
<td>Sediment Odour</td>
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<td>13.8</td>
<td>silt over fine-coarse sand</td>
<td></td>
<td>-130</td>
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<td>14.0</td>
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<td>silt, coarse sand and gravel over clay (iron particles also present from shore piles)</td>
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<td>black-brown silt with coal, iron sand and gravel (bloowolf from shore piles)</td>
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<td>15.0</td>
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<td>Sediment Odour</td>
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<td>Macrophytes</td>
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<td>-99</td>
<td>none</td>
<td>Chara</td>
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<td>2.3</td>
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<td>+276</td>
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ST. MARY'S RIVER

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<th>Depth (m)</th>
<th>Temp. (°C)</th>
<th>Sediment Appearance</th>
<th>Sediment Odour</th>
<th>Presence (K) of Oily/Phenolic Sheen</th>
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<td>SMD6.4E-230</td>
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<td>none</td>
<td>3.3</td>
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<td><em>Eloides, Potamogeton sp.</em></td>
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<td>7.0</td>
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<td>dark brown silt over sand, stones</td>
<td>-6</td>
<td>oily</td>
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<td>8.0</td>
<td>13.8</td>
<td>coarse sand and stones with little silt</td>
<td>+170</td>
<td>oily</td>
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<td>9.0</td>
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<td>coarse sand and stones with little silt</td>
<td>+60</td>
<td>none</td>
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<td>brown silt over coarse sand</td>
<td>+52</td>
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<td>7.0</td>
<td>13.7</td>
<td>fine silt (10 cm) over medium sand</td>
<td>-120</td>
<td>none</td>
<td>*algal scum</td>
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<td>14.0</td>
<td>19.0</td>
<td>brown silt over coarse sand and gravel</td>
<td>-75</td>
<td>none</td>
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<td>4.0</td>
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<td>organic silt with plant fibre over medium sand and gravel</td>
<td>-55</td>
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<td>1.5</td>
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<td>organic silt</td>
<td>-73</td>
<td>oily</td>
<td>*Eloides</td>
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Table D.3 (cont'd)

SEPTMBER 1983 ST. MARY'S RIVER SURVEY - FIELD OBSERVATIONS AND SEDIMENT DESCRIPTIONS

<table>
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<th>Station</th>
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<th>Depth (m)</th>
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<th>pH</th>
<th>Eh (mV)</th>
<th>Sediment Odour</th>
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<th>Macrophytes</th>
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<tr>
<td>101</td>
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<td>none</td>
<td>6.0</td>
<td>14.7</td>
<td>brown silt with organic detritus over clay</td>
<td>-162</td>
<td>none</td>
<td>x</td>
<td>(very slight)</td>
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<td>102</td>
<td>26.09.83</td>
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<td>13.8</td>
<td>brown silt over some medium sand</td>
<td>-153</td>
<td>none</td>
<td>x</td>
<td>(slight)</td>
<td>-</td>
</tr>
<tr>
<td>103</td>
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<td>brown silt over fine-medium sand</td>
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<td>104</td>
<td>26.09.83</td>
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<td>13.8</td>
<td>brown silt with little fine sand and abundant fine organic material</td>
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<td>none</td>
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<td>-</td>
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<tr>
<td>105</td>
<td>26.09.83</td>
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<td>brown silt with little fine-medium sand</td>
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<td>106</td>
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<td>13.8</td>
<td>silty medium sand</td>
<td>-95</td>
<td>none</td>
<td>x</td>
<td>(slight)</td>
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LITTLE LAKE GEORGE

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<th>Sediment Appearance</th>
<th>pH</th>
<th>Eh (mV)</th>
<th>Sediment Odour</th>
<th>Presence (X) of Oily/Phenolic Sheen</th>
<th>Macrophytes</th>
</tr>
</thead>
<tbody>
<tr>
<td>83</td>
<td>28.09.83</td>
<td>none</td>
<td>2.0</td>
<td>13.3</td>
<td>brown silt over fine sand</td>
<td>-120</td>
<td>organic</td>
<td>x</td>
<td>-</td>
<td>abundant Potamogeton sp.</td>
</tr>
<tr>
<td>86</td>
<td>28.09.83</td>
<td>none</td>
<td>8.0</td>
<td>13.3</td>
<td>brown silt over fine sand</td>
<td>-85</td>
<td>none</td>
<td>x</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>87</td>
<td>28.09.83</td>
<td>none</td>
<td>2.0</td>
<td>13.3</td>
<td>brown silt over clay</td>
<td>-90</td>
<td>organic</td>
<td>x</td>
<td>(very strong)</td>
<td>Potamogeton sp., Myriophyllum sp., Elodea</td>
</tr>
<tr>
<td>88</td>
<td>28.09.83</td>
<td>none</td>
<td>3.0</td>
<td>13.3</td>
<td>brown silt over clay</td>
<td>-95</td>
<td>none</td>
<td>x</td>
<td>-</td>
<td>Potamogeton sp.</td>
</tr>
<tr>
<td>89</td>
<td>28.09.83</td>
<td>none</td>
<td>3.0</td>
<td>13.3</td>
<td>brown silt over clay</td>
<td>-100</td>
<td>organic</td>
<td>x</td>
<td>-</td>
<td>Elodea</td>
</tr>
</tbody>
</table>

NICOLET LAKE

<table>
<thead>
<tr>
<th>Station</th>
<th>Date</th>
<th>Current Velocity</th>
<th>Depth (m)</th>
<th>Temp. (°C)</th>
<th>Sediment Appearance</th>
<th>pH</th>
<th>Eh (mV)</th>
<th>Sediment Odour</th>
<th>Presence (X) of Oily/Phenolic Sheen</th>
<th>Macrophytes</th>
</tr>
</thead>
<tbody>
<tr>
<td>108</td>
<td>27.09.83</td>
<td>slight</td>
<td>2.0</td>
<td>13.8</td>
<td>light brown fine-medium sand over clay</td>
<td>-200</td>
<td>none</td>
<td>-</td>
<td>Potamogeton sp.</td>
<td>-</td>
</tr>
<tr>
<td>109</td>
<td>27.09.83</td>
<td>slight</td>
<td>4.0</td>
<td>14.0</td>
<td>brown silty fine-coarse sand over clay</td>
<td>-100</td>
<td>none</td>
<td>-</td>
<td>Chara</td>
<td>-</td>
</tr>
</tbody>
</table>

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### Table D.3 (cont'd)

**SEPTEMBER 1983 ST. MARY'S RIVER SURVEY - FIELD OBSERVATIONS AND SEDIMENT DESCRIPTIONS**

<table>
<thead>
<tr>
<th>Station</th>
<th>Date</th>
<th>Current Velocity</th>
<th>Depth (m)</th>
<th>Temp. (°C)</th>
<th>Sediment Appearance</th>
<th>pH</th>
<th>Eh (mv)</th>
<th>Sediment Odor</th>
<th>Presence (X) of Oily/Phenolic</th>
<th>Sheen</th>
<th>Macrophytes</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>24.09.83</td>
<td>negligible</td>
<td>2.3</td>
<td>14.0</td>
<td>brown silty sand over soft clay</td>
<td></td>
<td>-90</td>
<td>slight organic</td>
<td>-</td>
<td>Potamogeton, Myriophyllum, Chara</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>24.09.83</td>
<td>strong</td>
<td>7.5</td>
<td>15.8</td>
<td>brown silt with fine sand</td>
<td></td>
<td>-120</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>24.09.83</td>
<td>negligible</td>
<td>3.8</td>
<td>15.5</td>
<td>brown silt over fine sand</td>
<td></td>
<td>-16</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>24.09.83</td>
<td>none</td>
<td>3.0</td>
<td>15.7</td>
<td>brown silt over fine sand</td>
<td></td>
<td>-20</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>24.09.83</td>
<td>none</td>
<td>6.0</td>
<td>15.7</td>
<td>brown silt over soft clay</td>
<td></td>
<td>-150</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>23.09.83</td>
<td>none</td>
<td>4.0</td>
<td>15.7</td>
<td>brown silt, fine sand over clay</td>
<td></td>
<td>-40</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td>Chara</td>
</tr>
<tr>
<td>91</td>
<td>23.09.83</td>
<td>none</td>
<td>4.0</td>
<td>15.2</td>
<td>brown silt, fine sand</td>
<td></td>
<td>-60</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td>Potamogeton spp.</td>
</tr>
<tr>
<td>92</td>
<td>23.09.83</td>
<td>none</td>
<td>7.0</td>
<td>14.8</td>
<td>brown silt</td>
<td></td>
<td>-95</td>
<td>none</td>
<td>x (slight)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>93</td>
<td>23.09.83</td>
<td>none</td>
<td>9.0</td>
<td>14.8</td>
<td>brown silt</td>
<td></td>
<td>-175</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>94</td>
<td>23.09.83</td>
<td>none</td>
<td>2.5</td>
<td>14.8</td>
<td>brown silt over medium sand and clay</td>
<td></td>
<td>-104</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td>Chara</td>
</tr>
<tr>
<td>95</td>
<td>23.09.83</td>
<td>none</td>
<td>6.0</td>
<td>15.1</td>
<td>brown silt over medium sand and clay</td>
<td></td>
<td>-140</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>96</td>
<td>23.09.83</td>
<td>none</td>
<td>3.0</td>
<td>14.9</td>
<td>brown silt</td>
<td></td>
<td>-142</td>
<td>none</td>
<td>x (slight)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>97</td>
<td>23.09.83</td>
<td>none</td>
<td>13.0</td>
<td>14.9</td>
<td>brown silt</td>
<td></td>
<td>-112</td>
<td>none</td>
<td>x (slight)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>98</td>
<td>23.09.83</td>
<td>none</td>
<td>7.0</td>
<td>14.9</td>
<td>brown silt</td>
<td></td>
<td>-90</td>
<td>none</td>
<td>x</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>99</td>
<td>23.09.83</td>
<td>none</td>
<td>2.0</td>
<td>13.9</td>
<td>medium sand with little silt</td>
<td></td>
<td>-85</td>
<td>none</td>
<td>x</td>
<td>Little algae on surface</td>
<td>-</td>
</tr>
<tr>
<td>100</td>
<td>23.09.83</td>
<td>none</td>
<td>14.0</td>
<td>13.1</td>
<td>brown silt</td>
<td></td>
<td>-130</td>
<td>none</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
LOCATION - 2901 (JUN 86)

VARIATION OF CURRENT DIRECTION, SPEED AND TEMPERATURE WITH TIME: LEIGH BAY ST. MARY'S RIVER

Figure D.4(a) Current Meter Velocity in Leigh Bay at Location 2901 - June 1986 - Lat. 46° 30' 1" N and Long. 84° 25' 52" W.
Figure D.4(b)  Current Rose in Leigh Bay at Location 2901 - 
June 1986 - Lat. 46° 30' 1" N and 
Long. 84° 25' 52" W.
LOCATION - 2901 (JUL 86)

TEMPERATURE

DEGREES

SPEED

STICK VECTOR

DAY OF MONTH

VARIATION OF CURRENT DIRECTION, SPEED AND TEMPERATURE WITH TIME: LEIGH BAY ST. MARY'S RIVER

Figure D.5(a) Current Meter Velocity in Leigh Bay at Location 2901 - July 1986 - Lat. 46° 30' 1" N and Long. 84° 25' 52" W.
Figure D.6(a) Current Meter Velocity in Leigh Bay at Location 2902 - June 1986 - Lat. 46° 30' 10" N and Long. 84° 25' 10" W.
Figure D.5(b) Current Rose in Leigh Bay at Location 2902 - June 1986 - Lat. 46° 30' 10" N and Long. 84° 25' 10" W.
LOCATION - 2902 (JUL 86)

TEMPERATURE

DIRECTION

SPEED

STICK VECTOR

DAY OF MONTH

VARIATION OF CURRENT DIRECTION, SPEED AND TEMPERATURE WITH TIME : LEIGH BAY ST. MARY'S RIVER

Figure D.7(a) Current Meter Velocity in Leigh Bay at Location 2902 - July 1986 - Lat. 46° 30' 10" N and Long. 84° 25' 10" W.
LOCATION - 2902 (JUL 86)

CURRENT ROSE HISTOGRAM: LEIGH BAY

ST. MARY'S RIVER

LEGEND

- 1.5-2.0CM/S
- 2.0-5.0CM/S
- 5.0+ CM/S

Figure D.7(b) Current Rose in Leigh Bay at Location 2902 -
July 1986 - Lat. 46° 30' 10" N and
Long. 84° 25' 10" W.
LOCATION - 2903 (JUN 86)

VARIATION OF CURRENT DIRECTION, SPEED AND TEMPERATURE WITH TIME: ALGOMA STEEL ST. MARY'S RIVER

Figure D.8(a) Current Meter Velocity at Algoma Steel - Location 2903 - June 1986 - Lat. 46° 30' 44" N and Long. 84° 22' 56" W.
Figure D.8(b) Current Rose at Algoma Steel - Location 2903 -
June 1986 - Lat. 46° 30' 44" N and
Long. 84° 22' 56" W.
LOCATION – 2903 (JUL 86)

TEMPERATURE

DIRECTION

SPEED

STICK VECTOR

DAY OF MONTH

VARIATION OF CURRENT DIRECTION, SPEED AND TEMPERATURE WITH TIME: ALGOMA STEEL ST. MARY'S RIVER

Figure D.9(a) Current Meter Velocity at Algoma Steel - Location 2903 - July 1986 - Lat. 46° 30' 44" N and Long. 84° 22' 56" W.
LOCATION - 2903 (JUL 86)

CURRENT ROSE HISTOGRAM: ALGOMA STEEL

ST. MARY'S RIVER

LEGEND

1.5-3.0 CM/S
3.0-6.7 CM/S
6.7+ CM/S

Figure D.9(b) Current Rose at Algoma Steel - Location 2903 - July 1986 - Lat. 46° 30' 44" N and Long. 84° 22' 56" W.
Note: See also Figs. 5.20 (a) to (d)
Figure D.12  Aerial Drogue Velocities for the Lake George Channel north of Sugar Island.
Figure D.13 Aerial Drogue Velocities for the Channel west of Sugar Island to Lake Nicolet.
APPENDIX E

VELOCITY VECTOR PLOTS FOR UPPER ST. MARYS RIVER
Overview.

In this appendix, a collection of the velocity vector diagrams computed by the FEM model for the Upper St. Marys River is documented for future reference. The velocity vectors are for a flow of 81,100 cfs (2,296 m³/s) with vertical eddy viscosity at 10 cm²/s and slip coefficient of 0.3. The following cases are compiled in this appendix:

(a) North 12 mph (19.3 km/h) wind - Figs. E1 (a) to (f);

(b) East 12 mph (19.3 km/h) wind - Figs. E2 (a) to (f);

(c) South 12 mph (19.3 km/h) wind - Figs. E3 (a) to (f);

(d) Southwest 12 mph (19.3 km/h) wind - Figs. E4 (a) to (f);

and

(e) West 12 mph (19.3 km/h) wind - Figs. E5 (a) to (f).

In each of the above cases, the velocity vector plots at the lake surface and at 0.2, 0.4, 0.6 and 0.8 of the total depth below the lake surface are given. A depth averaged velocity plot is also given for each of the cases.
Figure E.1(a) Surface Velocity Vectors - N Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.1(b) Velocity Vectors at 0.2 Depth Below Surface - N Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.1(c) Velocity Vectors at 0.4 Depth Below Surface -
N Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.1(d) Velocity Vectors at 0.6 Depth Below Surface — N. Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.1(e) Velocity Vectors at 0.8 Depth Below Surface - N Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.1(f) Depth Averaged Velocity Vectors - N Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.2(a) Surface Velocity Vectors – E Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.2(b) Velocity Vectors at 0.2 Depth Below Surface - E Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.2(c) Velocity Vectors at 0.4 Depth Below Surface —
E Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.2(d)  Velocity Vectors at 0.6 Depth Below Surface -
E Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.2(e) Velocity Vectors at 0.8 Depth Below Surface — E Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.2(f) Depth Averaged Velocity Vectors - E Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.3(a)  Surface Velocity Vectors - S Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.3(b) Velocity Vectors at 0.2 Depth Below Surface -
S Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.3(c)  Velocity Vectors at 0.4 Depth Below Surface - S Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.)
Figure E.3(d) Velocity Vectors at 0.6 Depth Below Surface -
South Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.3(e) Velocity Vectors at 0.8 Depth Below Surface -
3 Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.3(f) Depth Averaged Velocity Vectors - S Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.)
Figure E.4(a) Surface Velocity Vectors - SW Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.4(b) Velocity Vectors at 0.2 Depth Below Surface — SW Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.4(c) Velocity Vectors at 0.4 Depth Below Surface - SW Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.4(d)  Velocity Vectors at 0.6 Depth Below Surface -
SW Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.4(e) Velocity Vectors at 0.8 Depth Below Surface - SW Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.4(f) Depth Averaged Velocity Vectors - SW Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.5(a) Surface Velocity Vectors – W Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s.
Figure E.5(b)  Velocity Vectors at 0.2 Depth Below Surface - W Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.5(c) Velocity Vectors at 0.4 Depth Below Surface - W Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
Figure E.5(d) Velocity Vectors at 0.6 Depth Below Surface —
W Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed
Slip Coeff. of 0.3; and Vert. Eddy Viscosity
of 10 cm²/s).
Figure E.5(f) Depth Averaged Velocity Vectors – W Wind at 19.3 km/h; Flow of 2,296 m³/s; Bed Slip Coeff. of 0.3; and Vert. Eddy Viscosity of 10 cm²/s).
APPENDIX F

FEM MODEL USERS GUIDE
Overview.

An outline of the Galerkin finite element formulation and solution has been given in Chapter 3. The Upper St. Marys River is discretized using two dimensional simplex element. The model is able to do a numerical simulation of the hydrodynamics of the Upper River under different flow and wind conditions.

The input data to the Upper River is based on conditions in September when the flow is 81,100 cfs (2,296 m³/s) and the long term average water surface elevation is 601.37 feet (183.34 metre). However, the FEM model has interactive options that allow the user to change these values as well as other input parameters such as wind speed and direction, vertical eddy viscosity, bottom slip coefficient and with or without ice cover on the lake. An example of this interaction is shown in Fig. F.1.

A sample output listing of the results from the FEM model is illustrated in Fig. F.2. Some comments are embedded in Fig. F.2 to help clarify the significance of each part of the output listing. Finally, the input card arrangement of the FEM model is given in Fig. F.3. Again comments are embedded where necessary to help clarify the input data preparation. However, it should be emphasized that for the Upper River application, there is no necessity to make any modifications to these input cards. All anticipated changes are handled in the manner illustrated in Fig. F.1. The input data for the Upper River are on the program.
diskette provided, with the filename "STM.DAT". It is recommended that the user should read the "README.1ST" file on the program disk for any recent up-date information.

**System Requirements**

- CGA (Colour Graphics Adapter) monitor
- 512 kilobytes RAM
- Intel Math Co-processor (8087 or 80287 processor)
- IBM or MS DOS version 3.0 or later
A Finite Element Program for Steady Three Dimensional Circulation with Inflow and Ice Cover Conditions.

#### WARNING !!!!

a. Use UpperCase at (Y/N)? prompts.
b. Use Decimal Values at prompts for input constants.

** Enter Output Results FileName? --
STMARYS.RES
** Inflow/Outflow in cu.ft/s = 81100.000000
** Change Inflow/Outflow (Y/N)? --> Y
** Enter NEW Inflow/Outflow in cu.ft/s --> 125000.0
** Long term Ave. WSEL in ft = 601.3700000
** Change WSEL (Y/N)? --> Y
** Enter NEW WSEL in ft ? --> 605.0
** With Ice Cover (Y/N)? --> N
** Enter Wind Speed in MPH ? --> 24.0
** Wind Direction Selection :

```
N       NW
NW       WNW
NW        W
W        E
W        WSW
W        SW
W        S

** Direction in Upp.Case char.string? ---> ESE
** Bed Slip Permitted (Y/N)? --> Y
** Enter Slip Coeff. -- must be GT zero ---> 0.3
** Enter V.Eddy Viscosity? -- sq.cm/s --> 20.0
** Output Elem.,Node, No., Co-ord. (Y/N)? --> N
** Output Uz,Vz between Surface & Bed (Y/N)? --> Y
--- Please Wait ! ----
--- Please Wait ! ----
Stop - Program terminated.
```

Figure F.1 A Sample of the Screen-Keyboard Interaction.
This is an example output listing from the program STMARYS.EXE using the input data file STIM.DAT. Some comments are embedded in between the output print-out to help clarify their significances.

A Finite Element Program for Steady Three Dimensional Circulation with Inflow and Ice Cover Conditions.

A Microsoft FORTRAN 77 version developed at University of Windsor, Department of Civil Engineering. A User's Guide is available. For assistance consult:

Dr. J. A. McCorkodale
Dr. K. A. Ibrahim
Mr. E. M. Yuen

Version 1.0 (1986)

********** WIND DRIVEN CIRCULATION OF ST. MARYS RIVER

## Number of Nodes = 157
## Number of Elements = 248
## Size of Band Width = 17
## Coriolis (rad/s) = 1.055010E-004
## Inflow/Outflow (cu.ft/s) = 126000.000000000
## Water Surface Elev. (ft) = 665.000000000
## Length = 5.71515 Miles
## Ice Cover Over Lake? = No
## Bed Slip Coeff. = 3.000000E-001
## Wind Speed (cm/s) = 1072.9560000
## Wind Direction = ESE
## Wind stress T1 (sq.cm/sq.cm) = -3.1304450
## Wind stress T2 (sq.cm/sq.cm) = 1.3215270
## Vert. Eddy Viscosity (sq.cm/s) = 20.0000000

Figure F.2 Output Listing with Comments.
### Table

<table>
<thead>
<tr>
<th>Elem.</th>
<th>Node Number</th>
<th>X(1)</th>
<th>Y(1)</th>
<th>H(1)</th>
<th>X(2)</th>
<th>Y(2)</th>
<th>H(2)</th>
<th>X(3)</th>
<th>Y(2)</th>
<th>H(3)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1 6 7</td>
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<td>6.3</td>
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<td>.1</td>
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<td>.4</td>
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<td>1.3</td>
<td>.5</td>
<td>29.3</td>
</tr>
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<td>1.3</td>
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<td>.5</td>
<td>29.3</td>
<td>1.1</td>
<td>.2</td>
<td>29.3</td>
</tr>
<tr>
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<td>1.6</td>
<td>.3</td>
<td>8.3</td>
<td>1.6</td>
<td>.5</td>
<td>9.3</td>
<td>1.5</td>
<td>.6</td>
<td>15.3</td>
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<td>1.6</td>
<td>.3</td>
<td>8.3</td>
<td>1.5</td>
<td>.6</td>
<td>15.3</td>
<td>1.4</td>
<td>.4</td>
<td>11.3</td>
</tr>
<tr>
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<td>7 13 13</td>
<td>1.4</td>
<td>.4</td>
<td>11.3</td>
<td>1.5</td>
<td>.6</td>
<td>15.3</td>
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<td>29.3</td>
</tr>
<tr>
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<td>7 13 8</td>
<td>1.4</td>
<td>.4</td>
<td>11.3</td>
<td>1.5</td>
<td>.7</td>
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<td>1.3</td>
<td>.5</td>
<td>29.3</td>
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<td>.2</td>
<td>29.3</td>
<td>1.3</td>
<td>.5</td>
<td>29.3</td>
<td>1.2</td>
<td>.6</td>
<td>25.3</td>
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<tr>
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<td>3 9 4</td>
<td>1.1</td>
<td>.2</td>
<td>29.3</td>
<td>1.2</td>
<td>.6</td>
<td>25.3</td>
<td>1.0</td>
<td>.3</td>
<td>19.3</td>
</tr>
<tr>
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<td>4 9 10</td>
<td>1.0</td>
<td>.3</td>
<td>19.3</td>
<td>1.2</td>
<td>.6</td>
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<td>1.2</td>
<td>.7</td>
<td>7.3</td>
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<tr>
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<td>4 10 5</td>
<td>1.0</td>
<td>.3</td>
<td>19.3</td>
<td>1.2</td>
<td>.7</td>
<td>7.3</td>
<td>.9</td>
<td>.5</td>
<td>8.3</td>
</tr>
</tbody>
</table>

### Comments:

- **Elem.**: Element Number.
- **Node Number**: Each element has three nodes numbered in an anti-clockwise direction denoted as \( i, j, k \).
- **X(1), Y(1)**: \( x, y \) coordinates in miles based on a map scale of 1:40,000.
- **H(1)**: Depth at each node in feet.

---

**Figure F.2 Output Listing with Comments (cont'd).**
WIND DRIVEN CIRCULATION OF ST. MARYS RIVER

**Nodal Values Loading Case**

<table>
<thead>
<tr>
<th>El.No</th>
<th>Um cm/s</th>
<th>Ve cm/s</th>
<th>UVe cm/s</th>
<th>Dir</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-32E+01</td>
<td>25E+02</td>
<td>26E+02</td>
<td>71E+01</td>
</tr>
<tr>
<td>2</td>
<td>-20E+01</td>
<td>25E+02</td>
<td>26E+02</td>
<td>45E+01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>El.No</th>
<th>Um cm/s</th>
<th>Ve cm/s</th>
<th>UVe cm/s</th>
<th>Dir</th>
</tr>
</thead>
<tbody>
<tr>
<td>154</td>
<td>6200000000E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>155</td>
<td>6200000000E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>156</td>
<td>3150000000E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>157</td>
<td>0000000000E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Comments:**

Computed nodal distribution of stream function values in cubic feet per second across the lake boundaries.

**Table:**

<table>
<thead>
<tr>
<th>El.No</th>
<th>Um cm/s</th>
<th>Ve cm/s</th>
<th>UVe cm/s</th>
<th>Dir</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-32E+01</td>
<td>25E+02</td>
<td>26E+02</td>
<td>71E+01</td>
</tr>
<tr>
<td>2</td>
<td>-20E+01</td>
<td>25E+02</td>
<td>26E+02</td>
<td>45E+01</td>
</tr>
</tbody>
</table>

**Comments:**

El:Element Number.

Ua, Va: x, y component Depth Averaged Velocities.

UVa: Square Root of (Ua^2 + Va^2).

Uz, Vz: x, y component Horizontal Velocities at the lake surface, 0.2, 0.4, 0.6 and 0.8 Depths below the surface.

UVz: Square Root of (Uz^2 + Vz^2).

Dir: Velocity Direction from the North where, +ve values indicate angles anti-clockwise from the North, while -ve values are clockwise.

Figure F.2 Output Listing with Comments (cont'd).
### Wind Driven Circulation of St. Marys River

#### Nodal Values Loading Case

<table>
<thead>
<tr>
<th>Case</th>
<th>Values</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.000000000E+01 2.699999976E+00 3.51999991E+00</td>
<td>Computed nodal distribution of stream function values in non-dimensional units across the lake boundaries.</td>
</tr>
<tr>
<td>4</td>
<td>1.259999995E+00 5.000000000E+00 6.100000000E+01</td>
<td></td>
</tr>
</tbody>
</table>

---

**Figure P.2** Output Listing with Comments (cont'd).
Column no: 12345678901234567890123456789012345678901234567890

Card#1 Title: ************ WIND DRIVEN CIRCULATION OF ST. MARYS RIVER

Card#2 NP,NE,NSW,FCP,DISC,WSEL,DL :

157,246,17,0,105501E-3,81100.0,601.37,5.715151

where:

NP : Number of Nodes.
NE : Number of Elements.
NSW : Band Width.
FCP : Coriolis in rad/s.
DISCH : Inflow/Outflow in cu.ft/s.
WSEL : Water Surface Elevation in ft.

Cards #3 to #250 are element & node numbers, x,y coords., depths,
and Up-Winding codes :

1 1 6 7 6.40 0.50 5.30 5.10 8.30 5.70 1.501133002
2 1 7 2 6.40 0.50 5.70 1.501133 5.40 0.60 7.33001
3 2 7 8 5.40 0.60 7.33 5.70 1.501133 5.20 2.002933000
4 2 8 3 5.40 0.60 7.30 5.20 2.002933 4.60 1.002933000
5 6 11 12 6.30 1.30 8.34 5.50 1.90 9.34 6.10 2.401534002

Cards #251 to #261 are boundary node numbers and their nodal
values of dimensionless stream function :

1 6 11 10 20 29 38 1.00 1.00 1.00 1.00 1.00 1.00
47 56 65 74 83 92 1.00 1.00 1.00 1.00 1.00 1.00
101 110 115 120 127 125 1.00 1.00 1.00 1.00 1.00 1.00
125 132 139 140 141 146 1.00 1.00 1.00 1.00 1.00 1.00
152 153 154 148 143 149 1.00 0.75 0.50 0.50 0.50 0.50
155 156 157 151 145 138 0.50 0.25 0.00 0.00 0.00 0.00
131 124 119 114 105 106 0.00 0.00 0.00 0.00 0.00 0.00
107 108 109 100 91 82 0.00 0.00 0.00 0.00 0.00 0.00
73 64 55 46 37 28 0.00 0.00 0.00 0.00 0.00 0.00
19 18 17 15 15 10 0.00 0.00 0.00 0.00 0.00 0.00
4 5 4 3 2 -1 -1 0.00 0.13 0.52 0.90 0.00 0.00

Figure F.3 Layout of Input Cards for the FEM Model.
cards #262 to last card are repetition of cards #3 to #261:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>6</td>
<td>7</td>
<td>6.40</td>
<td>0.50</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
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<td>1.30</td>
</tr>
<tr>
<td>2</td>
<td>8.34</td>
<td>5.70</td>
<td>1.5011.33</td>
<td>5.40</td>
</tr>
<tr>
<td>3</td>
<td>5.40</td>
<td>0.60</td>
<td>7.33</td>
<td>5.20</td>
</tr>
<tr>
<td>4</td>
<td>5.20</td>
<td>2.0029.330000</td>
<td>7.33</td>
<td>5.20</td>
</tr>
<tr>
<td></td>
<td>4.60</td>
<td>1.0029.320000</td>
<td>2.0029.330000</td>
<td>4.60</td>
</tr>
</tbody>
</table>

24514915515021.7011.5025.4922.5011.5022.4921.4012.7019.48002
24615515615022.5011.5022.4922.4012.80 7.4921.4012.7019.48001
24715015515121.4012.7019.4922.4012.80 7.4920.5013.9025.47601
24815615715122.4012.80 7.4922.2013.5031.4920.5013.9025.47602

<table>
<thead>
<tr>
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<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>6</td>
<td>11</td>
<td>20</td>
<td>29</td>
</tr>
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<td>3.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
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<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>3</td>
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<td>73</td>
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</tr>
<tr>
<td>19</td>
<td>18</td>
<td>17</td>
<td>15</td>
<td>10</td>
</tr>
</tbody>
</table>

Last Card:
5 4 3 2 -1 -1 0.00 0.13 0.52 0.50 0.00 0.00

--- End of Input Data ---

Figure F.3 Layout of Input Cards for the FEM Model (cont'd).
APPENDIX G

KETOX USERS GUIDE
University of Windsor

KETOX Model

Version 3.0
October 1987

USER'S GUIDE

Introduction

This model will simulate the hydrodynamics and far field pollutant transport for most river systems with multiple inputs of conservative or non-conservative chemicals. The model will also simulate the water column and the active bed layer sediment chemical concentrations. This is achieved by incorporating in the model the diffusive exchange between the water column and the sediment as well as the chemical decay and transport mechanism of the particulate.

Outline of the Model

The model requires the user to segment the river into channels or reaches. River segmentation is a very powerful tool and can be used to analyse complex river systems. Analyses of the river then normally begin at a segment where the boundary conditions are known, and proceed sequentially downstream. Thus the results found for one segment are used as the upstream boundary condition for the next segment.

The model is programmed in FORTRAN 77. A brief outline of the model's program structure may assist the user's understanding of the data preparation. The program consists of:

(a) a DIRECTORY or MAIN program which calls the following four Sub-Models (i.e. subroutines):

- Dispx - Hydrodynamics and Transport
- Split - Divides flow into two channels
- Unfrn - Mixes pollutant uniformly across a channel
- Comb - Combines flow and pollutant from two channels into one;

and

(b) the Sub-Model itself which may or may not call on one or more of 13 other supporting subroutines (such as HYD, SYFLOW, RELAX, MIX, KE, ANALYT, TRIDG, SOLVE; TOXIC).
To run the model, the user must provide the necessary input data which are all confined within two input data files as described below:

(1) an executive command data file (e.g. KETOX.DIR) to specify the number of Sub-Models needed and to describe the calling sequence of the Sub-Model (i.e. either Dispx or Split or Unfrm or Comb). The calling sequence of the Sub-Models will depend on how the modeller have segmented the river starting from the upstream segment to the downstream segment. Each Sub-Model’s list of arguments will also be input along with the Sub-Model type.

and

(2) a second input data file (e.g. KETOX.RIV) to describe the boundary condition, decay and reaction rates constant, discretization, Manning’s n, channel cross-section and outfall information. These are the minimum input data requirements for the model to run. The units for these input data are in feet-second for discharges and velocities, while the concentrations are in S.I. units. However additional input data on settling velocity, resuspension velocity, sedimentation rate, active bed layer thickness and partition coefficients for the water column and the sediments will be required if the modeller needs the chemical concentration in the bed.

The filenames KETOX.DIR and KETOX.RIV will now be used consistently for the rest of this document. However, the user is at liberty to change these filenames when running the model. It is recommended that the user keeps the filename extensions "DIR" and "RIV" so as to avoid confusion.

**KETOX.DIR**

As mentioned the DIRECTORY or MAIN program may call in any logical order any of the four Sub-Models (namely, Dispx, Split, Unfrm, Comb) to describe a river system. Each of these Sub-Models has an argument or parameter list which will be discussed in detail in the sections to follow on each of the four Sub-Models.

A hypothetical river system will now be used to illustrate the input data preparation for the file KETOX.DIR. For example, to simulate a river with an island and a reach with high mixing (e.g. waterfalls) such as that shown in Fig. G.2, the following organization of the Sub-Models (i.e. Dispx, Comb, Split and Unfrm) should be used in the executive command input data file (i.e. KETOX.DIR):
It should be pointed out that the first card must contain the second input data filename which in this case is KETOX.RIV. The card arrangement above also illustrates how to number the water column concentration array in each river segment (i.e. the parameters NUMCON, NTOPC, NBOTC).

**SUB-MODELS**

As illustrated in the above example, the four sub-models were repeatedly called eight times in the KETOX.DIR file in a certain calling sequence as needed to describe the segmentation of the river system example. The four Sub-Models may in turn use various of the 13 subroutines depending on the values given to each argument of the Sub-Model’s argument or parameter list. Each of the Sub-Models and their individual arguments or parameters will now be explained in detail.

**DispX Sub-Model**

The Dispersion Sub-Model can be applied to any simple river reach. On being called by the DIRECTORY, it will in turn read the outfall data from the second input data file (i.e. KETOX.RIV). Then it calls the simplified flow distribution model HYD (one of the 13 subroutines) which in turn, for each cross-section, reads the channel width and radius of curvature followed by 40 equally spaced flow depths across the channel from the second input data file KETOX.RIV. The flow distribution is then computed including the secondary flow near the surface and bed at the centre line of
the river. At this point the model may use a constant dispersion
coefficient and proceeds with the far field dispersion
calculation. There is also an option to call the k-\(\varepsilon\) turbulence
model to obtain the dispersion coefficient.

There are 13 user definable arguments in the executive
command Dispx to be included in the command input data file.
These arguments are described below:

\[
\text{Dispx NUMBER QPERC AD NUMCON CEXP IC NS NC DXK FACT NHALF IDV ITX}
\]

where

- \(\text{Disp}\) = executive command of the Sub-Model;
- \(\text{NUMBER}\) = identification number of the reach;
- \(\text{QPERC}\) = flow in the reach as a percentage of the total
  river inflow, \(\text{QTOTAL}\);
- \(\text{AD}\) = depth adjustment in the reach (default value = 1.0);
- \(\text{NUMCON}\) = C array concentration identifier, i.e. storage
  location for current reach concentrations;
  (note: 0,1,2,3,4,5,6,7 could be used)
- \(\text{CEXP}\) = empirical exponent for the shape factor to account
  for bank effects on velocity distribution;
- \(\text{IC}\) = 1 calls HYD or
  0 reads flow pattern data;
- \(\text{NS}\) = number of cross-sections in the reach;
- \(\text{NC}\) = number of equal sub-divisions of \(\Delta X_T\) for
  computation of C;
- \(\text{DXK}\) = +'ve \(\Delta X_k\) for k-\(\varepsilon\) model or -'ve value bypasses the
  k-\(\varepsilon\) model;
- \(\text{FACT}\) = factor to adjust default value of the dispersion
  coefficient (default value is 15 \text{ ft}^2/\text{s} ); and
- \(\text{NHALF}\) = node at which transboundary estimate is made.
- \(\text{IDV}\) = an integer parameter and must be one of the
  following cases:
  0 no momentum modification is needed, that is the
  equilibrium velocity distribution calculated by
  the HYD subroutine is adequate for the reach.
  The corresponding k-\(\varepsilon\) model can be either
  activated or bypassed (i.e. DXK can be either
  +'ve or -'ve);
  1 same as for IDV = 0, except that in addition the
    user must now include in the second input data
    file, 40 equally equally spaced representative
    velocity values across the first cross-section
    of the reach. These velocities should be fairly
    representative of those actually observed at the
    reach.
  2 same as for IDV = 1, except that the k-\(\varepsilon\) model
    must be activated (i.e. the corresponding DXK
    parameter must always be +'ve). The momentum
    solution is implemented. In this case regions of
    jet flow can be adequately simulated by
    diffusing the excess or deficit momentum
    gradually across the reach. A momentum diffusion
    coefficient is required and is obtained from the
k-e model. The momentum excess or deficit is computed relative to the equilibrium velocity distribution as calculated by HYD while ensuring that mass is conserved at all times in the diffusion process.

\[ \text{ITX} = \text{an integer parameter and must be one of the following cases:} \]

0 no simulation of chemical concentration in the bed sediment is needed; and
1 option to simulate chemical concentration in the bed sediments. Additional input data is needed on partition coefficients in the water column and the sediments, settling velocity, resuspension velocity and sedimentation rate. User must include these additional input data in the second input data file KETOX.RIV.

Split Sub-Model

The Split Sub-Model divides the nodal concentrations e.g. C1, between two channels giving new nodal concentrations, e.g. C2 and C3 (see Fig. G3).

There are 5 user definable arguments in the executive command Split to be included as data in the command input file. These arguments are as follows:

\[ \text{Split PR1 PR2 NUSC NTOPC NBOTC} \]

where Split is executive command of the Sub-Model;
PR1 = percentage of total flow (not of QTOTAL) assigned to channel adjacent to node No. 1 of NUSC;
PR2 = percentage of total flow (not of QTOTAL) assigned to channel adjacent to node No. NOD of NUSC;
\{ note: NOD = total number of nodes in any cross-section; \}
PR1 + PR2 = 100.0% 
NUSC = nodal concentration array ID before flow division;
NTOPC = nodal concentration array ID corresponding to channel with PR1 % of flow; and
NBOTC = nodal concentration array ID corresponding to channel with PR2 % of flow;

Comb Sub-Model

The Combine Sub-Model combines and mixes the loads from two channels at their confluence. The combining of the two flows is assumed to be completed in a distance DX. This programme identifies the concentration discontinuity at the shear-line between the combining flows and uses an analytical solution (MIX) to disperse these concentrations. A turbulent dispersion using Dispx may subsequently be applied to the resulting concentrations (see Fig. G4).

The user must define 16 arguments as data in the command input file for the executive command Comb. These arguments are:
Comb NUMBER QPERC FR1 FR2 AD NUMC1 NUMC2 NUMC FDX CEXP IC NS NC
DXK DX IDV ITX

where Comb = executive command of the Sub-Model;
NUMBER = identification of the reach;
QPERC = fraction of flow entering from channel 1 which is adjacent to Node No. 1 in the resultant downstream channel;
FR1 = % fraction of flow entering from channel 2, i.e. adjacent to Node No. NOD in downstream channel;
FR2 = % number of lateral nodes
AD = depth adjustment in the reach (default value = 1.0);
NUMC1 = concentration array ID in channel 1;
NUMC2 = concentration array ID in channel 2;
NUMC = resultant concentration array ID (see Fig. G.4);
FDX = factor by which the normal dispersion coefficient at the middle of the channel should be multiplied to account for the increased mixing due to the impact of one flow on the other. If the junction is smooth (flows nearly parallel with similar average currents) then FDX = 1 as the flows meet at larger angled (\(\infty\)) (up to 180°) or larger differential currents the value of FDX will increase. The relative magnitude of each flow is also important. For a right angle confluence of approximately equal flows, it was found that 10.0 < FDX < 30.0;
CEXP = empirical exponent for the shape factor to account for bank effects on velocity distribution;
IC = 1 calls HYD or 0 reads flow pattern data;
NS = number of cross-section in a reach, normally = 2;
NC = number of equal sub-divisions of \(\Delta X_T\) for computation of C;
DXK = +ve \(\Delta X_k\) for k-e model or -ve value bypasses the k-e model; and
DX = assumed extent of confluence mixing effect.
IDV = an integer parameter that can be either 0, 1 or 2 (see detailed explanation in sub-model DispX).
ITX = an integer parameter and must be one of the following cases:
0 no simulation of chemical concentration in the bed sediment is needed; and
1 option to simulate chemical concentration in the bed sediments. Additional input data is needed on partition coefficients in the water column and the sediments, settling velocity, resuspension velocity and sedimentation rate. The user must include these additional input data in the second input data file KETOX.RIV.
Unfrm Sub-Model

Sometimes the contaminant in a channel can be assumed to be completely mixed vertically and laterally. This may occur along narrow channels, in whirlpools, on waterfalls or in hydraulic jumps.

The Uniform Sub-Model uniformly mixes the inflow with any local inputs and over-writes the qld C array with a new one. Unfrm is used as an executive command in the input file with the following arguments:

\[ \text{Unfrm NUMBER QPERC NUMBC QO CO ITX} \]

where

- **Unfrm** = executive command for the Sub-Model;
- **NUMBER** = identification of the reach location;
- **QPERC** = flow entering this section as a percentage of QTOTAL;
- **NUMBC** = concentration array ID for the channel to be uniformly mixed;
- **QO** = local outfall discharge in cu.ft/s; and
- **CO** = local outfall concentration.
- **ITX** = an integer parameter and must be one of the following cases:
  - 0 no simulation of chemical concentration in the bed sediment is needed; and
  - 1 option to simulate chemical concentration in the bed sediments. Additional input data is needed on partition coefficients in the water column and the sediments, settling velocity, resuspension velocity and sedimentation rate. User must include these additional input data in the second input data file KETOX.RIV.

KETOX.RIV

The filename "KETOX.RIV" must be specified in Card 1 of KETOX.DIR. A summary of the input data required for KETOX.RIV is given in Table G.1. It is made up of two groups of input data described as data Group A and Group B.
Data Group A

The first five input cards complete this group. Their card arrangement are illustrated below:

Column:  1  2  6  7  8
          12345678901234567890          012345678901234567890

Card 1:TT..........................TT
Card 2:AA BB
Card 3:C1 C2 C3 .................... CAA
Card 4:D1 D2 D3 .................... DAA-1 100.
Card 5:EE

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card1:TT..TT</td>
<td>Title</td>
<td>Title of river simulated</td>
</tr>
<tr>
<td>Card2:AA</td>
<td>Nodes</td>
<td>Number of nodal points laterally across each river cross-section (typically AA = 15)</td>
</tr>
<tr>
<td>:BB</td>
<td>DX(^*)</td>
<td>Space step between two adjacent cross-section of the river ((^*) see additional note on DX)</td>
</tr>
<tr>
<td>Card3:C1..CAA</td>
<td>Conc.</td>
<td>Initial (ambient) chemical concentrations at the upstream boundary (typically 15 values)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>S.I.</td>
</tr>
<tr>
<td>Card4:D2..100.0</td>
<td>n</td>
<td>Initial upstream boundary stream function values for node 2 to node AA: ( D_1 = 0.0 % )</td>
</tr>
<tr>
<td>Card5:EE</td>
<td>Decay</td>
<td>A combined effective decay constant</td>
</tr>
</tbody>
</table>

* Additional Note on DX

The value of DX will remain the same for the entire river to be modelled once its numeric value is chosen by the modeller. DX will determine how many cross-sections the modeller must provide in order to segment the entire river to be simulated. For instance the length of a river segment such as Dispx divided by the value of DX will give the number of river cross-sections (NS parameter) in the segment which the modeller must discretize. The modeller must then provide river depths at each node (typically 15 nodes are used) for each river cross-section. Hence the spatial resolution to describe the actual river bathmetry is controlled by the value of DX chosen. However it should not be confused with the numerical spatial resolution of the model which can be controlled by the value chosen for the NC parameter.
Data Group B

Only the river segments in the KETOX.DIR file that call the Sub-Models DispX and Comb will have additional input data requirements in this group. The card arrangement for these additional input data are shown in Table G.1 under the sub-heading Data Group B.

Table G.1

<table>
<thead>
<tr>
<th>Card/Item</th>
<th>Variables</th>
<th>Explanation</th>
<th>Integer</th>
<th>Decimal</th>
<th>Format</th>
<th>Units</th>
</tr>
</thead>
</table>

Data Group A

MAIN Programs

1 1 :TITLE River System Example
2 1 :NOD No. of nodes
3 1 to :C Initial Concentrations at nodes ( ML^-3 )
4 1 to :UPR Accumulated Y of flow from base shore
5 1 :DECAY Decay constant per second

Data Group B

* * For Each Executive Command DispX

6-1 1 :INFALL No. of point or non-point sources to
be considered in this reach
1 :INFALL Distance from start of reach to outfall
2 :INFALL The node at which outfall input is assigned
3 :INFALL Concentration of outfall ( ML^-3 )
4 :INFALL Outfall discharge

For ITI of 1 (i.e. suspended and bed sediments included) the following input data are needed

6-2 1 :NLAY Number of layers : Layer 1 => Water Column
2 :NSYSTEM Number of Systems :
3 :INFAR = 0 , use previously read kinetic constants
4 :ISY Print-out control selection :
5 1 :INFAR = 1 , read in new kinetic constants
6 1 :INFAR = 0 , print only Conc. C(i,j) in layer 1, i.e.
7 1 :INFAR = 1 , print C(i,j) and C(2lay,nsystem,j), i.e.
8 1 :INFAR = 2 , print the same as ISY = 1 and CD(layer,j)
9 1 :INFAR = 3 , print the same as ISY = 1 and CBED(j),
i.e. total bed conc.

\[ = 4 \text{ \text{print the same as ISY = 3 and THALF}(1,j)} \]

and \( \text{THALF}(2,j) \): 

\( \text{THALF}(1,j) = \text{time for bed conc. to increase} \)

\( \text{from} \ 0 \ \text{to} \ \text{CBED}(j)/2 \)

\( \text{THALF}(2,j) = \text{time for bed conc. to decrease} \)

\( \text{from} \ \text{CBED}(j) \ \text{to} \ \text{CBED}(j)/2 \)

5 \text{ \text{POROSITY}} \text{ Bed layer porosity} \quad \text{x \ Free \ ---}

6-3 \text{ \text{PHK}} \text{ Photolysis rate constant} \quad \text{x \ Free \ \text{sec}^{-1}}

2 \text{ \text{HYK}} \text{ Hydrolysis rate constant} \quad \text{x \ Free \ \text{sec}^{-1}}

3 \text{ \text{BDK}} \text{ Biodegradation rate constant} \quad \text{x \ Free \ \text{sec}^{-1}}

4 \text{ \text{IOK}} \text{ Oxidation rate constant} \quad \text{x \ Free \ \text{sec}^{-1}}

5 \text{ \text{EVK}} \text{ Volatilization rate constant} \quad \text{x \ Free \ \text{feet} \text{/s}}

6 \text{ \text{IBK}} \text{ Effective decay rate in the bed sediment} \quad \text{x \ Free \ \text{sec}^{-1}}

7 \text{ \text{BD}} \text{ Diffusion coefficient for the bed layer} \quad \text{x \ Free \ \text{feet} \text{/s}}

6-4 \text{ \text{BEDH2}(1..15)} \text{ Active bed layer thickness at 15 bed nodes} \quad \text{x \ Free \ \text{feet}}

15

For Each Layer \text{ (Layer = 1 to NLAY \text{,})}, \text{repeat the following input data for System (System = 1 to NSYSTEM)}

6-5 \text{ \text{HPYSyll}} \text{ Settling velocity of the System} \quad \text{x \ Free \ \text{feet} \text{/s}}

2 \text{ \text{HWS}} \text{ Resuspension velocity of the System} \quad \text{x \ Free \ \text{feet} \text{/s}}

3 \text{ \text{WS}} \text{ Sedimentation rate by the System} \quad \text{x \ Free \ \text{feet} \text{/s}}

6-6 \text{ \text{PIL1}} \text{ Partition coeff. in Layer 1 of the System} \quad \text{x \ Free \ ---}

2 \text{ \text{AMC1}} \text{ Mass Conc. in Layer 1 of the System} \quad \text{x \ Free \ \text{mg} / \text{L}}

6-7 \text{ \text{PIL2}} \text{ Partition coeff. in Layer 2 of the System} \quad \text{x \ Free \ ---}

2 \text{ \text{AMC2}} \text{ Mass Conc. in Layer 2 of the System} \quad \text{x \ Free \ \text{mg} / \text{L}}

For 10V of 1 or 2 observed velocities must be included as data 10 values per card

6-8 \text{ \text{UA1(1)}} \text{ 40 velocities equally distributed across the channel in ft/s.} \quad \text{x \ Free \ \text{feet} \text{/s}}

6-9 \text{ \text{IDW}} \text{ Section width in ft.} \quad \text{x \ Free \ \text{feet}}

2 \text{ \text{RC}} \text{ Radius of curvature to middle of channel} \quad \text{x \ Free \ \text{feet}}

( \text{from Node 1} )

6-10 \text{ \text{DB1(1)}} \text{ 40 depths uniformly distributed across the channel in ft. (cannot specify zero depths)} \quad \text{x \ Free \ \text{feet}}

3

For Each Executive Command Comb ( NS = 2 )

It is assumed that there is only one outfall.

7-1 \text{ \text{IFALL}} \text{ Usually 0.0 (ML-3)} \quad \text{x \ Free \ \text{feet}}

2 \text{ \text{VVFALL}} \text{ Usually 0.0} \quad \text{x \ Free \ \text{cu} / \text{ft} / \text{s}}

3 \text{ \text{ICFALL}} \text{ Usually 0.0} \quad \text{x \ Free \ \text{S.I.}}

4 \text{ \text{OFALL}}
For IDV of 1 or 2 observed velocities must be included as data 10
values per card

7-2 : 1 to :4V(1) 40 velocities equally distributed across the
        1 : 40 : channel in ft/s.

For HYD (........) repeat twice the 40 depths data

7-3 : 1 to :4D(1) 40 depths uniformly distributed across the
        1 : 40 : channel in ft. (cannot specify zero depths)

Program Implementation

The present version of the program is compiled using
Microsoft FORTRAN 77 Optimizing Compiler Version 4.0 and is
written with the intention of enabling the user a greater
flexibility in the set-up of the input data without having to
modify the source program itself. It also provides the user with
the option to vary the defaulted input parameters such as the
total river flow, the river depth adjustment for each reach and
the provision for ice cover simulation through an interactive
capability. This version of the model requires two input data
files presently referred to in this document as KETOX.DIR and
KETOX.RIV. The file KETOX.DIR is also referred to as the
executive command input data file, while KETOX.RIV is described
as the second input data file in the entire document. The input
data cards for KETOX.DIR have been clearly illustrated for a
simple river system example. Table 6.1 shows the required
arrangement of input data cards for the file KETOX.RIV.

The program is written to run on IBM PC/XT/AT or any IBM
compatible microcomputer. The user must ensure that the following
files are on the program diskettes:

<table>
<thead>
<tr>
<th>File</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>KETOX87.EXE</td>
<td>Executable image to run on machines with 8087</td>
</tr>
<tr>
<td></td>
<td>Math coprocessor installed.</td>
</tr>
<tr>
<td>KETOX.EXE</td>
<td>Executable image to run on machines without</td>
</tr>
<tr>
<td></td>
<td>8087 Math processor installed.</td>
</tr>
<tr>
<td>KETOX.DIR</td>
<td>Executive command input data file.</td>
</tr>
<tr>
<td>KETOX.RIV</td>
<td>Supporting input data file.</td>
</tr>
</tbody>
</table>
Figure 61 Definition of Computational Grids for Input Data, C and k-e.
Figure 62 Example of River System Showing the Appropriate Sub-Model and Definition of the C Array.
Figure G3 Definition Diagram for the SPLIT Sub-Model.
Figure G4 Definition Sketch for COMB Sub-Model.
Figure G.5  Layout of the KETOX.DIR Input File.
Figure G.6  Layout of the KETOX.RIV Input File.
<table>
<thead>
<tr>
<th>POROSITY</th>
<th>** PHK HYK BICX OXK EVK BK BD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00</td>
<td>** WP WRS WS Biotic Solids System 1</td>
</tr>
<tr>
<td>0.50</td>
<td>** PI &amp; Mass Conc. of Layer 1 &amp; System 1</td>
</tr>
<tr>
<td>0.50</td>
<td>** WP WRS WS Abiotic Solids System 1</td>
</tr>
<tr>
<td>0.50</td>
<td>** PI &amp; Mass Conc. of Layer 2 &amp; System 1</td>
</tr>
<tr>
<td>0.50</td>
<td>** WP WRS WS Abiotic Solids System 2</td>
</tr>
<tr>
<td>0.50</td>
<td>** PI &amp; Mass Conc. of Layer 2 &amp; System 2</td>
</tr>
<tr>
<td>0.50</td>
<td>** WP WRS WS Abiotic Solids System 3</td>
</tr>
<tr>
<td>1000.0, -9800.0</td>
<td>** PI &amp; Mass Conc. of Layer 2 &amp; System 3</td>
</tr>
</tbody>
</table>

** X'SECT. 1

** X'SECT. 2

** X'SECT. 3

** X'SECT. 4

** X'SECT. 5

---

Figure G.6  Layout of the KETOX.RIV Input File (cont'd).
Figure G.6  Layout of the KETOX.RIV Input File (cont'd).
<table>
<thead>
<tr>
<th>POROSITY</th>
<th>1.E-7,1.E-7,1.E-7,1.E-8,2.E-6,1.E-7,1.E-4</th>
<th>PHK HYK BIDK DXK EVK BK BD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.05E05,1.0</td>
<td>Pi &amp; Mass Conc. of Layer 1 &amp; System 1</td>
</tr>
<tr>
<td></td>
<td>0.02E05,0.3E04</td>
<td>Pi &amp; Mass Conc. of Layer 2 &amp; System 1</td>
</tr>
<tr>
<td></td>
<td>0.01E05,0.3E05</td>
<td>Pi &amp; Mass Conc. of Layer 2 &amp; System 2</td>
</tr>
<tr>
<td></td>
<td>0.00E02,1.0</td>
<td>Pi &amp; Mass Conc. of Layer 1 &amp; System 3</td>
</tr>
<tr>
<td></td>
<td>0.01E02,0.3E05</td>
<td>Pi &amp; Mass Conc. of Layer 2 &amp; System 3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>POROSITY</th>
<th>1.E-7,1.E-7,1.E-7,1.E-8,2.E-6,1.E-7,1.E-4</th>
<th>PHK HYK BIDK DXK EVK BK BD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.05E05,1.0</td>
<td>Pi &amp; Mass Conc. of Layer 1 &amp; System 1</td>
</tr>
<tr>
<td></td>
<td>0.02E05,0.3E04</td>
<td>Pi &amp; Mass Conc. of Layer 2 &amp; System 1</td>
</tr>
<tr>
<td></td>
<td>0.01E05,0.3E05</td>
<td>Pi &amp; Mass Conc. of Layer 2 &amp; System 2</td>
</tr>
<tr>
<td></td>
<td>0.00E02,1.0</td>
<td>Pi &amp; Mass Conc. of Layer 1 &amp; System 3</td>
</tr>
<tr>
<td></td>
<td>0.01E02,0.3E05</td>
<td>Pi &amp; Mass Conc. of Layer 2 &amp; System 3</td>
</tr>
</tbody>
</table>

---

**Figure G.6  Layout of the KETOX.RIV Input File (cont’d).**
Figure G.6  Layout of the KETOX.RIV Input File (cont'd).
Figure G.6  Layout of the KETOX.RIV Input File (cont'd).
Figure G.6 Layout of the KETOX.RIV Input File (cont'd).
Figure G.6 Layout of the KETOX.RIV Input File (cont'd).
APPENDIX H

TABLES
Table 4.1.
Flow Distribution at the Soo Locks

<table>
<thead>
<tr>
<th>Structure</th>
<th>Percent of Total Flow</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>May - Nov.</td>
<td>Dec.- April</td>
</tr>
<tr>
<td>Edison Power Canal</td>
<td>25%</td>
<td>28%</td>
</tr>
<tr>
<td>U.S. Navigational Canal</td>
<td>0.6%</td>
<td>0.2%</td>
</tr>
<tr>
<td>U.S. Power Canal</td>
<td>13%</td>
<td>15%</td>
</tr>
<tr>
<td>Regulating Works (Rapids)</td>
<td>26%</td>
<td>21%</td>
</tr>
<tr>
<td>Canadian Navigational Canal</td>
<td>0.3%</td>
<td>0.2%</td>
</tr>
<tr>
<td>Great Lakes Power Canal</td>
<td>36%</td>
<td>35%</td>
</tr>
<tr>
<td>Domestic Usage</td>
<td>0.2%</td>
<td>0.3%</td>
</tr>
</tbody>
</table>
Table 5.1
A Comparison of the F.E. Model and Corps of Engineers (1984) Velocities (Deep Zones)

Vertical Eddy Viscosity, $\eta = 10.0 \text{ cm}^2/\text{s}$
Bottom Slip Coefficient = 0.3
Flow at 81,100 cfs (2,298 $\text{m}^3/\text{s}$)

<table>
<thead>
<tr>
<th>Element Number</th>
<th>Corps of Engineers (1984) Station No.</th>
<th>Wind Direction/Speed</th>
<th>Distance Below Lake Surface</th>
<th>F.E. Model Velocity</th>
<th>Corps of Engineers (1984) Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>216</td>
<td>NW 19.3 km/h (12 mph)</td>
<td>0.2 Depth 0.4 Depth 0.8 Depth</td>
<td>0.46 m/s 0.41 m/s 0.22 m/s</td>
<td>0.46 m/s 0.43 m/s 0.39 m/s</td>
</tr>
<tr>
<td>26</td>
<td>210</td>
<td>NW 19.3 km/h (12 mph)</td>
<td>0.2 Depth 0.4 Depth 0.8 Depth</td>
<td>0.76 m/s 0.71 m/s 0.42 m/s</td>
<td>0.58 m/s 0.52 m/s 0.43 m/s</td>
</tr>
<tr>
<td>248</td>
<td>262</td>
<td>NW 19.3 km/h (12 mph)</td>
<td>0.2 Depth 0.4 Depth 0.8 Depth</td>
<td>0.34 m/s 0.26 m/s 0.13 m/s</td>
<td>0.31 m/s 0.39 m/s 0.67 m/s</td>
</tr>
<tr>
<td>126</td>
<td>233</td>
<td>ESE 19.3 km/h (12 mph)</td>
<td>0.2 Depth 0.4 Depth 0.8 Depth</td>
<td>0.37 m/s 0.35 m/s 0.19 m/s</td>
<td>0.34 m/s 0.34 m/s 0.24 m/s</td>
</tr>
<tr>
<td>157</td>
<td>241</td>
<td>ESE 19.3 km/h (12 mph)</td>
<td>0.2 Depth 0.4 Depth 0.8 Depth</td>
<td>0.32 m/s 0.32 m/s 0.19 m/s</td>
<td>0.31 m/s 0.31 m/s 0.21 m/s</td>
</tr>
<tr>
<td>180</td>
<td>244</td>
<td>ESE 19.3 km/h (12 mph)</td>
<td>0.2 Depth 0.4 Depth 0.8 Depth</td>
<td>0.32 m/s 0.34 m/s 0.20 m/s</td>
<td>0.31 m/s 0.34 m/s 0.21 m/s</td>
</tr>
</tbody>
</table>
Table 5.2

Qualitative Current Data (MOE 1985) in Leigh Bay Area.

<table>
<thead>
<tr>
<th>Station</th>
<th>Date</th>
<th>Current Velocity</th>
<th>Depth (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>123-1850</td>
<td>04.10.85</td>
<td>none</td>
<td>2.5</td>
</tr>
<tr>
<td>124</td>
<td>04.10.85</td>
<td>none</td>
<td>1.0</td>
</tr>
<tr>
<td>SMU2.5-1300</td>
<td>04.10.85</td>
<td>none</td>
<td>4.0</td>
</tr>
<tr>
<td>SMU2.5-1830</td>
<td>04.10.85</td>
<td>none</td>
<td>4.0</td>
</tr>
<tr>
<td>SMU2.5-2470</td>
<td>04.10.85</td>
<td>none</td>
<td>1.5</td>
</tr>
<tr>
<td>125-980</td>
<td>04.10.85</td>
<td>slight</td>
<td>12.0</td>
</tr>
<tr>
<td>126-2000</td>
<td>04.10.85</td>
<td>none</td>
<td>4.5</td>
</tr>
</tbody>
</table>
### Table 5.3

A Comparison of Velocity from Different Sources.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Element Number</td>
<td>Velocity</td>
<td>Station</td>
<td>Velocity</td>
</tr>
<tr>
<td>Leigh</td>
<td>ESE 19.3 km/h (12 mph)</td>
<td>135</td>
<td>2.8 cm/s</td>
<td>229</td>
<td>79.3 cm/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>163</td>
<td>3.1 cm/s</td>
<td>236</td>
<td>85.4 cm/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>166</td>
<td>7.4 cm/s</td>
<td>-</td>
<td>51.5 cm/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>174</td>
<td>1.8 cm/s</td>
<td>238</td>
<td>51.5 cm/s</td>
</tr>
<tr>
<td>Pointe</td>
<td>NW 19.3 km/h</td>
<td>39</td>
<td>3.4 cm/s</td>
<td>215</td>
<td>12.8 cm/s</td>
</tr>
<tr>
<td></td>
<td>(12 mph)</td>
<td>41</td>
<td>2.5 cm/s</td>
<td>212</td>
<td>35.4 cm/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>48</td>
<td>0.87 cm/s</td>
<td>213</td>
<td>25.9 cm/s</td>
</tr>
<tr>
<td>Aux</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pins</td>
<td>ESE 19.3 km/h</td>
<td>72</td>
<td>6.7 cm/s</td>
<td>220</td>
<td>16.5 cm/s</td>
</tr>
<tr>
<td>Bay</td>
<td>(12 mph)</td>
<td>78</td>
<td>6.0 cm/s</td>
<td>221</td>
<td>56.4 cm/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>105</td>
<td>4.4 cm/s</td>
<td>-</td>
<td>126-2000</td>
</tr>
<tr>
<td>Others</td>
<td>ESE 19.3 km/h</td>
<td>128</td>
<td>12.0 cm/s</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>(12 mph)</td>
<td>204</td>
<td>24.0 cm/s</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>232</td>
<td>16.0 cm/s</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>248</td>
<td>22.0 cm/s</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

**Note:**

* Information on wind direction and speed not available.
Table 5.4

Statistical Comparison of FEM Velocities.

<table>
<thead>
<tr>
<th>Locations</th>
<th>Finite Element Element No.</th>
<th>Velocity ( P_i ) cm/s</th>
<th>Ontario MOE ( O_i ) cm/s</th>
<th>Integrated Exploration ( O_i ) cm/s</th>
<th>((P_i - O_i)) cm/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leigh</td>
<td>135</td>
<td>2.8</td>
<td>4.88</td>
<td>-</td>
<td>-2.08</td>
</tr>
<tr>
<td>Bay</td>
<td>163</td>
<td>3.1</td>
<td>3.27</td>
<td>-</td>
<td>-0.17</td>
</tr>
<tr>
<td></td>
<td>166</td>
<td>7.4</td>
<td>none</td>
<td>2.5</td>
<td>4.90</td>
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<tr>
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<td>174</td>
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<td>none</td>
<td>0.0</td>
<td>1.80</td>
</tr>
<tr>
<td>Other</td>
<td>128</td>
<td>12.0</td>
<td>slight</td>
<td>8.0</td>
<td>4.00</td>
</tr>
<tr>
<td>regions</td>
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<td>24.0</td>
<td>moderate</td>
<td>3.0</td>
<td>21.00</td>
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<tr>
<td></td>
<td>232</td>
<td>16.0</td>
<td>negligible</td>
<td>2.0</td>
<td>14.00</td>
</tr>
<tr>
<td></td>
<td>248</td>
<td>22.0</td>
<td>strong</td>
<td>16.0</td>
<td>6.00</td>
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</tbody>
</table>
Table 5.5

Summary of the Verification Process.

<table>
<thead>
<tr>
<th>Verification</th>
<th>Comments</th>
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</thead>
<tbody>
<tr>
<td>(2) Using a separate and independent data source (Integrated Exploration, 1985).</td>
<td>Reasonable agreement of velocity trends in both Leigh Bay and other shallow zones.</td>
</tr>
<tr>
<td>(3) Aerial photographs compared with model's surface velocities under ESE wind.</td>
<td>Excellent agreement in the current circulation patterns.</td>
</tr>
</tbody>
</table>
Table 5.6
Comparison of DYNHYD4 Velocities (cm/s).

<table>
<thead>
<tr>
<th>Location</th>
<th>Finite Element Method</th>
<th>DYNHYD4</th>
<th>Field data*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Elem. No.</td>
<td>Velocity</td>
<td>Velocity</td>
</tr>
<tr>
<td>Shipping</td>
<td>32</td>
<td>36.3</td>
<td>39.5</td>
</tr>
<tr>
<td>Channel</td>
<td>26</td>
<td>63.0</td>
<td>43.2</td>
</tr>
<tr>
<td></td>
<td>248</td>
<td>24.3</td>
<td>18.1</td>
</tr>
<tr>
<td></td>
<td>126</td>
<td>30.3</td>
<td>23.4</td>
</tr>
<tr>
<td></td>
<td>157</td>
<td>25.5</td>
<td>22.7</td>
</tr>
<tr>
<td></td>
<td>180</td>
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<td>20.7</td>
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<td>135</td>
<td>2.8</td>
<td>1.9</td>
</tr>
<tr>
<td>Bay</td>
<td>163</td>
<td>3.1</td>
<td>13.0</td>
</tr>
<tr>
<td></td>
<td>166</td>
<td>7.4</td>
<td>1.2</td>
</tr>
<tr>
<td></td>
<td>174</td>
<td>1.8</td>
<td>1.6</td>
</tr>
</tbody>
</table>

* Note: Sources of field data are from Ontario MOE, Corps of Engineers and Integrated Exploration Inc.
Table 6.1

<table>
<thead>
<tr>
<th>Source</th>
<th>Load (kg/d)</th>
<th>Flow (m³/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Algoma Steel</td>
<td>200</td>
<td>550,000</td>
</tr>
<tr>
<td>(Terminal Basin Outfall)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2. Abitibi Paper</td>
<td>7</td>
<td>69,000</td>
</tr>
<tr>
<td>3. Domtar Chemical</td>
<td>25</td>
<td>17</td>
</tr>
<tr>
<td>(via STP)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(via Bennett Creek)</td>
<td>0.024</td>
<td>430</td>
</tr>
</tbody>
</table>
Table 6.2
Phenol Loading to the St. Marys River - Ontario MOE 1983.

<table>
<thead>
<tr>
<th>Outfall Sources</th>
<th>Flow (m³/d)</th>
<th>Phenol (ug/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Algoma Steel</td>
<td>360,000</td>
<td>280 - 50</td>
</tr>
<tr>
<td>2. Abitibi Paper</td>
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<td>66 - 20</td>
</tr>
<tr>
<td>3. Domtar Chemical</td>
<td>62,000</td>
<td>-</td>
</tr>
</tbody>
</table>
Table 6.3

Values of Constants in KETOX.

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<thead>
<tr>
<th></th>
<th>$c_\mu$</th>
<th>$c_{1e}$</th>
<th>$c_{2e}$</th>
<th>$c_{3e}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
<th>$\sigma_t$</th>
<th>$n$</th>
<th>$k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rodi</td>
<td>0.09</td>
<td>1.43</td>
<td>1.92</td>
<td>2.0</td>
<td>1.0</td>
<td>1.3</td>
<td>0.5</td>
<td>0.025</td>
<td>0.42</td>
</tr>
<tr>
<td>St. Marys</td>
<td>0.09</td>
<td>1.43</td>
<td>1.92</td>
<td>1.0</td>
<td>1.0</td>
<td>1.3</td>
<td>0.5</td>
<td>0.024</td>
<td>0.42</td>
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</tbody>
</table>
Table 6.4

<table>
<thead>
<tr>
<th>Location</th>
<th>Sample Size</th>
<th>MOE Mean (ug/L)</th>
<th>1974 Std. Devs (s/y/n)</th>
<th>KETOX Values (ug/L)</th>
<th>MOE - KETOX (ug/L)</th>
<th>Normal Distribution Test</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Canadian Shoreline</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SMD-0.2</td>
<td>26</td>
<td>24.0</td>
<td>7.0</td>
<td>1.3728</td>
<td>22.0</td>
<td>2.0</td>
</tr>
<tr>
<td>SMD-0.8</td>
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<td>1.3416</td>
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<td>1.0</td>
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<tr>
<td>SMD-1.2</td>
<td>53</td>
<td>12.0</td>
<td>4.0</td>
<td>0.5494</td>
<td>12.0</td>
<td>0.0</td>
</tr>
<tr>
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<td>4.0</td>
<td>0.5963</td>
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<tr>
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<td>3.5</td>
<td>1.0104</td>
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<td>0.5</td>
</tr>
<tr>
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<td>4.0</td>
<td>0.5443</td>
<td>8.0</td>
<td>0.0</td>
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<tr>
<td><strong>U.S. Shoreline</strong></td>
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<td></td>
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<td></td>
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<tr>
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<td>1.0</td>
<td>0.1429</td>
<td>2.0</td>
<td>0.0</td>
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<tr>
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<td>1.0</td>
<td>0.1429</td>
<td>2.0</td>
<td>0.0</td>
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<tr>
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<td>1.0</td>
<td>0.1429</td>
<td>2.0</td>
<td>0.0</td>
</tr>
<tr>
<td>SMD-2.6</td>
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<td>1.0</td>
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<td>2.0</td>
<td>0.0</td>
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<tr>
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<td>0.5547</td>
<td>3.0</td>
<td>2.0</td>
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<tr>
<td>SMD-5.3W</td>
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<td>1.6</td>
<td>0.2667</td>
<td>1.5</td>
<td>1.5</td>
</tr>
</tbody>
</table>

* Note: Location failed the normal distribution test.
Table 6.5

<table>
<thead>
<tr>
<th>Ontario Sample Size</th>
<th>MOE Mean ug/L</th>
<th>MOE Std. Devs.</th>
<th>1983 Values (s/j/n)</th>
<th>KETOX Values ug/L</th>
<th>MOE - KETOX ug/L</th>
<th>Normal Distribution Test</th>
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<tbody>
<tr>
<td><strong>Reach 10</strong></td>
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<td></td>
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<td></td>
</tr>
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<td>1.395</td>
<td>0.698</td>
<td>1.95</td>
<td>0.45</td>
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<tr>
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<td>0.80</td>
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<tr>
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<td>0.36</td>
<td>0.219</td>
<td>0.098</td>
<td>0.37</td>
<td>-0.01</td>
</tr>
<tr>
<td><strong>Reach 12</strong></td>
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<td></td>
<td></td>
<td></td>
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<td>1.81</td>
<td>1.106</td>
<td>0.418</td>
<td>1.80</td>
<td>0.01</td>
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<td>0.877</td>
<td>0.332</td>
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<td>0.492</td>
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<tr>
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</table>

* Note: Location failed the normal distribution test.
Table 6.6
Comparison of DYNHYD4 Velocities (ft/s).

<table>
<thead>
<tr>
<th>Channel</th>
<th>Corps of Engineers Current Meter</th>
<th>Engineers Drogue Values</th>
<th>KETOX with Momentum Adjustment</th>
<th>DYNHYD4 Values</th>
<th>(DYNHYD4 - COE)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
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<td>3.0</td>
<td>2.7</td>
<td>2.94</td>
<td>0.26</td>
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<tr>
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<td>3.0</td>
<td>2.6</td>
<td>2.8</td>
<td>2.91</td>
<td>0.09</td>
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<td>2.4</td>
<td>2.9</td>
<td>2.64</td>
<td>0.16</td>
</tr>
<tr>
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<td>1.9</td>
<td>1.8</td>
<td>1.73</td>
<td>-0.13</td>
</tr>
<tr>
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<td>1.0</td>
<td>1.7</td>
<td>1.32</td>
<td>0.46</td>
</tr>
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<td>1.4</td>
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<td>-0.56</td>
</tr>
<tr>
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<td>0.7</td>
<td>0.32</td>
<td>0.16</td>
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<tr>
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<td>0.17</td>
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<td>1.1</td>
<td>1.7</td>
<td>1.22</td>
<td>0.08</td>
</tr>
<tr>
<td>33</td>
<td>1.5</td>
<td>1.2</td>
<td>1.7</td>
<td>1.28</td>
<td>0.22</td>
</tr>
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<td>1.8</td>
<td>1.6</td>
<td>1.19</td>
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</table>
Table 6.7
Comparison of KETOX and DYNHYD4 Velocities.

<table>
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<tr>
<th>Channel</th>
<th>KETOX with Momentum Adjustment (ft/s)</th>
<th>DYNHYD4 Values (ft/s)</th>
<th>(KETOX - DYNHYD4) (ft/s)</th>
<th>Remarks</th>
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<td>-0.11</td>
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<td>7</td>
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<td>2.64</td>
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<td>Std. Dev. of the</td>
</tr>
<tr>
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<td>1.8</td>
<td>1.73</td>
<td>0.07</td>
<td>Mean = 0.0802</td>
</tr>
<tr>
<td>10</td>
<td>1.7</td>
<td>1.32</td>
<td>0.38</td>
<td>( t_{\text{model}} = 2.573 )</td>
</tr>
<tr>
<td>12</td>
<td>1.4</td>
<td>1.56</td>
<td>-0.16</td>
<td>( t_{\text{table}} = 3.169 )</td>
</tr>
<tr>
<td>29</td>
<td>0.7</td>
<td>0.32</td>
<td>0.38</td>
<td>at 1% level of</td>
</tr>
<tr>
<td>30</td>
<td>1.0</td>
<td>0.62</td>
<td>0.38</td>
<td>significance</td>
</tr>
<tr>
<td>32</td>
<td>1.7</td>
<td>1.22</td>
<td>0.48</td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>1.7</td>
<td>1.28</td>
<td>0.42</td>
<td></td>
</tr>
<tr>
<td>34</td>
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<td>1.19</td>
<td>0.41</td>
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</table>
## Table 7.1

Spreadsheet for KETOX's Results

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<th>4</th>
<th>6</th>
<th>8</th>
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<td>-12</td>
</tr>
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<td>0.09</td>
<td>0.09</td>
<td>0.09</td>
</tr>
<tr>
<td>BedPar</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Note:

This spreadsheet is obtained by using the "FILE - IMPORT - STRUCTURED" keys sequence in Symphony.

The ASCII/numeric file imported is KETOX.WAT as created by the KETOX model automatically. The sheet runs from column A to P with each column denoting a node on the river cross-section. Each row on the sheet therefore contains computed results for a river cross-section.

<table>
<thead>
<tr>
<th>LxDist</th>
<th>4125 Dxc</th>
<th>4250 Dxc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distan</td>
<td>0</td>
<td>31.5</td>
</tr>
<tr>
<td>Distant</td>
<td>0</td>
<td>31.5</td>
</tr>
<tr>
<td>Depth</td>
<td>-10</td>
<td>-11</td>
</tr>
<tr>
<td>Veloci</td>
<td>1.6</td>
<td>2.3</td>
</tr>
<tr>
<td>WaterC</td>
<td>3.9</td>
<td>3.7</td>
</tr>
<tr>
<td>WatCD1</td>
<td>3.8</td>
<td>3.5</td>
</tr>
<tr>
<td>BedPar</td>
<td>20</td>
<td>20</td>
</tr>
</tbody>
</table>

LxDist = distance in ft, Distant = distance across the river width in feet, WaterC = total toxicant conc. in the water column at each of 15 nodes in mg/L, WatCD1 = dissolved toxicant conc. in the water column at each of 15 nodes in mg/L, BedPar = particulate toxicant conc. in the bed column at each of 15 nodes in mg/g.
Table 7.2
Estimated Loads at Algoma Diffuser.

<table>
<thead>
<tr>
<th>Toxic Organics</th>
<th>1986 Terminal Basin Loads (kg/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ammonia</td>
<td>2,631 to 5,056</td>
</tr>
<tr>
<td>Cyanide</td>
<td>29 to 53</td>
</tr>
<tr>
<td>Phenol</td>
<td>9 to 110</td>
</tr>
<tr>
<td>Oil and Grease</td>
<td>1,413 to 10,000</td>
</tr>
<tr>
<td>Suspended Solids</td>
<td>4,200 to 6,700</td>
</tr>
</tbody>
</table>
Table 7.3
Receiving Water Guidelines

<table>
<thead>
<tr>
<th>Toxic Organics</th>
<th>Concentration Level Guidelines</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ammonia</td>
<td>&lt; \left( 16.0 - 106.66 \times \text{Cyanide}_{\text{mg/L}} \right) \quad 0.5 \text{ mg/L} \quad \text{see ammonia}^*</td>
</tr>
<tr>
<td>Cyanide</td>
<td></td>
</tr>
<tr>
<td>Phenol</td>
<td>5.0 \text{ ug/L}</td>
</tr>
<tr>
<td>Oil and Grease</td>
<td>1 \text{ ppm (no sheen)}</td>
</tr>
<tr>
<td>Suspended Solids</td>
<td>5 \text{ ppm above background}</td>
</tr>
</tbody>
</table>

*Note: It is noted the guidelines for ammonia and cyanide are coupled, i.e. the allowable concentration of ammonia decreases linearly as free cyanide increases. For example, if cyanide = 0 then ammonia = 16 \text{ mg/L}, while if cyanide = 0.15 \text{ mg/L} then ammonia = 0.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Length of LUZ for 1986 Terminal Basin Loads (ft)</th>
<th>1986 Loads (kg/d)</th>
<th>Loads Required to achieve guidelines within a 1000 ft LUZ (kg/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ammonia</td>
<td>&lt; 1000</td>
<td>4000</td>
<td>2890 c</td>
</tr>
<tr>
<td>Cyanide</td>
<td>&lt; 1000</td>
<td>53</td>
<td>27 c</td>
</tr>
<tr>
<td>Phenol</td>
<td>&gt; 10000</td>
<td>100</td>
<td>20 a</td>
</tr>
<tr>
<td>Oil &amp; Grease</td>
<td>&lt; 1000</td>
<td>1400</td>
<td>850 d</td>
</tr>
<tr>
<td>Suspended</td>
<td>&lt; 1000</td>
<td>6000</td>
<td>4250 e</td>
</tr>
</tbody>
</table>

Solids

a. median summer flow 87000 cfs.
b. extreme low flow 54000 cfs.
c. load to eliminate toxic conditions at outfall.
d. load to prevent surface sheen.
e. for aesthetics near outfall at low flow.
APPENDIX I

FIGURES
ST. MARYS FALLS CANAL
AND
THE SOO LOCKS

Figure 1.2  Layout at the Soo Locks.
Figure 1.3 Study Limits of the Upper and Lower St. Marys River.
Figure 2.1 Schematic of a Side Discharge Outfall in a River (Rodi et al., 1981).
Figure 2.2 Sketch of Physical-Chemical Processes in a Lake (Mills et al., 1985).
Figure 2.3 Schematic of Physical-Chemical Processes in a River (Thomann and Muller, 1987).
Figure 3.2 A Sketch of the Excess Momentum Adjustments at a River Cross-Section.
Figure 3.3 Definition Sketch of Lateral Adjustments of Node Locations Across a River Cross-Section.
Figure 3.5 Model Segmentation of WASP4 (Ambrose et al., 1988).
WIND GRAPH
(SAULT STE. MARIE, MICHIGAN)

WIND SPEED
RANGE LIMITS IN MPH

ALL CEILING AND VISIBILITY CONDITIONS

Figure 4.3  Wind Graph at Sault Ste. Marie Airport.
Figure 4.4 Ice Cover Analysis for East Center Pier Station.
Figure 4.5  Ice Cover Analysis for Pittsburg Dock Station.
Figure 5.2a  Vertical Eddy Viscosity Variation Under No Wind - Element 25.

\( \eta_v \text{ cm}^2/\text{s} \)

- EDDY \( \rightarrow 1.0 \)
- \( \rightarrow 10.0 \)
- \( \circ \circ \rightarrow 20.0 \)
- \( \rightarrow 40.0 \)
- \( \star \star \rightarrow 80.0 \)
Figure 5.2b Vertical Eddy Viscosity Variation Under No Wind - Element 46.

\( \eta_v \text{ cm}^2/\text{s} \)

- EDDY \( \rightarrow \) 1.0
- \( \rightarrow \) 10.0
- \( \rightarrow \) 20.0
- \( \rightarrow \) 40.0
- \( \rightarrow \) 80.0
Figure 5.2c  Vertical Eddy Viscosity Variation Under No Wind – Element 98:

\[ \eta_v \text{ cm}^2/\text{s} \]

EDDY: 1.0  
10.0  
20.0  
40.0  
80.0
Figure 5.2d  Vertical Eddy Viscosity Variation Under No Wind - Element 125.

\( (\eta_v \text{ cm}^2/\text{s}) \)

- EDDY  \( \rightarrow \) 1.0
- \( \rightarrow \rightarrow \) 10.0
- \( \rightarrow \rightarrow \rightarrow \) 20.0
- \( \rightarrow \rightarrow \rightarrow \rightarrow \) 40.0
- \( \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \) 80.0
Figure 5.2e Vertical Eddy Viscosity Variation Under No Wind - Element 164.

\[ \eta_v \text{ cm}^2/\text{s} \]

EDDY \[ \leftarrow 1.0 \rightarrow 10.0 \leftarrow 20.0 \rightarrow 40.0 \leftarrow 80.0 \]
Figure 5.2f  Vertical Eddy Viscosity Variation Under No Wind — Element 201.

\[
\eta_v \text{ cm}^2/\text{s}
\]

\begin{align*}
\text{EDDY} & \quad 1.0 & 10.0 & 20.0 & 40.0 & 80.0
\end{align*}
Figure 5.3a  Vertical Eddy Viscosity Variation Under NW 19.3 km/h Wind - Element 25.

\( \eta_v \text{ cm}^2/\text{s} \)

- E007  \( \rightarrow \) 1.0
- 10.0  \( \rightarrow \) 10.0
- 20.0  \( \rightarrow \) 20.0
- 40.0  \( \rightarrow \) 40.0
- 80.0  \( \rightarrow \) 80.0
Figure 5.3b  Vertical Eddy Viscosity Variation Under NW 19.3 km/h Wind - Element 46.
Figure 5.3c  Vertical Eddy Viscosity Variation Under NW 19.3 km/h Wind - Element 98.

\( \eta_v \, \text{cm}^2/\text{s} \)

- **EDDY**
  - 1.0
  - 10.0
  - 20.0
  - 40.0
  - 80.0
Figure 5.3d  Vertical Eddy Viscosity Variation Under NW 19.3 km/h Wind - Element 125.

($\eta_v \text{ cm}^2/\text{s}$)

EDDY $\leftarrow 1.0 \quad \leftarrow 10.0 \quad \leftarrow 20.0 \quad \leftarrow 40.0 \quad \leftarrow 80.0$
Figure 5.3e  Vertical Eddy Viscosity Variation Under NW 19.3 km/h Wind - Element 164.

\( \eta_v \text{ cm}^2/\text{s} \)

EDDY  \( \rightarrow \) 1.0 \( \rightarrow \) 10.0 \( \rightarrow \) 20.0 \( \rightarrow \) 40.0 \( \rightarrow \) 80.0
Figure 5.3f Vertical Eddy Viscosity Variation Under NW 19.3 km/h Wind - Element 201.

\[ \eta_v \text{ cm}^2/\text{s} \]

- EDDY: 1.0  
- 10.0  
- 20.0  
- 40.0  
- 80.0
Figure 5.4a  Vertical Eddy Viscosity Variation Under ESE 19.3 km/h Wind - Element 25.

\( \eta_v \ cm^2/s \)

- EDDY 1.0
- 10.0
- 20.0
- 40.0
- 80.0
Figure 5.4b Vertical Eddy Viscosity Variation Under ESE 19.3 km/h Wind - Element 46.

\( \eta_v \text{ cm}^2/\text{s} \)

- Eddy 1.0
- 10.0
- 20.0
- 40.0
- 80.0
Figure 5.4c  Vertical Eddy Viscosity Variation Under ESE 19.3 km/h Wind - Element 98.

\( \eta_v \text{ (cm}^2\text{/s)} \)
Figure 5.4d Vertical Eddy Viscosity Variation Under ESE 19.3 km/h Wind - Element 125.

(\(\eta_v \text{ cm}^2/\text{s}\))

EDDY \(\rightarrow\) 1.0 \(\rightarrow\) 10.0 \(\rightarrow\) 20.0 \(\rightarrow\) 40.0 \(\rightarrow\) 80.0
Figure 5.4e  Vertical Eddy Viscosity Variation Under ESE 19.3 km/h Wind - Element 164.

$\eta_v$ cm$^2$/s

- EDDY --- 1.0
- 10.0
- 20.0
- 40.0
- 80.0
Figure 5.4f  Vertical Eddy Viscosity Variation Under ESE 19.3 km/h Wind - Element 201.

\( \eta_v \) cm\(^2\)/s

Eddy: 1.0, 10.0, 20.0, 40.0, 80.0
Figure 5.5a Effects of Bottom Slip Coefficients Varying Under No Wind - Element 25.
Figure 5.5b  Effects of Bottom Slip Coefficients Varying Under No Wind - Element 46.
Figure 5.5c Effects of Bottom Slip Coefficients Varying Under No Wind - Element 98.
Figure 5.5d, Effects of Bottom Slip Coefficients Varying Under No Wind - Element 125.
Figure 5.5e  Effects of Bottom Slip Coefficients Varying Under No Wind - Element 164.
Figure 5.5f Effects of Bottom Slip Coefficients Varying Under No Wind - Element 201.
Figure 5.6a Effects of Bottom Slip Coefficients Varying Under NW 19.3 km/h Wind - Element 25.
Figure 5.6b Effects of Bottom Slip Coefficients Varying Under NW 19.3 km/h Wind - Element 46.
Figure 5.6c  Effects of Bottom Slip Coefficients Varying Under NW 19.3 km/h Wind - Element 98.
Figure 5.6d Effects of Bottom Slip Coefficients Varying Under NW 19.3 km/h Wind - Element 125.
Figure 5.6e Effects of Bottom Slip Coefficients Varying Under NW 19.3 km/h Wind - Element 164.
Figure 5.6f Effects of Bottom Slip Coefficients Varying Under NW 19.3 km/h Wind - Element 201.
Figure 5.7a Surface Velocity Vectors Under NW 19.3 km/h Wind.
Figure 5.7b Velocity Vectors at 0.2 Depth Below Surface.

NW 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
NW 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3

Figure 5.7c Velocity Vectors at 0.4 Depth Below Surface.
Figure 5.7d  Velocity Vectors at 0.6 Depth Below Surface.
Figure 5.7e  Velocity Vectors at 0.8 Depth Below Surface.

NW 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
Figure 5.7f Depth Averaged Velocity Vectors.

NW 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
Figure 5.8a Surface Velocity Vectors Under ESE 19.3 km/h Wind.

ESE 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm³/s and Slip 0.3
ESE 12 mph (19.3 km/h) wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3

Figure 5.8b Velocity Vectors at 0.2 Depth Below Surface.
Figure 5.8c  Velocity Vectors at 0.4 Depth Below Surface.

ESE 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
Figure 5.8d Velocity Vectors at 0.6 Depth Below Surface.
Figure 5.6e Velocity Vectors at 0.8 Depth Below Surface.

ESE 12 mph (19.3 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
Figure 5.8f Depth Averaged Velocity Vectors.
No Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3

Figure 5.9a Surface Velocity Vectors Under No Wind.
Figure 5.9b  Velocity Vectors at 0.2 Depth Below Surface.
Figure 5.9c, Velocity Vectors at 0.4 Depth Below Surface.

No Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
Figure 5.9d  Velocity Vectors at 0.6 Depth Below Surface.
Figure 5.9e  Velocity Vectors at 0.8 Depth Below Surface.

No Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3
Figure 5.9f  Depth Averaged Velocity Vectors.
NW 12 mph (19.3 km/h) Wind
Eddy 10.0 cm²/s
Slip 0.3
Flow 81,100 cfs (2,298 m³/s)

Figure 5.11 Stream Circulation Pattern Under NW 19.3 km/h Wind.
Figure 5.13 Stream Circulation Pattern Under E 19.3 km/h Wind.
ESE 12 mph (19.3 km/h) Wind
Eddy 10.0 cm²/s
Slip 0.3
Flow 81,100 cfs (2,298 m³/s)

Figure 5.14 Stream Circulation Pattern Under ESE 19.3 km/h Wind.
Figure 5.15 Stream Circulation Pattern Under S 19.3 km/h Wind.
Figure 5.16 Stream Circulation Pattern Under SW 19.3 km/h Wind.
W 12 mph (19.3 km/h) Wind
Eddy 10.0 cm²/s
Slip 0.3
Flow 01,100 cfs (2,298 m³/s)

Figure 5.17  Stream Circulation Pattern Under W 19.3 km/h Wind.
THE QUALITY OF THIS MICROFICHE IS HEAVILY DEPENDENT UPON THE QUALITY OF THE THESIS SUBMITTED FOR MICROFILMING.

UNFORTUNATELY THE COLOURED ILLUSTRATIONS OF THIS THESIS CAN ONLY YIELD DIFFERENT TONES OF GREY.
Upper St. Marys River - Chloropleth Map

With No Wind Condition
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cm³/s (81,100 cfs)

Velocity Levels (cm/s) 

- < 15
- < 61
- < 3.0
- < 30

Figure 5.18(a) With No Wind Condition
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cu.m/s (81,100 cfs)

Velocity Levels (cm/s) ▁▁▁▁▁▁ (15.) ▁▁▁▁▁▁ (30.)
▁▁▁▁▁▁ (61.) ▁▁▁▁▁▁ (61.)

Figure 5.18(b) With North Wind
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cum/s (81,100 cfs)

Velocity Levels (cm/s)  

Figure 5.18(c)  With East Wind
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cum/s (81,100 cfs)

Velocity Levels (cm/s)  

Figure 5.18(d) With East South-East Wind
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cu.m/s (81,100 cfs)

Velocity Levels (cm/s)
- - 15
- - - 3.0
- - - - 30

Figure 5.18(e) With South Wind
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cum/s (81,100 cfs)

Velocity Levels (cm/s) 

Figure 5.18(f) With South-West Wind
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vert. Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 c.u.m/s (81,100 cfs)

Velocity Levels (cm/s)  
\[
\begin{array}{c}
\text{< 15.} \\
\text{< 30.} \\
\text{< 61.} \\
\text{61.} \\
\end{array}
\]

Figure 5.18(g) With West Wind
Upper St. Marys River - Chloropleth Map

Wind Speed 19.3 kmph (12 mph)
Vertical Eddy Viscosity 10 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cu.m/s (81,100 cfs)

Figure 5.18(h) With North-West Wind
Figure 5.19a Circulation Pattern Under N 38.6 km/h Wind

Flow 81.100 cfs (2,298 m³/s)

Density 10.0 cm/s and slip 0.3

X-DISTANCES IN MILE

Y-DISTANCES IN MILE

N 24 mph (38.6 km/h) Wind
Figure 5.19c  Circulation Pattern Under ESE 38.6 km/h Wind.
W 24 mph (38.6 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and slip 0.3

Figure 5.19f  Circulation Pattern Under W 38.6 km/h Wind.
NW 24 mph (38.6 km/h) Wind
Flow 81,100 cfs (2,298 m³/s)
Eddy 10.0 cm²/s and Slip 0.3

Figure 5.19g  Circulation Pattern Under NW 38.6 km/h Wind.
Figure 5.20a Corps of Engineers (1984) Velocity Vectors at 0.2 Depth Below Surface.
Figure 5.20b  Corps of Engineers (1984) Velocity Vectors at 0.4 Depth Below Surface.
Figure 5.20c  Corps of Engineers (1984) Velocity Vectors at 0.8 Depth Below Surface.
Figure 5.20d Corps of Engineers (1984) Composite Velocity Vectors.
Figure 5.21 Aerial Photograph of Upper St. Marys River Under ESE Wind.
Figure 5.22a  Velocity Vectors at 0.5 Depth, Below Surface With Ice Cover Condition.
Ice Cover
Eddy 1.0 cm²/s
Slip 0.3
Flow 81,100 cfs (2,298 m³/s)

Figure 5.22b Velocity Vectors at 0.6 Depth Below Surface With Ice Cover Condition.
Figure 5.22d  Velocity Vectors at 0.8 Depth Below Surface With Ice Cover Condition.
Figure 5.22e Velocity Vectors at 0.9 Depth Below Surface With Ice Cover Condition.
Ice Cover
Eddy 1.0 cm$^2$/s
Slip 0.3
Flow 81,100 cfs (2,298 m$^3$/s)

Figure 5.22f  Depth Averaged Velocity Vectors Under Ice Cover.
Upper St. Marys River - Chloropleth Map

With Ice Cover Condition
Vert. Eddy Viscosity 1.0 sq.cm/s
Slip Coefficient 0.3
Flow 2,298 cu.m/s (81,100 cfs)

Velocity Levels (cm/s)

Figure 5.23 With Ice Cover Condition
Figure 5.28 Upper St. Marys River Surface Elevations (relative to the mean water level - DYNHYD4.)
Figure 6.1 Ambient Phenol Data (Ontario MOE 1974).
Figure 6.2  Variation in Phenol Loading to Algoma Terminal Basin (Ontario MOE 1972-74).
Figure 6.3 St. Marys River – Municipal Intakes, Outfalls and Industrial Waste Discharges.
Figure 6.4 Definition of Reaches for the KETOX model of the Lower St. Marys River.
Cross-Sectional Velocity Profiles
Flow 104,000 CFS - No Ice Cover
Reach 1 LX = 500

Figure 6.5a Comparison of Measured and Computed Velocity Profiles - Reach 1 LX = 500.
Cross-Sectional Velocity Profiles
Flow 104,000 CFS - No Ice Cover
Reach 18  LX = 1000

COE Measured 1984 ■
K-E Momentum Adj. ●
Fully Developed ★

Figure 6.5b  Comparison of Measured and Computed Velocity Profiles - Reach 18 LX = 1000.
Cross-Sectional Velocity Profiles
Flow 104,000 CFS - No Ice Cover
Reach 10  LX = 500

Figure 6.5c  Comparison of Measured and Computed Velocity Profiles - Reach 10 LX = 500.
Cross-Sectional Velocity Profiles
Flow 104,000 CFS - No Ice Cover
Reach 10 \( LX = 1000 \)

Figure 6.5d  Comparison of Measured and Computed Velocity Profiles - Reach 10 \( LX = 1000 \).
Figure 6.5e  Comparison of Measured and Computed Velocity Profiles – Reach 12 LX = 1000.
Cross-Sectional Velocity Profiles
Flow 104,000 CFS - No Ice Cover
Reach 12 LX = 2500

COE Measured 1984 ●
K-E Momentum Adj. ●
Fully Developed ★

Figure 6.5f Comparison of Measured and Computed Velocity Profiles - Reach 12 LX = 2500.
Figure 6.5g  Comparison of Measured and Computed Velocity Profiles - Reach 19 LX = 500.
Figure 6.6  Measured (Ontario MOE 1974) and Predicted (KETOX)
Figure 6.7a Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 8 Combine.
Figure 6.7b  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 18 LX = 1000.
Figure 6.7c  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser — Flow 81,000 cfs — Reach 18 LX = 2000.
Figure 6.7d Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 10 LX = 1000.
Figure 5.7e  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 10 LX = 2000.
Figure 6.7f Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 12 LX = 1000.
Figure 6.7g  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 µg/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 12 LX = 2000.
Figure 6.7h Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 12 LX = 3000.
Figure 6.7i  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 19 LX = 1000.
Figure 6.7j  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 19 LX = 3000 FT.
Figure 6.7k  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 13 LX = 3000.
Figure 6.8a  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 126,000 cfs - Reach 8 Combine.
Figure 6.8b  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 126,000 cfs - Reach 18 LX = 1000.
Figure 6.8c Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 126,000 cfs - Reach 18 LX = 2000.
Figure 6.8d Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser – Flow 126,000 cfs – Reach 10 LX = 1000.
Figure 6.3e  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 126,000 cfs - Reach 10 LX = 2000.
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Note: Selected Value for Level 3 MUST NOT be less than 2.35

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Time in Hours

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NOMENCLATURE

\( A \)  \quad \text{domain enclosed by the boundary } \Gamma

\( A^e \)  \quad \text{triangular elemental area}

\( A_j \)  \quad \text{cross-sectional area of panel } j \text{ between nodes } j \text{ and } j+1

\( A_j' \)  \quad \text{the corrected area for panel } j

\( A_s \)  \quad \text{surface area of a water cell}

\( A_T \)  \quad \text{total flow area of a river cross-section}

\( A(x,y) \)  \quad \text{a constant coefficient in Eq. (3.11)}

\( a_1, a_2, a_3 \)  \quad \text{constant coefficients in Eq. (3.37)}

\( (a,b,c)_i \)  \quad \text{functions of the } x, y, z \text{ coordinates of node } i

\( (a,b,c)_j \)  \quad \text{functions of the } x, y, z \text{ coordinates of node } j

\( (a,b,c)_k \)  \quad \text{functions of the } x, y, z \text{ coordinates of node } k

\( B(x,y) \)  \quad \text{a constant coefficient in Eq. (3.11)}

\( C \)  \quad \text{depth averaged chemical concentration}

\( C_a \)  \quad \text{chemical concentration in air}

\( C_{area} \)  \quad \text{area correction coefficient}

\( C_B \)  \quad \text{bottom friction factor}

\( C_{D1} \)  \quad \text{effective dissolved chemical concentration in the water column}

\( C_{D2} \)  \quad \text{effective dissolved chemical concentration in the sediment}

\( C_{drag} \)  \quad \text{wind drag coefficient}

\( C_d \)  \quad \text{dissolved toxicant concentration on a bulk volume basis}

\( C_{d}^- \)  \quad \text{dissolved toxicant concentration in water}
C_{d1} \quad \text{dissolved chemical concentration in the water column}

C_{d2} \quad \text{dissolved chemical concentration in the sediment}

C_f \quad \text{a friction coefficient}

C_{M, M-1} \quad \text{depth averaged chemical concentrations at grid locations M and (M-1)}

C_{p1} \quad \text{effective particulate chemical concentration in the water column}

C_{p2} \quad \text{effective particulate chemical concentration in the sediment}

C_p \quad \text{concentration of toxicant absorbed to particulate in the water column or sediment}

C_{p1} \quad \text{particulate chemical concentration in the water column}

C_{p2} \quad \text{particulate chemical concentration in the sediment}

C_o \quad \text{chemical concentration at the outfall location}

C_T \quad \text{total toxicant concentration}

C_{T_0} \quad \text{total toxicant concentration from adjoining upstream segment}

C_{T1} \quad \text{total toxicant concentration in water column}

C_{T2} \quad \text{total toxicant concentration in sediment column}

C_w \quad \text{dissolved chemical concentration in water column}

C(x, y) \quad \text{a constant coefficient in Eq. (3.11)}

\text{c_1, c_2} \quad \text{empirical constants in the K-E equations}

\text{c_c, c_{1c}, c_{2c}} \quad \text{empirical constants in the K-E equations}

\text{c_{\mu}, c_{\kappa}} \quad \text{empirical constants in the K-E equations}

D \quad \text{diffusion factors as defined in Eq. (3.33)}

D_i \quad \text{diffusion factors}
\(D_{\text{cell}}\) average depth of a cell
\(D_{1,1}\) diffusion factors as defined in Eq. (3.33)
\(D_{M,M}\) diffusion factors at grid locations \(M\) and \(m\)
\(D_{xc}\) space step used by KETO in the direction of flow
\(D_{z}\) diffusion factors
\(d\Gamma\) incremental length on the outer surface boundary
\(E\) energy dissipation rate
\(E_{t}\) transverse mixing coefficient in Eq. (2.26)
\(E_{z}\) lateral turbulent mixing coefficient
\{\(F\)\} a force matrix
\(F_{i}\) external forces
\(F_{b}\) driving force or the source
\(F(\rho,T,S)\) an empirical function
\(f\) Coriolis coefficient
\(f_d\) dissolved fraction of a chemical
\(f_{d1}\) effective dissolved fraction in water column
\(f_{d2}\) effective dissolved fraction in sediment column
\(f_d\) dissolved fraction
\(f_{d1}\) dissolved fraction in water column
\(f_{d2}\) dissolved fraction in sediment column
\(f_{p}\) particulate fraction
\(f_{p1}\) particulate fraction in water column
\(f_{p2}\) particulate fraction in sediment column
\(f_{p\text{1},i}\) effective particulate fraction in water column
\(f_{p\text{2},i}\) effective particulate fraction in sediment column.
\( g \)  
gravity

\( \vec{g} \)  
gravitational force vector

\( g_1 \)  
fast decay rate

\( g_{1c} \)  
effective fast decay rate

\( g_2 \)  
slow decay rate

\( g_{2c} \)  
effective slow decay rate

\( H \)  
Henry's Law constant

\( H_1 \)  
depth of the water column

\( H_2 \)  
depth of the sediment column

\( h, h(x,y) \)  
local flow depth

\( h_j, h_{j+1} \)  
local flow depths at nodes \( j \) and \( j+1 \)

\( i, j, k \)  
unit vectors in the \( x, y, z \) directions respectively

\( J \)  
relationship as defined in Eq. (3.32)

\( K \)  
kinetic energy of the turbulent motion

\( [K] \)  
global stiffness matrix

\( K_1 \)  
sum of hydrolysis, oxidation, biodegradation, photolysis and volatilization rates in water column

\( K_{1c} \)  
combined effect of the sum of hydrolysis, oxidation, biodegradation, photolysis and volatilization rates in water column

\( K_2 \)  
sum of hydrolysis, oxidation and biodegradation rates in sediment column

\( K_c \)  
gas phase transfer coefficient

\( K_l \)  
water-sediment diffusion exchange coefficient

\( K_{lp} \)  
liquid phase transfer coefficient

\( K_s \)  
sedimentation rate coefficients
effective sedimentation rate coefficients

apparent total removal rates of the chemical

effective apparent total removal rates of the chemical

net volatilization rate constant

conductivity rate constant

direction cosines normal to the outer surface boundary, \( \Gamma \)

molecular transport coefficient

solids concentration

solids concentration in water column

solids concentration in sediment column

coefficients for stream function coordinates

number of unknowns

Manning's roughness coefficient

empirical exponent

parameter as defined in Eq. (3.41)

parameter as defined in Eq. (3.41)

parameter as defined in Eq. (3.41)

pressure

time mean static pressure

atmospheric pressure

river flow rate

flow rate in the water column

flow rate at the outfall location

velocity vector with \( u, v \) and \( w \) components

cumulative discharge
q_{mean} \quad \text{mean component of the fluctuating physical quantity of the fluid}

q(x,y,z,t) \quad \text{instantaneous value of a fluctuating physical fluid quantity}

q'(x,y,z,t) \quad \text{randomly fluctuating component about the mean value of the physical fluid quantity}

R \quad \text{gas constant}

r \quad \text{toxicant concentration on a per unit dry weight solids basis}

r_1 \quad \text{toxicant concentration on a per unit dry weight solids basis in the water column}

r_{1e} \quad \text{effective toxicant concentration on a per unit dry weight solids basis in the water column}

r_2 \quad \text{toxicant concentration on a per unit dry weight solids basis in the sediment column}

r_{2e} \quad \text{effective toxicant concentration on a per unit dry weight solids basis in the sediment column}

r_c \quad \text{radius of curvature of the channel centre line}

r_{loc} \quad \text{local radius of curvature}

S \quad \text{salinity}

S_e \quad \text{energy slope}

S_o \quad \text{an effective frictional slope}

S_{1c} \quad \text{parameter as defined in Eq. (3.81)}

S_{2c} \quad \text{parameter as defined in Eq. (3.82)}

s \quad \text{slip coefficient}

s_1 \quad \text{parameter as defined in Eq. (3.63)}

s_2 \quad \text{parameter as defined in Eq. (3.64)}
T  temperature

t  time

$\tau_D$  detention time of the cell

$\tau_{half/1}$  half life of the fast decay rate

$\tau_{\text{eff}/1}$  effective half life of the fast decay rate

$\tau_{half/2}$  half life of the slow decay rate

$\tau_{\text{eff}/2}$  effective half life of the slow decay rate

$U, V$  depth averaged velocity components in the $x,y$ directions respectively

$U_{i,j}^m$  excess momentum corrected velocity at node $j$ of cross-section $i$

$U_{i,j+1}^m$  excess momentum corrected velocity at node $j+1$ of cross-section $i$

$U_s$  shear velocity

$U(x,y)$  depth averaged velocity component in the $x$-direction

$u, v, w$  instantaneous velocities in the $x, y, z$ directions respectively

$\bar{u}, \bar{v}, \bar{w}$  time mean velocities in the $x, y, z$ directions respectively

$u_b, v_b$  time mean bottom velocities in the $x, y$ direction respectively

$\bar{u}_b, \bar{v}_b$  time mean bottom velocities in the $x, y$ direction respectively

$\bar{u}_i, \bar{u}_j$  time mean velocity vector ($i$ or $j = 1, 2, 3$)

$\bar{u}, \bar{S}$  turbulent correlation for the scalar quantity

$\bar{u}_s, \bar{v}_s, \bar{w}_s$  time mean surface velocities in the $x, y, z$ directions respectively
V  volume of a water cell
V_1  volume of the water column
V_2  volume of the sediment column
VolatR volatilization rate coefficient
V  wind velocity at 4 metres above the water surface
V(x,y) depth averaged velocity component in the y-direction
v_x  channel velocity in the x-direction
W  width of the river
W_T mass inflow rate of toxicant
w_x, w_y wind velocities in the x,y direction respectively
w_s settling velocity
w_r resuspension velocity
w_s sedimentation velocity
\vec{X} body force vector
x_i, x_j coordinates in space (i or j = 1, 2, 3)
x, y, z Cartesian coordinate system
y_j, y_{j+1} lateral distances of nodes j and j+1 from one side of the shore
y_{j, n}, y_{j, m} new excess momentum adjusted locations at nodes j and j+1
z lateral distance of the local grid point from the shore
z_j \Delta \omega between nodes j and (j - 1)
z_{j+1} \Delta \omega between nodes j and (j + 1)
\beta sediment capacity factors
\beta_e effective sediment capacity factors
\( \beta_s \)  
\( \beta^T \)  
\( \Gamma \)  
\( \Delta \omega \)  
\( \Delta \omega_j \)  
\( \delta U \)  
\( \xi \)  
\( \eta_H \)  
\( \eta_V \)  
\( \Theta \)  
\( \lambda \)  
\( \mu \)  
\( \nu_m \)  
\( \nu_t \)  
\( \Xi \)  
\( \Pi \)  
\( \Pi' \)  
\( \Pi_1 \)  
\( \Pi_2 \)  
\( \rho, \rho_o \)  
\( \rho_a \)  
\( \rho u_i u_j \)  
\( \sigma_k, \sigma_c \)  
\( \tau_{bx}, \tau_{by} \)

molecular salinity diffusion coefficient  
molecular thermo-diffusion coefficient  
outer surface boundary  
incremental change in \( \omega \) across the river width  
unitless stream function value between nodes \( j \) and \( j+1 \)  
excess depth average velocity at each node  
lake surface elevation variation  
horizontal eddy viscosity  
vertical eddy viscosity  
porosity  
latitude of the earth  
dynamic viscosity  
turbulent traverse mixing coefficient for excess momentum  
turbulent eddy viscosity  
Coriolis parameter matrix  
partition coefficient  
porosity corrected partition coefficient  
partition coefficient in the water column  
partition coefficient in the sediment column  
fluid densities  
air density  
Reynolds stresses  
empirical diffusion constants  
bottom stresses due to friction in the \( x, y \) direction respectively
\( \tau_s \)  
surface wind shear in the prevailing wind direction

\( \tau_x, \tau_y \)  
surface wind stresses in the \( x,y \) direction respectively

\( \chi(z) \)  
a shape factor for river bank effects

\( \psi \)  
stream function defined in Eq. (3.9)

\( \Phi \)  
an approximation of \( \psi \)

\( \{ \psi \} \)  
matrix of stream function nodal values

\( \psi_{i,j,k} \)  
nodal stream function values at the nodes \( i,j,k \) respectively

\( \Omega \)  
angular velocity of the earth

\( \omega \)  
dimensionless cumulative discharge

\( \nabla \)  
vector operator

\( \bar{X} \)  
time mean scalar quantity (i.e. temperature or salinity) per unit mass
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Krishnappan B.G., and Lau Y.L., 1983. RIVMIX Transport Model, Computer programme developed by CCIW.


Lake Superior Regulation - Plan 1977.


VITA AUCTORIS

1953  Born on the 24th day of January in Singapore.

1972  Graduated from pre-university at St. Joseph's Institution, Singapore.

1975  Completion of mandatory military service with the 7th Infantry Regiment, Singapore Armed Forces.

1981  Graduated from the University of Windsor, Windsor, Ontario, Canada, with the degree of Bachelor of Applied Science in Civil Engineering.

1984  Received the degree of Master of Applied Science in Civil Engineering from the University of Windsor, Windsor, Ontario, Canada.

1984  Accepted into the Faculty of Graduate Studies and Research, University of Windsor, Windsor, Ontario, Canada, in a programme leading to the degree of Doctor of Philosophy in Civil Engineering.
Figure 6.7d  Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 µg/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 10 LX = 1000.
Figure 5.7e Comparison of Ontario MOE Measured and KETOX Predicted Phenol Concentrations Based on 1973-74 Loading of 700 ug/L at the Algoma Diffuser - Flow 81,000 cfs - Reach 10 LX = 2000.