WATER QUALITY BRANCH
ENVIRONMENTAL PROTECTION DEPARTMENT
MINISTRY OF ENVIRONMENT, LANDS AND PARKS

A Compendium of Water Quality Models

Compiled by SARAH RIECKEN
JANUARY 1995

Canadian Cataloguing in Publication Data
Riecken, Sarah.
A compendium of water quality models

Includes bibliographical references: p.
ISBN 0-7726-2358-9

1. Water quality - Simulation methods. 2. Water quality management. I. BC Environment. Water Quality Branch.

TD227.B7R53 1994 363.73'942 C95-960048-5

Abstract

This compendium is a catalog of literature-cited surface water quality models that pertain to the nutrient dynamics of lakes, reservoirs, and rivers, and the fate and transport of toxic contaminants in freshwater environments. Water quality models are useful as predictive tools for assessing the state of water quality in most water mediums. There is much variety in the type and complexity of the water quality models that are available, and there are many factors involved in the selection of an appropriate model that meets user capabilities and study objectives. The models are presented in three general categories based on their theoretical origins and format: empirical, mechanistic, or computer simulation. There is no standard for the information included with each model description; the models are summarized based on the information available in the literature or from the developer. The goal of the report is to provide a reference source of water quality models that could be followed up on by the regional Environmental Protection staff of the Ministry of Environment, Lands and Parks. This compendium does not contain evaluations of the models that are cited. A general introduction to the classification and use of water quality models is provided. Models that are specific to watersheds, and groundwater, marine, or waste treatment systems are not included.

Acknowledgements

This compendium was written under the supervision of Dr. Rick Nordin. Thank-you to all of the model developers and distributors who contributed information; to Jim Bryan, Bob Grace, Brent Moore, and Murray Sexton for their initial guidance; and to Bill Duncan, Liz Freyman, Les Swain and Larry Pommen for their review comments.

Glossary and Abbreviations

Adsorption: The action of a solid (sediment) that holds molecules of a gas, liquid or solid to its surface, causing a thin film to form.

Aggradation: An interpretation of aggradation as used in the context of the CHARIMA description on page64 is an antonym for degradation.

Armouring: (Also known as paving) The process whereby larger particles (sediments) form a layer over a stream bed preventing finer particles from being released. (Forrest Holly, Section 3.1.4)

BOD: Abbreviation for biochemical oxygen demand

Calibration: Using a predetermined optimization criterion, the best values for the parameters of the model are estimated (along with error terms) (Chapra and Reckhow, Section 1.4).

Confirmation: (Often called verification or validation) Testing the model's outputs by rigourous statistical methods using a new set of data (different from calibration) (Chapra and Reckhow, Section 1.4).

Desorption: Release of an adsorbed substance.

DO: Abbreviation for dissolved oxygen.

Epilimnion: The warm upper layer of a thermally stratified lake.

Eutrophic: A body of water with an abundant suppply of nutrients and a high rate of formation of organic matter by photosynthesis.

External Load: The addition of nutrients (i.e. phosphorus and nitrogen) to a lake from external sources such as surface runoff and air.

Flushing Time: The relationship between the volume of a lake and the inflow or outflow volume. Can be expressed as the time (in years) of theoretical emptying or filling.

Flushing Rate: The number of times per a year the water of a lake is completely renewed. The flushing rate is reciprocal of the flushing time.

Fugacity:	A thermodynamic quantity related to the chemical potential or activity that characterizes the escaping tendency from a phase. Fugacities have units of pressure (Pa).
Hypolimnion:	The cool waters that make up the lowest layer of a thermally stratified lake.
Internal Loading:	The release of phosphorus from sediment sources to the water column.
Littoral Zone:	An interface region between the land of a drainage basin and the open water of a lake.
Mesotrophic:	A body of water with a moderate supply of nutrients and a moderate rate of formation of organic matter by photosynthesis. Intermediate between oligotrophic and eutrophic conditions.
Mixing Zone:	[Known in B.C. as an Initial Dilution Zone (IDZ)] An area where two water sources meet. (i.e. where a river runs into a lake, or where an outfall pipe enters a river).
Monte Carlo Simulation:	An empirical approach to sampling distribution that is often resorted to when the ideal or mathematical sampling distribution seems intractible.
Oligotrophic:	A body of water with a poor supply of nutrients and a low rate of formation of organic matter by photosynthesis.
pE:	Abbreviation for electrical potential.
Secchi Disc Transparency	(Often called Secchi disc depth or Secchi depth) The mean depth of the point where a weighted white disc, 20cm in diameter, disappears when viewed from the shaded side of a vessel, and that point where it reappears upon raising after it has been lowered out of sight.
Sorption:	Absoption or adsorption happening jointly or separately.
Stochastic:	Determined by a random distribution of probabilities.
Thermocline:	The plane of maximum rate of decrease of temperature with respect to depth.
Volatilization:	Evaporation.

TABLE OF CONTENTS

1.0 Introduction

This document is intended as guidance for persons who are directly involved in researching and managing water quality processes in B.C., particularly the regional Environmental Protection staff of the Ministry of Environment, Lands and Parks.

A model is defined as a simplified (often mathematical) description of a system that assists in calculations and predictions of the condition of that system in a given situation (Concise Oxford Dictionary, 1990). The use of models is becoming an integral part of the water quality management process. This is an indication that water resource managers find value in the insight a model can provide. The use of the computer for the simulation of water-related processes has made water quality-modelling a relatively inexpensive tool to investigate the impact of alternative development approaches before any irreversible action is taken. Because technology is advancing so rapidly, it is worthwhile for the prospective model user to keep track of the most recent modelling innovations.

The purpose of this compendium is to provide an accessible reference source of surface water quality models to prospective model users. This compendium is by no means comprehensive, although it does demonstrate the extent to which water quality models can be applied. For example, included in this compendium are models that can be used in either river or lake systems to predict trophic status or chemical transport. Water management models that can be used for reservoir and river basin regulation, and mixing zone models that can simulate the conditions of effluent outfall areas have also been compiled.

1.1 Classification of Water Quality Models

The models presented in this compilation are generally mathematical. A mathematical model is an equation, or a set of equations, that relates input parameters and variables to quantified outputs, based on specific assumptions and simplifications of the real system being modelled[1]. Mathematical models can be described by many different criteria. Chapra and Reckhow[2] provided the following descriptions of the descriptive terms for models that are used in this manual.

[1]U.S. EPA Seminar on the transport and fate of contaminants in the subsurface. Slide copies. Technology Transfer, CERI-87-45. [2]Chapra and Reckhow, 1983. See Section 1.4 for complete reference.

1. **Empirical or mechanistic.** An empirical model is developed primarily from an analysis of data. Empirical models are based more on fitting a set of data and less on theoretical principles. Mechanistic models, on the other hand, are intended to be mathematical descriptions of theoretical principles. It should be emphasized that any good model has both empirical and mechanistic features, but it is possible to classify most models according to a stronger basis in either empiricism or theory.

2. **Simulation or optimization.** Simulation models are designed to describe the functioning of a system. Optimization models are used to find a solution that is best (minimum or maximum) in some sense (often subject to constraints, such as cost or environmental quality).

> Many of the models described here have been adapted to a computer program format for simulation purposes. The program forms an interface between the user and the model. The degree of complexity of the programs vary with the programmer. Some of the programs have user-friendly interfaces while others require a sophisticated knowledge of the program. For example, the lake eutrophication model, EUTROMOD, is fairly user-friendly as it is run from the IBM software program AsEAsyAs, while the stream transport model, BLTM, requires that the user be able to program in Fortran to input much of the data.

3. **Static or dynamic.** These terms refer to the presence or absence of a time-dependency. Static or steady-state models describe behavior that is constant over time and is thus time-independent. Dynamic models describe behavior that varies with time and thus is time-dependent.

4. **Lumped parameter or distributed parameter.** These terms refer to the presence or absence of a space-dependency. Lumped-parameter models are zero-dimensional in space; they are based on an assumption of uniform conditions throughout the system modelled. An example of a zero-dimensional model is the continuously-stirred-tank-reactor (CSTR) that is used to estimate the concentration of a pollutant as a function of time. In contrast, distributed-parameter models, are developed to describe systems with variable conditions in one or more spatial dimension. An example of a distributed parameter model would be one that is used to describe the oxygen profile in a stratified lake.

> Distributed parameter models are categorized further according to how they represent the real world in terms of spatial resolution. One-dimensional models are considered to be the most simple. They simulate either the vertical or

longitudinal behavior of a water body. Two-dimensional models simulate the longitudinal and either transverse behavior or depth of a water body. Three-dimensional models are the most complex. They attempt to simulate the behavior of a whole system by taking into account all types of water movement. The decision of what type of model to use is usually limited by the amount of data available and the objective of the modelling study. A model is not a feasible water quality tool unless the appropriate data are available.

5. **Deterministic or stochastic.** Deterministic models use expected values (i.e. no real data) for all parameters and variables and yield predictions that are also expected values. Stochastic models incorporate variability, and possibly error, in probability density functions for selected parameters and/or variables. This results in a probability density function for the prediction.

6. **Cross-sectional or longitudinal.** Cross-sectional models describe behavior among cases (e.g., a cross section of the lakes in the U.S.), in contrast to longitudinal models, which describe behavior for a single case over time. As a rule cross-sectional models are more often empirical, whereas longitudinal models may be either empirical or mechanistic.

1.3 Use of Models

Models can be used to answer questions regarding the environmental impact of existing and potential loadings and waste discharges. Water quality investigators may use models to predict the future phosphorus content of a lake resulting from a newly developed pulp mill, or to evaluate the present condition of a system to determine what effects current use is inflicting on it. Models can also help to understand the complex relationships among the biotic and abiotic components of water systems. The extent to which a model can be useful depends on the suitability of the chosen model to the desired application, and the ability of the individuals interpreting the outputs. (i.e., the individuals need to know the theoretical components on which the model is based in order to understand why certain outputs occur.) No model will provide a definitive solution to any problem because there is risk, in the form of uncertainty, associated with all methods of prediction. The "best" models are those that have a solid basis of theoretical concepts, and have been confirmed by comparing actual measurements to predicted results.

There are many factors involved in the selection of a model that best suits the user's needs. Ultimately, the model that is selected should meet set standards for cost and data limitations, reliability, and capability. However, in reality the model that is selected will reflect a compromise of all standards. The major expense in implementing a model results from the acquisition of accurate and appropriate data. The most appropriate data are site-specific. However site-specific data are not always feasible to obtain for reasons of expense and time limitations. An alternative to providing site-specific data is to make use of either data gathered in the literature or "default" values for parameters that are included in some complex models. The consequence of using non-site-specific data is an increase in uncertainty of the model's output (Chapra and Reckhow, 1983). Some guidelines to follow when researching models for a specific application are:

1. Attempt to find a model that suits the expertise of the persons who will be implementing it. If the model user lacks programming capabilities, do not select a model that requires this knowledge. User-friendly programs are becoming more prevalent. It may be possible for a consultant to adapt a complex program to a user-friendly interface.
2. Be able to meet the requirements of the selected model and still maintain reliable results and budget requirements. If the amount of available data does not meet the requirements of a complex model, it may be worthwhile to select a more simple model instead of using default values in place of missing data.
3. Check the model documentation to make sure that the model has been successfully calibrated and confirmed.
4. Research past applications of the model in terms of recent application and success.
5. Understand the assumptions the model is based on and ensure these assumptions reflect the characteristics of the water system that is to be simulated.
6. Determine the uncertainty associated with the model's predictions, and whether this level of uncertainty will allow the study objectives to be met.
7. Of all equally capable models, choose the most simple. A complex model will prove to be more difficult to implement than a simple one, and its results may be more unreliable because of the implementation problems the user will encounter.

1.3 Model Review Methods

The process involved in documenting current model information for this compendium involved three steps:

1. Model identification. The search for available models was initiated by selective review of journal abstracts and applicable CD-ROM disks. In general the search was limited to documentation published after 1989.

Models that involved only watersheds, groundwater, marine, or waste treatment systems were not included.

2. Detailed information search. Using the names of developers and distributing agencies gathered during the identification process, an attempt to acquire detailed information about the capabilities and applications of each model was made. If no contact was made with the developer, a distributor, or a current user, the model was deleted from inclusion in this compendium. No attempt was made to contact the authors of empirical and mechanistic models identified in the literature search unless further clarification on the applicability of the model was necessary.

3. Summarization. The model documentation that was gathered was used to formulate a short description of each model's capabilities. Provided with each model description is the information necessary to find out more about each model. The best person to talk with about how to apply each model is either the model developer or the person who is distributing the model. Often, technical support is provided by phone or by a tutorial course. The developer may suggest using a consulting agency to determine whether the model is applicable for the desired water quality investigation or to re-calibrate and re-confirm the model.

1.4 Sources of General Water Quality Modelling Information

1. Bowie, G.L., W.B. Mills, D.B. Porcella, C.L. Campbell, J.R. Pagenkopf, G.R. Rupp, K.M. Johnson, P.W.H. Chan, S.A. Gherini, and C.E. Chamberlin. 1985. Rates, constants, and kinetic formulations in surface water quality modeling (2nd ed.). U.S. Environmental Protection Agency, Athens, GA. EPA 600/3-85/040.

This manual is intended to be used by practitioners as a convenient reference on modelling formulations, constants, and rates commonly used in surface water quality simulations. Chapters are presented that discuss the following topics: physical processes of dispersion and temperature; dissolved oxygen; pH and alkalinity; nutrients; algae; zooplankton; and coliforms.

2. Chapra, S.C. and K.H. Reckhow. 1983. Engineering approaches for lake management. Vol.1: Data analysis and empirical management. Vol.2: Mechanistic modeling. Butterworth Publishers. ISBN 0-250-40392-7.

Chapra and Reckhow apply their combined knowledge of modelling, applied statistics, and environmental engineering to this two-volume tutorial on the concepts and analytical techniques behind lake management. The format of *Engineering Approaches* enables readers to use the two-volume set as either reference texts to lake water quality modelling issues, or as educational reading. While both volumes focus on the development of the mathematical aspect of models, these books provide basic information about the subject of water quality management and how water quality modelling can be undertaken.

3. Henderson-Sellers, B., Ed. 1991. Water quality modeling. Volume IV; decision support techniques for lakes and reservoirs. CRC Press. Boca Raton, Florida.

Decision Support Techniques for Lakes and Reservoirs is a compilation of simulation modelling case studies contributed by various authors. The first chapter contains a comprehensive introduction to the concepts of simulation modelling and the methodology behind decision support systems, and a detailed summary of eutrophication simulation. The remaining chapters are summaries of specific modelling applications.

4. Kenney, B.C. 1990a. On the dynamics of phosphorus in lake systems. National Hydrology Research Institute Paper No. 45. Inland Waters Directorate, NHRI, Saskatoon, Saskatchewan.

   Kenney, B.C. 1990b. Dynamics of phosphorus in a chain of lakes: The Fishing Lakes. National Hydrology Research Institute Paper No. 44. Inland Waters Directorate, NHRI, Saskatoon, Saskatchewan.

   Kenney, B.C. 1994. Phosphorus dynamics in riverine lakes. Water Poll. Res. J. Can. 29(2/3): 185-202.

In these publications Kenney presents a review of phosphorus modelling concepts and a summary of the necessary components to phosphorus loading models. The models are developed to predict the phosphorus concentration of very shallow, or riverine, lakes.

5. Reckhow, K.H. 1979. Quantitative techniques for the assessment of water quality. U.S. Environmental Protection Agency, Washington, D.C. EPA 440/5-79-015.

This report is useful as a guide to the original empirical phosphorus models that many current models are based on.

2.0 Modelling the Water Quality of Lakes and Reservoirs

Lakes have a number of characteristics that lend themselves to modelling approaches. The major contributing factors are that lakes have discrete boundaries (in contrast to oceans) and they have less spatial and temporal complexity than flowing waters.

The majority of models proposed at this time fit into the category of empirical models however, a significant number of mechanistic models and simulation models have been described in the past few years.

Two workers who have been involved with lake modelling for many years and who are both preparing new books are Dr. Kenneth Reckhow and Dr. Steven Chapra. Their earlier two-volume set on lake modelling is a key reference source of lake modelling information (see section 1.4).

2.1 Lake Nutrient/ Productivity Models

2.1.1 EUTROMOD: Eutrophication Model

Type: An easy-to-use watershed and lake modelling procedure for eutrophication management, with an emphasis on uncertainty analysis. Computer simulation.

Description:

Based on inputs of data pertaining to land use, pollutant concentrations, and lake characteristics EUTROMOD estimates nutrient loading, various trophic state concentrations, and trihalomethane concentrations.

The EUTROMOD file is run from the IBM spreadsheet software program AsEasyAs. EUTROMOD's outputs are based both on statistical relationships and a continuously-stirred-tank-reactor (CSTR) model.

Comments:

EUTROMOD is a powerful and handy tool which greatly decreases the time required for tedious calculations. At present, EUTROMOD is specific to watersheds in Kansas, Missouri, Oklahoma, Arkansas, Iowa, Nebraska, Indiana, Illinois, Ohio, Florida, and northeast United States. The user's responsibilities are significant, and substantial time may be required to gather the data necessary for running the model. The model is subject to a certain amount of uncertainty (which is addressed in the uncertainty analysis portion of the spreadsheet), so the user should not assume that predictions are definitive. Finally, since the model simply expresses cross-sectional associations among variables, a thorough evaluation of lake management options likely requires a more detailed lake-specific study involving field sampling.

EUTROMOD requires some improvements before it can be considered complete. Although it is available for distribution users should consult the developer before implementing this program.

Availability:

For ordering information contact:

North American Lake Management Society, 1 Progress Boulevard, Box 27, Alachua, Florida 32615. Phone (904) 462-2554. Fax (904) 462-2568.

Reference:

1. Reckhow, K. EUTROMOD. Lake and watershed modeling software. Summary description provided by Bruce Wilson: Minnesota Pollution Control Agency, 520 Lafayette Road, St. Paul, MN 55155. Phone (612) 296-9210; Fax (612) 297-8683.

Other Sources of Information:

1. Kenneth Reckhow, Duke University, School of Forestry and Environmental Studies, Durham, North Carolina 27708-0328. Phone (919) 613-8026. Fax (919) 684-8741. Internet: RECKHOW@acpub.duke.edu

2.1.2 PHOSMOD: Long-Term Total Phosphorus Model for Lake/Sediment Interactions

Type: A modelling framework that is designed to model the seasonal and long-term trends of total phosphorus and oxygen in stratified lakes. Computer simulation. Based on the model described in Chapra and Canale (1991).

Description:

The modelling framework is implemented via a personal-computer oriented software package--PHOSMOD 1.0. It is designed for interactive implementation and is self-documented. PHOSMOD allows the user to rapidly generate and analyze scenarios. The software includes graphical displays and can be run on IBM-PC compatible microcomputers. It is presently designed for implementation with EGA color graphics.

Comments:

The author outlines the limitations of PHOSMOD in the user's manual. Chapra warns that the model has not been "beta tested," a process whereby users, other than the original developer, test the model by running it for new applications. As well, the computer program does not contain an efficient "error trapping" system. In other words, the program will attempt to process all data that the user inputs, even if the data represents an unrealistic scenario. Due to these weaknesses in the PHOSMOD program users must be familiar with the requirements for applying the model properly.

Availability:

For ordering information contact:

NALMS, 1 Progress Boulevard, Box 27, Alachua, Florida 32615. Phone (904) 462-2554. Fax (904) 462-2568.

Reference:

1. Chapra, S.C. 1991. PHOSMOD 1.0. Software to model seasonal and long-term trends of total phosphorus and oxygen in stratified lakes. CADSWES Working Paper No. 14.

Other Sources of Information:

1. Chapra, S.C. and R.P. Canale. 1991. Long-term phenomenological model of phosphorus and oxygen in stratified lakes. Water Res. 25(6):707-715.

This paper describes an empirical modelling framework that is used to predict the long-term response of a lake to changes in its phosphorus loading. Included in the framework are two models: a total phosphorus model and a hypolimnetic oxygen model. The paper demonstrates the application of the model to Shagawa Lake, Minnesota. The conclusions state that the results obtained from the study are a credible representation of a future recovery of the lake although revisions to the model are necessary.

2. Steven Chapra, CADSWES, Campus Box 428, University of Colorado, Boulder, CO 80309-0428.Phone: (303) 492-3972.

2.1.3 BATHTUB/ FLUX/ PROFILE Model

Type: Eutrophication model for impoundments. Computer simulation.

Description:

BATHTUB is a simple eutrophication model that predicts the response of impoundment areas to nutrient loading. FLUX and PROFILE are associated programs that calculate data to be used by BATHTUB. FLUX calculates the nutrient loadings while PROFILE calculates the annual impoundment water quality. The model does not consider temperature, oxygen or dissolved materials. A separate river water quality model is required in order to provide inputs about the upstream water quality.

Reference:

1. Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for Inland Waters Directorate, Environment Canada, Regina, Saskatchewan. (Bill Gummer may be reached at 306-780-5322)

2. Cooke, G.D., E.B. Welch, S.A. Peterson, and P.R. Newroth. 1993. Restoration and management of lakes and reservoirs. Second edition. Lewis Publishers. ISBN 0-87371-397-4.

Other Sources of Information:

1. Walker, W.W., Jr. 1987. Empirical methods for predicting eutrophication in impoundments. Technical Report E-81-9. U.S. Army Engineer Waterways Experiment Station, Environmental Laboratory, Vicksburg, Mississippi.

2.1.4 SED -- A Simple Dynamic Model for the Release of Phosphorus from Sediments in Shallow, Eutrophic Systems

Type: A dynamic model that describes the release of phosphorus from sediments in shallow, eutrophic lakes. Computer simulation.

Description:

Based on model inputs of sediment temperature, concentration of dissolved phosphorus in the overlying water, and the phosphorus loaded to the sediment, SED estimates the net phosphorus release from lake sediments.

SED describes the diffusive transport of dissolved phosphorus from sediments to the overlying water, mineralization of organic phosphorus in the sediment, and adsorption, desorption and fixation of inorganic phosphorus from the water column to the sediment. The main principle used in SED is that mineralization of organic matter not only produces dissolved phosphorus, but also determines the conditions of the sediment.

Calibration of SED was performed using data set form Lake Veluwe, The Netherlands. SED is capable of reproducing phosphorus retention in Lake Veluwe and yields realistic values for the net phosphorus release from the sediment, both in magnitude and in seasonal pattern.

System Requirements and Availability:

SED is written for a MS DOS personal computer in TURBO-PASCAL. It is menu-directed and user-friendly. According to Van der Molen (1991) it is available free of charge from the author: Institute for Inland Water Management and Wastewater Treatment, P.O. Box 17, 8200 AA Lelystad, The Netherlands.

Reference:

1. Van der Molen, D.T. 1991. A simple, dynamic model for the simulation of the release of phosphorus from sediments in shallow, eutrophic systems. Wat. Res., 25(6): 737-744.

2.1.5 TSM -- Lake Trophic Status Model

Type: A trophic model for lakes based on empirical and semi-empirical equations. Computer simulation.

Description:

The TSM is a refinement of the Dillon, Rigler (1975) model. It is based on empirical and semi-empirical equations that can predict the mean phosphorus concentration of a lake or values for other trophic status indicators such as chlorophyll a and Secchi depth. The TSM is now operated as a PC-based program that has the capabilities of modelling watersheds. The model can include up to 15 tributary streams for a study lake, and up to three lakes (> 10 ha in size) upstream in each tributary. Each of these lakes, in turn, may have up to 15 tributaries. This feature enables lake managers to predict the effect of lakeshore development throughout an entire watershed, including downstream lakes.

Hutchison *et al.*. (1991) describe how the TSM functions to predict total phosphorus concentrations. These estimates can then be used to derive phosphorus objectives which are lake specific. The paper outlines the use of the TSM in the Boshkung Lake and its catchment, which has a combined area of 879.1 km^2.

The TSM has been designed to model trophic status indicators in Precambrian Shield lakes, although adaption of the model to other geographical areas is feasible.

References:

1. Dillon, P.J. and F.H. Rigler. 1975. A simple method for predicting the capacity of a lake for development based on lake trophic status. J. Fish. Res. Bd. Canada. 32:1519-1531.

2. Hutchison, N.J., B.P. Neary, and P.J. Dillon. 1991. Validation and use of Ontario's Trophic Status Model for establishing lake development guidelines. Lake and Reserv. Manage. 7(1): 13-23.

Other Sources of Information:

1. Ontario Ministry of Environment. 1991. Users Manual for PC-based Lakeshore Capacity Study Trophic Status Model, Version 1.0 (Draft). 49pp.

2.1.6 BETTER -- Box Exchange Transport Temperature Ecology Reservoir Model

Type: A two-dimensional reservoir water quality model. Computer simulation.

Description:

BETTER has been designed to reproduce observed seasonal patterns of temperature, DO, nutrients, pH, and algal biomass in reservoirs. The two-dimensional structure of the model allows the effects of both thermal stratification and inflow/outflow advection to be simulated. The philosophy of the most recent BETTER model has been to create a generalized model that does not incorporate a code designed for a specific problem. However code modifications may still be required for complex applications that are beyond the scope of the latest version. A detailed discussion of the capabilities and limitations of BETTER is included in the technical reference manual and user's guide.

System Requirements and Availability:

IBM PC (or 100% compatible computer); DOS 2.0 or higher; 1 double-sided diskette drive and a hard disk with at least 10MB free spce; at least 640K RAM memory; a pen plotter; a math coprocessor.

The BETTER software is being made available in part for broader testing in order to identify potential applications, program options, debugging, and other code modifications that could enhance future versions. Suggestions for revision, inquiries on how to obtain the BETTER software and documentation, and questions regarding user support, should be directed to: Mr. Don Anderson, HB 2C-C, TVA Water Quality Department, 311 Broad Street, Chattanooga, TN 37402-2801. Phone: (615) 751-7329.

Reference:

1. Bender, M.D., G.E. Hauser, M.C. Shiao, and W.D. Proctor. 1990. BETTER: A two-dimensional reservoir water quality model. Technical reference manual and user's guide. Tennessee Valley Authority Engineering Laboratory. Report No. WR28-2-590-152.

2.2 Mechanistic Models

2.2.1 A Trophic Status Model Based on Total Phosphorus Concentrations

Type: Mechanistic.

Description:

Swiss modellers Imboden and Gachter (1978) present a model of trophic state prediction. Inputs to the model are descriptions of lake morphometry, hydraulic loading, respiration rate, sedimentation, vertical eddy diffusion, depth of thermocline, and exchange of phosphorus at the sediment-water interface.The dynamic, one-dimensional model is used to predict the primary production of a lake as a measure of total phosphorus.

The model is applied to two lakes in Switzerland that are similar in depth and volume in order to compare field measurements and model calculations. The model is also described as it is applied to a much larger lake, Lake Washington, in order to predict the lake's response to various external and internal eutrophication control measures such as reduction of phosphorus loading, discharge of hypolimnetic water, aeration of the hypolimnion, and destratification. The conclusions of the study find that the model successfully describes the response of Lake Washington to the diversion of sewage effluent over a four-year period.

Reference:

1. Imboden, D.M. and R. Gachter. 1978. A dynamic lake model for trophic state prediction. Ecol. Modelling. 4: 77-98.

2.2.2 Three Mass Balance Models of Phosphorus -- An Analysis of Their Sedimentation Assumptions

Type: Mechanistic

Description:

Phosphorus loading models differ in that some assume the mass of phosphorus lost to the sediments is a function of the mass of phosphorus in the lake (in-lake mass decay) while others assume it to be a function of the loading mass (loading decay). Examination of the empirical basis of both hypotheses shows that a loading decay model describes the behavior of a large number of lakes better than the more common in-lake mass decay. However, further analysis indicates that a model of the form

$$[P] = L\ (1-R')/(q_S + \sigma'\ z)$$

which incorporates both assumptions, appears even more justified (Author's abstract). ([P] = lake phosphorus concentration, L = phosphorus loading, q_S = areal water loading, z = mean depth, σ = sedimentation coefficient, R = retention coefficient.)

Reference:

1. Prairie, Y.T. 1988. A test of the sedimentation assumptions of phosphorus input-output models. Arch. Hydrobiol. 111(3): 321-327.

2.2.3 Mass Balance Models of Phosphorus in Sediments and Water

Type: Mechanistic.

Description:

Lam *et al.* (1982) present models in order of progressively more complex spatial resolution in which the effects on the sediment-water interactions are emphasized. For simple models, the diagnostic approach of calculating the net settling and return of total phosphorus is demonstrated with data from Lake Erie. For more complex models, the effects of interbasin transport and vertical mixing are shown to be important in determining the pathways of the sediment-released or sediment-bound phosphorus in the water column (Author's abstract).

Reference:

1. Lam. D.C.L., W.M. Schertzer, and A.S. Fraser. 1982. Mass balance models of phosphorus in sediments and water. Hydrobiol. 91: 217-225.

2.2.4 Eutrophication Model

Type: Mechanistic. A mathematical lake eutrophication model that can assume steady-state or dynamic conditions.

Description:

Based on inputs of total phosphorus loads, lake mean depth, volume, flushing rate, algal growth coefficients, and rates of photosynthesis, mineralization, and settling, the model predicts concentrations of total phosphorus, algal phosphorus, dissolved phosphorus, and chlorophyll in lakes.

The model is based on simplification of the lake structure into either a two-compartment completely mixed system, a system consisting of an epilimnion compartment with inputs from the hypolimnion, or a single completely mixed system. It is considered to be intermediate in complexity to nutrient loading models and multivariable models.

Comments:

The main difficulty in implementing this model is the estimation of four coefficients. These calculations are more feasible when sufficient field data and gross productivity measurements are available.

Reference:

1. Schooner, J.L., and D.L. O'Connor. 1980. A steady state eutrophication model for lakes. Wat. Res., 14: 1651-1665.

2.2.5 Internal Phosphorus Load Models for Anoxic Lakes

Type: Mechanistic.

Description:

Nurnberg (1984) describes two methods of calculating the internal phosphorus load in anoxic lakes in order to aid in calculating the total phosphorus concentration in such lakes. The internal phosphorus load in anoxic lakes represents the release of phosphorus from the sediment under reducing conditions therefore this source of phosphorus in the lake must be taken into account when calculating total phosphorus. The first model calculates internal load as the difference between the observed phosphorus retention in anoxic lakes and that predicted by a formula that adequately describes phosphorus retention in oxic lakes. However, values for observed phosphorus retention are not always available therefore an alternative method is described. The second model predicts internal load as the product of an average rate of phosphorus release from anoxic sediments, the surface area of the anoxic sediment, and the period of anoxia. This predicted value can then be combined with a retention-based budget model for external load.

Comments:

The author notes that the information used to derive her conclusions are based on data from lakes that are not naturally anoxic but anoxic by cultural processes.

Reference:

1. Nurnberg, G. 1984. The prediction of internal phosphorus load in lakes with anoxic hypolimnia. Limnol. Oceanogr., 29(1): 111-124.

Other Sources of Information:

1. Nurnberg, G., and R.H. Peters. 1984. The importance of internal phosphorus load to the eutrophication of lakes with anoxic hypolimnia. Verh. Int. Ver. Limnol. 22:190-194.

2. Dr. Gertrud Nurnberg, Freshwater Research, R.R.1, Baysville, Ontario P0B 1A0. Phone and Fax: (705) 767-3718.

2.2.6 Sedimentation and Resuspension Models

Type: Mechanistic.

Description:

A 2-D vertical flow and suspended matter transport model and a 3-D transport model are described by Podsetchine and Huttula (1994). Existing parameterizations of resuspension and deposition of sediments on the bottom are discussed. Models were applied for calculation of unsteady sediment transport in Lake Karhijarvi, Finland, for a five-year period with high winds and heavy rain in Autumn 1992. A parabolic distribution of vertical eddy diffusivity was found to be applicable. Erosion was approximated with cubic dependance on bed dhear stress. The 3-D model showed that the observed turbidity peak in the middle of the lake was caused by suspended matter transport through the River Susikoski. Sediment resuspension was found to be limited in the areas with depth less than 1m. The 2-D vertical model was useful for determination of erosion under certain weather conditions, but for detailed analysis in space and time a 3-D model with high resolution is required (Author's abstract).

Reference:

1. Podsetchine, V. and T. Huttula. 1994. Modelling sedimentation and resuspension in lakes. Water Poll. Res. J. Canada 29 (2/3): 309-342.

2.3 Empirical Models

2.3.1 An Introduction to Empirical Models for Lakes and Reservoirs

Over the past 25 years a large number of models have been described that arise from the principle of empiricism. These models generally draw some mathematical relationship between two or more quantitative measurements in lakes. The classic example of this is Vollenweider's (1968) relationship between phosphorus loading and trophic status of lake. Another early use of empiricism was by Satamoto (1966) in describing the relationship between phosphorus and chlorophyll in lakes. Since Vollenweider's landmark publication the method of using reported results from the literature, and sample results for a wide range of lakes, to derive an understanding of the relationship between the components of a lake ecosystem has been widely used.

Frank Rigler was an advocate of empiricism and one of his students, Robert Peters, and subsequently his students, have used this approach - many of the publications cited in this section are a result of the ideas of Rigler and Peters.

References:

1. Sakamoto, M. 1966. Primary production by phytoplankton commumity in some Japanese lakes and its dependence on lake depth. Arch. Hydrobiol. 62: 1-28.

2. Vollenweider, R.A. 1968. The scientific basis of lake and stream eutrophication, with particular reference to phosphorus and nitrogen as eutrophication factors. Tech. Rpt. OECD Paris OAS/CSI/68, 27: 1-182.

2.3.2 Hypolimnetic Oxygen Deficit Model for Oligotrophic Lakes

Type: Empirical.

Description:

Rates of hypolimnetic oxygen depletion can be predicted from a knowledge of a lake's phosphorus retention, the average hypolimnetic temperature, and the mean thickness of the hypolimnion. Areal oxygen deficits cannot be used to index lake trophic status because areal calculations do not eliminate the influence of hypolimnetic morphometry (Author's abstract).

Comments:

The regression equation for this model was developed from data for 12 lakes. The model's predictions were found to be highly correlated with observed data for 20 oligotrophic lakes. There is no reference to the location or the type of lakes that were used to develop the regression equation.

Reference:

1. Cornett, R.J. and F.H. Rigler. 1979. Hypolimnetic oxygen deficits: their prediction and interpretation. Science 205:580-581.

2.3.3 Hypolimnetic Oxygen Deficit Model Based on Chlorophyll Concentrations

Type: Empirical.

Description:

Until recently, hypolimnetic oxygen consumption was thought to be a way of comparing the productivity of lakes. This study shows that hypolimnion oxygen represents hypolimnion thickness and temperature as well as productivity. A relationship based on the multiplicative effects of chlorophyll (productivity), thickness, and temperature closely fits the observed oxygen depletion in the Laurentian Great Lakes and in many small lakes. Applied to Lake Erie, the relationship suggests that although a 50% decrease in productivity may result in higher oxygen concentrations, significant oxygen depletion would still occur. The use of oxygen concentrations, depletion rates, or areal deficits to compare the productivity of lakes is not justified without reference to hypolimnion thickness and temperature (Author's abstract).

This linear regression model was developed from data collected from 26 small and large lakes in North America, including the Great Lakes.

Reference:

1. Charlton, M.N. 1980. Hypolimnion oxygen consumption in lakes: discussion of productivity and morphometry effects. Can. J. Fish. Aquat. Sci. 37:1531-1539.

2.3.4 A Trophic Status Model Based on Oxygen Deficit Rate

Type: Empirical

Description:

Welch and Perkins (1979) present a linear regression equation that relates phosphorus loading and oxygen deficit rate (ODR). ODR is defined as the rate of oxygen depletion per unit hypolimnetic surface during summer stratification. Data from 26 lakes, including 13 Precambrian Shield lakes in Ontario, and others that had been previously determined as stratified and showing a measurable reduction in oxygen content in the hypolimnion during the summer, were used to develop this model.

The authors use this model to estimate a level of phosphorus loading that they predict will have a negative effect on fisheries and recreational lake use.

Reference:

1. Welch, E.B., and M.A. Perkins. 1979. Oxygen-deficit--phosphorus loading relation in lakes. J. WCPF. 51(12): 2823-2828.

2.3.5 A Nutrient Budget Model for the Prediction of Total Phosphorus Concentration

Type: Empirical.

Description:

The total phosphorus budgets for a number of lakes in the Haliburton-Kawartha region of southern Ontario were measured over a 20-month period. These data, combined with the lakes' morphometry and water budgets, were used to test a simple nutrient budget model similar to that proposed by Vollenweider (1969) purporting to predict the total phosphorus concentration in lakes. Except in the case of two very shallow lakes, the concentrations predicted by the model were very close to those measured in the lakes at spring overturn. Additional data from the literature supported the belief that this model could be used effectively for oligotrophic and mesotrophic lakes. Its value lies in the fact that quantitative changes in the phosphorus loading can be interpreted in terms of changes in phosphorus concentration, which in turn, can be related to changes in parameters that reflect the lake's trophic state such as summer chlorophyll *a* concentration (Dillon and Rigler, 1974/Authors' Abstract).

Reference:

1. Dillon, P.J. and F.H. Rigler. 1974. A test of a simple nutrient budget model predicting the phosphorus concentration in lake water. J. Fish. Res. Board. Can. 31: 1771-1778.

2. Vollenweider, R.A. 1969. Moglichkeiten und Grenzen elementarer Modelle der Stoffbilanz von Seen. Arch. Hydrobiol. 66: 1-36.

2.3.6 Phosphorus Retention Capacity of Lakes

Type: Empirical.

Description:

Mean annual lake phosphorus concentrations ($[P]_X$) in a steady state system can be described as a function of two variables, the mean annual influent phosphorus concentration and the net annual phosphorus sedimentation: $[P]_X = [p] (1 - R_p)$ (see Rigler, 1975). [p] is the annual phosphorus supply/annual water supply and R_p is that fraction of inflowing phosphorus retained by the sediments annually. Since R_p is critical in determining $[P]_X$, lake properties were examined for their influence on R_p: the best fit empirical expressions developed related R_p to either areal water supply (annual water inflow rate/lake surface area) or hydraulic washout coefficient (annual water ouflow rate/lake volume). The expressions were derived from characteristics of low productivity in lakes; their validity for more productive lakes was not examined.

A graph of [p] vs. R_p is proposed to illustrate the relationship between $[P]_X$, [p], and R_p, and if lake phosphorus concentrations are used as measures of trophic state, this graph is useful for predicting trophic state and changes in trophic state caused by altering [p] and/or R_p (Larson and Mercier, 1975/Authors' abstract edited).

References:

1. Larson, D.P. and H.T. Mercier. 1975. Phosphorus retention capacity in lakes. J. Fish. Board. Can. 33:1742-1750.

2. Rigler, F.H. 1975. Nutrient kinetics and the new typology. Verh. Int. Ver. Limnol. 19:197-210.

2.3.7 Prediction of Phosphorus Release Rates from Total and Reductant-Soluble Phosphorus in Anoxic Lake Sediments

Type: Empirical

Description:

Release rates of phosphorus from anoxic sediment surfaces in seven North american lakes were determined from core tube incubations. These rates were compared with several phosphorus fractions within the 0-5 and 5-10 cm layers of the corresponding sediment. Regressions of release rates both on total sediment phosphorus and on reductant-soluble phosphorus were highly significant. Analysis of literature data from lakes worldwide also showed significant relationships between the release rates and total sediment phosphorus and citrate dithionite bicarbonite extractable phosphorus. Mass balance calculations for individual cores indicated that reductant-soluble phosphorus decreases in wet surficial sediments, while total phosphorus in the overlying water increases. The release rates of different phosphorus fractions in the water - total, soluble reactive, and total reactive phosphorus - were very similar, indicating the high biological availability of the released phosphorus.

Reference:

1. Nurnberg, G. 1988. Prediction of phosphorus release rates from total and reductant-soluble phosphorus in anoxic lake sediments. Can. J. Fish. Aquat. Sci. 45: 453-462.

2.3.8 Prediction of Total Phosphorus Concentration in North Temperate Lakes

Type: Empirical.

Description:

This model was developed in order to predict the average phosphorus concentration throughout a lake during the growing season. It is based on data from 47 north temperate lakes included in the EPA's National Eutrophication Survey.

The text describing this model applies to most empirical phosphorus models. It includes step by step instructions for calculating total phosphorus concentrations, and a good discussion of uncertainty analysis and the applicability of this model to lakes unlike those in the original data set.

Reference:

1. Reckhow, K.H. and S.C. Chapra. 1983. Engineering approaches for lake management. Volume 1: Data analysis and empirical modeling. Butterworth Publishers. p.272-279.

2.3.9 Prediction of Total Phosphorus Concentrations, Chlorophyll *a* , and Secchi Depths in Natural and Artificial Lakes

Type: Empirical.

Description:

Based on inputs of total phosphorus loads, lake mean depth, and flushing rate, this model predicts the total phosphorus concentration of a lake. This model was developed using data from 704 natural and artificial lakes therefore it is applicable to most natural and artificial lakes in the temperate region. Estimates for Secchi depths and chlorophyll *a* concentrations are based on empirical phosphorus-chlorophyll *a*, and chlophyll *a*-Secchi depth relationships.

Canfield and Bachmann (1981) give a comprehensive discussion of aspects involved in the prediction of total phosphorus concentrations. Specifically, it contains a recommendation that empirical phosphorus models should only be used for making order of magnitude estimates of phosphorus concentrations in lakes because of the uncertainty associated with the predictions. For example the Canfield-Bachmann model has a 95% confidence interval of 31-288% of the calculated total phosphorus concentration while other models are less precise.

Reference:

1. Canfield, D.E., Jr. and R.W. Bachmann. 1981. Prediction of total phosphorus concentrations, chlorophyll *a* , and Secchi depths in natural and artificial lakes. Can. J. Fish. Aquat. Sci. 38: 414-423.

2.3.10 Prediction of Secchi Disc Depths in Florida Lakes: Impact of Algal Biomass and Organic Color

Type: Empirical.

Description:

A model for the prediction of Secchi disc depths in Florida lakes was developed and tested using data from 205 lakes. A statistical analysis showed that the best estimate of lake Secchi disc depths could be obtained by $\ln(SD) = 2.01 - 0.370 \ln(Chla) - 0.278 \ln(C)$ where SD is Secchi disc depth (m), Chla is the chlorophyll *a* concentration (mg/m^3), and C is the organic color concentration (mg/l as Pt.). The model yields unbiased estimates of lake Secchi disc depths over a wide range of algal and organic color concentrations and has a 95% confidence interval of 47-224% of the calculated Secchi disc depth. Other published Secchi-Chlorophyll models are less precise but can be used almost equally well. This indicates organic color concentrations do not affect Secchi disc depths as much as algal levels. Further reductions in the remaining error term, however, might be accomplished by including a variable for suspended inorganic sediment (Author's abstract).

Reference:

1. Canfield, D.E., Jr. and L.M. Hodgson. 1983. Prediction of Secchi disk depths in Florida lakes: Impact of algal biomass and organic color. Hydrobiol. 99: 51-60.

2.3.11 Photosynthesis Model

Type: Empirical.

Description:

Based on inputs of total phosphorus loads, lake mean depth, flushing rate, epilimnetic total phosphorus and total nitrogen this model predicts epilimnetic volumetric rates of photosynthesis.

This model is an extension of an earlier phosphorus loading model (Dillon and Rigler, 1974,1975) that is used to predict volumetric rates of photosynthesis in north temperate lakes where the total nitrogen to total phosphorus ratio is greater than or equal to 13, indicating dominance of photosynthesis by phosphorus.

Comments:

Smith (1979) includes a discussion of volumetric rates of photosynthesis versus integral rates of photosynthesis. In short, Smith finds that it is more valuable to use volumetric rates because they are strongly correlated with lake nutrient concentration as compared with integral rates which are not strongly correlated with nutrient concentrations.

Reference:

1. Dillon, P.J. and F.H. Rigler. 1974. The phosphorus-chlorophyll relationship in lakes. Limnol. Oceanogr. 19: 767-773.

2. Dillon, P.J. and F.H. Rigler. 1975. A simple method for predicitng the capacity of a lake for development based on lake trophic status. J. Fish. Res. Bd. Can. 31: 731-738.

3. Smith, V.H. 1979. Nutrient dependence of primary productivity in lakes. Limnol. Oceanogr. 24(6):1051-1064.

2.3.12 Phosphorus-Phytoplankton Model

Type: Empirical.

Description:

Many of the published empirical nutrient-phytoplankton relationships are based on analysis of global data sets in which variables typically span 2-4 orders of magnitude. In some regions of the world, the variability in trophic status between lakes is much less than this. To see if useful relationships exist over a smaller trophic gradient, Dillon *et al.* (1988) studied 16 oligotrophic and mesotrophic lakes for a 4-year period. The range in both total phosphorus and chlorophyll *a* between these lakes was only 3-fold. Nevertheless, excellent relationships between these parameters were found, with typically 80% of the variability in chlorophyll *a* being explained by total phosphorus. The residual variance was in all cases, most strongly correlated to the total phosphorus:total nitrogen ratio. Substitution of phytoplankton biomass for chlorophyll *a* resulted in even better relationships as long as the diatom fraction was excluded from the biomass. Zooplankton biomass did not explain a significant amount of the residual variance in any case (Author's abstract).

Reference:

1. Dillon, P.J., K.H. Nicholls, B.A. Locke, E. DeGrosbois, and N.D. Yan. 1988. Phosphorus-phytoplankton relationships in nutrient-poor soft-water lakes in Canada. Verh. Int. Ver. Limnol. 23: 258-264.

2.3.13 U.S. OECD Phosphorus-Loading Eutrophication Response Models

Type: Empirical.

Description:

In this paper, the predictive capability of the "U.S. Organization for Economic Cooperation and Development (OECD) - Vollenweider-Rast-Lee and Jones" phosphorus load-response models is examined.

The models presented are an outgrowth of the Cooperative program on Eutrophication Control of OECD. This program was initiated to define quantifiable relationships between nutrient loads and eutrophication-related responses of water bodies, which could be used as management tools in the assessment and control of eutrophication in lakes and impoundments. Through the OECD program, a detailed evaluation was made of loadings and responses of over 200 water bodies exhibiting a variety of trophic conditions and physiographic factors in about 20 nations around the world. These water bodies were grouped into four regional projects. Approximately 34 lakes were included in the OECD-North American Project. The OECD eutrophication study program is described in detail by Rast and Lee (1978), and Vollenweider and Kerekes (1980).

References:

1. Rast, W., R.A. Jones, and G.F.Lee. 1983. Predictive capability of U.S. OECD phosphorus loading-eutrophication response models. J. WCPF. 55(7): 990-1003.

2. Rast, W. and G.F. Lee. 1978. Summary analysis of the North American (U.S. portion) OECD eutrophication project: Nutrient loading-lake response relationships and trophic state indices. EPA 600/3-78-008, Corvallis, Oregon.

3. Vollenweider, R.A. and J.J. Kerekes. 1980. Synthesis report: Cooperative Programme on Monitoring of Inland Waters (Eutrophication Control), Report prepared for the Organization for Economic Cooperation and Development (OECD), Paris.

2.3.14 A Model of Species Density in Shoreline Vegetation

Type: Empirical.

Description:

Predicting the species density (number of species per unit area) of communities is a major goal of ecology. Shipley *et al.* (1991) present a regression model of species density on a local ($0.25m^2$) scale for the vegetation of freshwater shorelines in southwestern Quebec. Two attributes of the vegetation, the amount of aboveground biomass (in grams) and the proportion of the vegetation composed of obligate perennial species, predicted 76% of the variation in species density. the success of the predictor variables suggested that competitive intensity, as reflected in biomass levels, and the time elapsed since the last disturbance event, as reflected in the proportion of the vegetation composed of obligate perennials, are important determinants of local variation in species density. The model was then tested against independent data from shoreline vegetation in southeastern Ontario. There were no significant differences in the two data sets in their response to the two independent variables in the full model. However, only 42% of the variance in species density was explained in the combined data set (Author's abstract).

Reference:

1. Shipley, B., P.A. Keddy, C. Gaudet, and D.R.J. Moore. 1991. Ecology 72(5): 1658-1667.

2.3.15 Empirical Relationship Between Bacterial Abundance and Chlorophyll Concentration in Fresh and Marine Waters

Type: Empirical.

Description:

A strong, positive relationship was found between bacterial abundance and chlorophyll concentration in fresh and marine waters. Freshwater and marine linear regression equations are statistically indistinguishable. The overall equation is log AODC = 5.867 + 0.776 log chla, $r^2 = 0.88$, where AODC (acridine orange direct count) is the number of bacteria per millilitre and chla is micrograms of chlorophyll *a* per litre. It is apparent that planktonic bacteria and algae are tightly linked in lakes and the sea. The slope of the regression line, however, shows that bacterial numbers do not increase as rapidly as algal biomass with an increase in nutrient concentration. We suggest that this disproportionately smaller increase in bacterial numbers needs not signify a smaller role for bacteria in lake metabolism with increasing nutrient availability, if bacterial productivity per unit bacterial biomass increases between systems (Author's abstract).

Reference:

1. Bird, D.F. and J. Kalff. 1984. Empirical relationship between bacterial abundance and chlorophyll concentration in fresh and marine waters. Can. J. Fish. Aquat. Sci. 41:1015-1023.

2.3.16 Empirical Prediction of Crustacean Zooplankton Biomass and Profundal Macrobenthos Biomass in Lakes

Type: Empirical.

Description:

Hanson and Peters (1984) used data taken from the literature to develop and compare several estimators of crustacean zooplankton biomass (49 lakes) and profundal macrobenthos (38 lakes). Both mean zooplankton biomass ($r^2 = 0.72$, $P < 0.001$) and mean profundal macrobenthos biomass ($r^2 = 0.48$, $P < 0.001$) correlated better with mean total phosphorus than with Secchi depth, mean depth, maximum depth, or lake surface area. Mean total phosphorus concentration was also superior to mean chlorophyll *a* concentration ($r^2 = 0.57$, $P < 0.001$) as an estimator of macrobenthos biomass. Inclusion of maximum depth as a variable in a multiple regression resulted in a slight but significant ($P < 0.030$) improvement in the zooplankton-total phosphorus relationship ($R^2 = 0.75$, $P < 0.001$). Inclusion of lake surface area as a variable in a multiple regresssion significantly ($P < 0.001$) improved the predictive power of the profundal macrobenthos-total phosphorus relationship ($R^2 = 0.59$, $P < 0.001$) (Author's abstract).

Reference:

1. Hanson, J.M. and R.H. Peters. 1984. Empirical prediction of crustacean zooplankton biomass and profundal macrobenthos biomass in lakes. Can. J. Fish. Aquat. Sci. 41: 439-445.

2.3.17 Empirical Models for Zooplankton Biomass in Lakes

Type: Empirical.

Description:

Estimates of macrozoobenthos from the literature were regressed against a series of limnological variables to yield empirical models for zoobenthic biomass in the profundal, sublittoral, and littoral zones of lakes. Variables indicative of phytoplankton biomass (chlorophyll concentration, total phosphorus concentration, and Secchi disk transparency) explained between 14% and 57% of the variance of zoobenthic biomass. Other factors such as humic color, morphometry (slope, mean depth, ratio of mean to maximum depth, and lake area), and mean annual air temperature substantially increased the amount of explained variance. In the profundal and sublittoral zones, the best models explain 70% of the variance in zoobenthic biomass. Littoral zone models explained less than 50%, and this deficiency was attributed to sampling difficulties and to high local variability of slope and wave exposure in the littoral zone (Author's abstract).

Reference:

1. Rasmussen, J.B. and J. Kalff. 1987. Empirical models for zoobenthic biomass in lakes. Can. J. Fish. Aquat. Sci. 44: 990-1001.

2.3.18 Prediction of Algal Bioaccumulation and Uptake Rate of Nine Organic Compounds by 10 Physicochemical Properties

Type: Empirical.

Description:

Many quantitative structure-activity relationships describe steady-state levels of accumulation of organic contaminants in aquatic organisms, but few treat the dynamics by which these levels are achieved. This paper extends this approach by developing relations to describe the time course of uptake for different organic compounds. The instantaneous rates of uptake and the bioconcentration factors (BCF) of nine organic compounds were determined by following the bioaccumulation of radioactively-labeled-compounds in the green alga *Selenastrum capricornutum* . When all nine compounds are used in regression, capacity ratio and the octanol/water partition coefficient predict BCF equally well. However, if the hydrocarbons alone are considered, the capacity ratio predicts BCF most effectively. The uptake rate, which could only be measured effectively for five compounds, is best predicted by the connectivity index. These two regressions were effective in reconstructing the original experiment; they may also be effective at predicting the time course of contaminant bioaccumulation (Author's abstract).

Reference:

1. Mailhot, H. 1987. Prediction of algal bioaccumulation and uptake rate of nine organic compounds by ten physicochemical properties. Environ. Sci. Techno. 21(10):1009-1013.

2.3.19 The Nitrogen and Phosphorus Dependence of Algal Biomass in Lakes

Type: Empirical.

Description:

An analysis of mean growing season concentrations of chlorophyll, total phosphorus (TP), and total nitrogen (TN) in 228 north latitude lakes confirms previous observations that chlorophyll yield is dependent both on the phosphorus concentration and on the TN;TP ratio. Of two modified chlorophyll models which depend explicitly on both nitrogen and phosphorus developed and tested, one, a multiple regression model, appears to greatly reduce the error of chlorophyll prediction in lakes. A theoretical framework is presented which provides an explanation for the observed effects of N:P ratios (Author's abstract).

Reference:

1. Smith, V.H. 1982. The nitrogen and phosphorus dependence of algal biomass in lakes: An empirical and theoretical analysis. Limn. Oceanogr. 27(6) 1101-1112.

2.3.20 Ratio to Indicate Blue-Green Algae Scarcity

Type: Empirical.

Description:

An analysis of growing season data from 17 lakes throughout the world suggests that the relative proportion of blue-green algae (Cyanophyta) in the epilimnetic phytoplankton is dependent on the epilimnetic ratio of total nitrogen to total phosphorus. Blue-green algae tended to be rare when this ratio exceeded 29 to 1 by weight, suggesting that modification of this ratio by control of nutrient additions may provide a means by which lake water quality can be managed (Author's abstract).

Reference:

1. Smith, V.H. 1983. Low nitrogen to phosphorus ratios favor dominance by blue-green algae in lake phytoplankton. Science 221: 669-671.

2.3.21 Predictive Models for the Biomass of Blue-Green Algae in Lakes

Type: Empirical.

Description:

In lakes which experience water quality problems due to nuisance growth of blue-green algae, summer concentrations of chlorophyll *a* may not always be a meaningful measure of water quality for making management decisions. Models for the prediction of summer mean blue-green algal biomass were thus developed from data collected from five systems located in North America and Sweden.

It is suggested that the model of choice is $BG = -0.142 + 0.596 \log TP - 0.963 \log Z$, where BG is the biomass of blue-green algae (gm^{-3}), TP is the concentration of total phosphorus ($mg\ m^{-3}$), and Z is the mean depth of the lake (m). When coupled to current loading models, this model can potentially be used to assess the impacts of phosphorus loading reductions on threshold odor in water supplies (Author's abstract).

Reference:

1. Smith, V.H. 1985. Predictive models for the biomass of blue-green algae in lakes. Water Res. Bull. 21(3) 433-.

2.3.22 Empirical Relationships Between the Element Composition of Aquatic Macrophytes and Their Underlying Sediments

Type: Empirical

Description:

A simple view of the role of rooted macrophytes in element cycling sees them as pumps retrieving buried elements from the sediment profile. To investigate the relationship between the elemental composition of plants and sediments, we analysed published data for 39 elements. The best general model explained 84% of the variance of the log of plant element concentrations:

LPE = -0.81 + 0.90 Log Sediment Element (ug/g dry wt.) - 0.12 Sediment Organic Content (ug/g drt wt.) + 0.67 Atomic radius (nm) ($r^2 = 0.84$; n=39)

This close relationship between the concentration of an element in plant tissues and in the underlying sediment indicates that aquatic plants do not differ markedly in element composition from the sediments in which they grow (Author's abstract edited).

Reference:

1. Jackson, L.J., J.B. Rasmussen, R.H. Peters and J. Kalff. 1991. Empirical relationships between the element composition of aquatic macrophytes and their underlying sediments. Biogeochem. 12: 71-86.

2.3.23 Empirical Physiological Models of Ecosystem Processes

Type: Empirical.

Description:

A continuing hope, for many biologists, is the erection of general theories which will predict interesting attributes of ecological systems from a limited number of state variables. This paper describes one attempt to link those equations which empirically describe physiological rates as a function of animal body weight in order to provide interesting, if qualitative, predictions about holistic ecosystem properties such as successional change or material flow (Author's abstract edited).

Reference:

1. Peters, R.H. 1978. Empirical physiological models of ecosystem processes. Verh. Int. Verein. Limnol. 20: 110-118.

2.3.24 Time Series Modelling of Water Quality

Type: Empirical.

Description:

Time series models of reservoir water quality are water resource management tools and provide insight into reservoir dynamics since they account for autocorrelation, seasonality, and trends present in the data. Autoregressive integrated moving average (ARIMA) models were applied to describe patterns in selected water quality variables of Red Rock Lake, Iowa. Models were generated for total phosphorus, total nitrogen, and suspended solids for an 8-year period (1972-1979). Patterns in lake concentration and the usefulness of time series models to lake and reservoir management are described (Author's abstract).

Reference:

1. Montgomery, R.H. 1984. Time series modelling of reservoir water quality. In: Lake and Reservoir Management. EPA 440/5/84-001.

2.3.25 An Allometric Model for Pesticide Bioaccumulation

Type: Empirical.

Description:

A combination of the frequency distribution of body sizes and appropriate allometric relationships may permit a more operational approach to pesticide bioaccumulation than the more traditional level concept. To demonstrate this potential, we describe patterns of bioaccumulation as functions of time and body size in a computer ecosystem in which no differences in trophic level exist. The qualitative similarity between these patterns and those reported in the literature from laboratory and field experiments suggests that empirical relations describing contaminant fluxes as functions of body weight could form a powerful base for the prediction of contaminant body burden in natural systems. We believe this approach could prove useful for any persistant contaminant with high biological affinity (Author's abstract).

Reference:

1. Griesbach, S. and R.H. Peters. 1982. An allometric model for pesticide bioaccumulation. Can. J. Fish. Aquat. Sci. 39: 727-735.

2.3.26 Evaluation of Models Predicting Mixing Depth

Type: Empirical.

Description:

Since mixing depth affects many aspects of lake productivity, including nutrient recycling, Hanna (1990) evaluated the predictive power of 17 empirical models that relate mixing depth to morphometric variables to identify the best predictor. These models were tested empirically by compiling data from 123 temperate lakes of differing morphometry, geometry, and trophy. Four statistical indices of precision and bias, indicate that the model published by Shuter *et al.*. (1983) using maximum effective length of the lake was the best published model for predicting mixing depth, although it is slightly biased.

Hanna (1990) then examined the effect of alternate predictors, reflecting lake configuration, basin shape, and geographical indices, to formulate an improved model. The best single predictor of thermocline depth (THER) was maximum effective length (MEL): Log THER = 0.336 Log MEL - 0.245. No improvement in predictive power was obtained by combining other variables. This model is statistically superior to that of Shuter *et al.*. (1983) because it is not biased, it represents a greater number of lakes, and it covers a broader range of lake sizes and shapes over a more extensive geographical region. Two other models, using lake area and length of shoreline are proposed as alternative predictive tools, if MEL is not readily available (Author's abstract).

Reference:

1. Hanna, M. 1990. Evaluation of models predicting mixing depth. Can. J. Fish. Aquat. Sci. 47: 940-947.

2. Shuter, B.J., D.A. Schlesinger, and P.A. Zimmerman. 1983. Empirical predictions of annual surface water temperature cycles in North American lakes. Can. J. Fish. Aquat. Sci. 40: 1838-1845.

2.3.27 A Simple Model for Predicting the Date of Spring Stratification in Temperate and Subtropical Lakes

Type: Empirical.

Description:

The date of onset of spring stratification in northern hemisphere lakes is predictable from mean annual air temperature. The prediction is further improved by also considering lake surface area (surrogate of wind exposure) and by the ratio (R) of lake surface to mean depth, with R reflecting aspects of lake morphometry and heat storage capacity. Mean annual air temperature and R together explain 68% of the variance in the date of onset of stratification in a combined 70-lake data set from North America, Europe, and Asia. Nearly identical fractions were explained when the lakes were separated into dimictic and warm monomictic data sets. The remaining unexplained variation is probably largely attributable to interyear variation in weather, but also to unexamined differences in regional wind strength, local protection from the winds, lake shape, and lake turbidity, as well as differences in the intervals at which temperature profiles were taken (Author's abstract).

Reference:

1. Demers, E. and J. Kalff. A simple model for predicting the date of spring stratification in temperate and subtropical lakes. Limnol. Oceanogr. 38(5): 1077-1081.

2.3.28 A Simple Model for Predicting the Date of Fall Turnover in Thermally Stratified Lakes

Type: Empirical.

Description:

The date of fall turnover can be predicted from average midsummer hypolimnetic temperature in acidic and non-acidic lakes in central Ontario. The prediction of fall turnover date is improved by inclusion of two further independent variables, mean depth, and adjusted latitude (for altitude), in a global data set (ranges of mean depth, 1.1-86m; adjusted latitude, 38° - 65°). The models explain 67-80% of the variance of fall turnover date and are potentially useful in the design of monitoring programs and for predicting impacts of anthropogenic activities that influence lake thermal budgets, e.g. diversion for cooling waters or damming of cold inflows (Author's abstract).

Reference:

1. Nurnberg, G. 1988. A simple model for predicting the date of fall turnover in thermally stratified lakes. Limnol. Oceanogr. 35(5): 1190-1195.

2.4 Models Developed for Specific Lake and Reservoir Applications

2.4.1 A Cross-Sectional Model for Phosphorus in Southeastern U.S. Lakes

Type: Empirical/cross-sectional.

Description:

Data from 42 lakes and reservoirs in Virginia, North Carolina, South Carolina, and Georgia were used to develop a cross-sectional regression model for the prediction of phosphorus concentration. The development of this model was chosen as an alternative to using one of the many north temperate climate models that are available. After evaluation of the model it was determined that the linear relation between phosphorus input and lake phosphorus concentration is not entirely consistent with the southeastern lakes data available. Application of the model to Lake Rhodhiss, North Carolina is described. This application illustrated how error reduction methods might be employed with the model (Reckhow and Clements, 1984).

Comments:

The descriptive paper contains a good discussion on the theory and application of cross-sectional models. It also contains evaluations of other cross-sectional models including the Larson-Mercier (1976) model that has been used for a variety of applications worldwide.

References:

1. Reckhow, K.H. and J.T. Clements. 1984. A cross-sectional model for phosphorus in southeastern U.S. lakes. In: Lake and reservoir management. EPA 440/5/84-001.

2. Larson, D.P., amd H.T. Mercier. 1976. Phosphorus retention capacity of lakes. J. Fish. Board Can. 33:1742-50.

2.4.2 Total Phosphorus Simulation - Lake Wallenpaupack

Type: Computer simulation.

Description:

A mechanistic ecosystem simulation model developed in order to model total phosphorus in lakes. The model was designed for use on a microcomputer. The model simulates the physical transport, settling, vertical exchange through the thermocline, sediment release of total phosphorus. The model was applied to Lake Wallenpaupack, Pennsylvania in order to determine what, if any, changes in discharge from the resident hydroelectric power plant would produce a significant reduction in the summer epilimnetic phosphorus concentrations. (Horstman *et al.,* 1984)

Comments:

The descriptive paper contains a summary of the model theory, limitations, and equations. The equations are also described in Chapra and Reckhow (1983). The results of the study at Lake Wallenpaupack are discussed with possible explanations for the results outlined. The paper does not indicate that the ecosystem model is restricted in application to Lake Wallenpaupack.

References:

1. Horstman, K.H., R.S. Copp, and F.X. Browne. 1984. Use of a predictive phosphorus model to evaluate hypolimnetic discharge scenarios for Lake Wallenpaupack. In: Lake and reservoir management. EPA 440/5/84-001.

2. Chapra, S.C., and K.H. Reckhow. 1983. Engineering approaches for lake management. Vol.2: Mechanistic modeling. Ann Arbor Sci. Publishers., Ann Arbor, MI.

2.4.3 Modelling the Water Quality of a Proposed Impounded Lake of a Tidally Influenced River - River Usk, UK

Type: Computer simulation.

Description:

The unsatisfying water quality of the tidally influenced River Usk, Wales, UK, has resulted in a proposal for a barrage across the river in order to eliminate the tidal influence upstream. The area will then not be subject to high changes in water levels, which at low water leave the sediment banks dry and sometimes smelling and looking bad. The barrage project is proposed to increase the recreational and touristic value of the area. The water of the resulting impoundment upstream of the barrage would be almost stagnant and the impoundment would be receiving treated and untreated municipal waste water. Eutrophic conditions and a periodically two-layered structure of the water masses, due to the development of a thermocline, must be foreseen (Bach and Kjensen, 1994/Author's abstract edited).

Using MIKE 12, a PC-based two-layer model package, the hydrodynamic and water quality conditions of the proposed impoundment of the River Usk were analyzed. The MIKE 12 simulation system comprises three modules: a hydrodynamic module, an advection-dispersion module, and a water quality module. The water quality module consists of different submodules describing the physical, chemical, and biological processes of importance to eutrophication, oxygen depletion, toxicity of chemicals and bacterial problems.

A two-layered model was considered adequate to describe the proposed impoundment as it was predicted to be shallow (about 10m). In shallow reservoirs the probability of vertical circulation and transport within each layer is less than for deep reservoirs where a multilayered or three-dimensional model would be appropriate.

References:

1. Bach, H.K., and J.K. Kjensen. 1994. Modelling of the water quality of a proposed impounded lake of a tidally influenced river. Ecol. Model., 74: 77-90.

2. Ecological Modelling Centre (EMC). 1992. MIKE 12, a short description. Report from the Ecological Modelling Centre, Horsholm, Denmark.

2.4.4 Water Quality Simulation of the Proposed Jordanelle Reservoir, Utah

Type: Multiple model approach.

Description:

In order to assess the environmental impact of the proposed Jordanelle Reservoir on the downstream water quality in the Provo River and Deer Creek Reservoir and evaluate the design and water quality criteria for the Reservoir two different models were implemented (1). A combination model of both the Vollenweider (2) and Canfield and Bachmann (3) approaches were used to estimate the trophic state of the proposed reservoir. The Corps of Engineers Water Quality for River and Reservoir Systems (WQRRS) mathematical simulation model was used to estimate the thermal stratification and hypolimnetic oxygen concentrations.

Reference:

1. Wegner, D.L. 1984. Water quality simulation of the proposed Jordanelle reservoir, Utah. In: Lake and reservoir management. EPA 440/5/84-001.

2. Canfield, D.E. Jr., and R.W. Bachmann. 1981. Prediction of total phosphorus concentrations, chlorophyll *a*, and Secchi depths in natural and artificial lakes. Can. J. Fish. Aquat. Sci. 38:414-423.

3. Vollenweider, R.A. 1975. Input-output models with special reference to the phosphorus loading concept in limnology. Schweiz. Z. Hydrol. 37(1):53-84.

2.4.5 Kootenay Lake Fertilization Response Model

Type: Computer simulation.

Background:

The model was developed in response to a severe decline in the kokanee salmon (Oncorhynchus nerka) population due to competition with Mysis relicta, an introduced species, for grazing zooplankton. The kokanee is the most important source of food for the Gerrard rainbow trout (Oncorhynchus mykiss) therefore the prevention of extinction of two fish species was of primary concern. The model was calibrated using historical data to support predictions of nutrient loadings, water flow patterns, and changes in kokanee habitat.

Description:

The Kootenay Lake model has two functions: 1) to predict the long term response of phytoplankton, grazing zooplankton, Mysis, kokanee, and Gerrard trout to lake nutrient loading from an external source, and 2) to simulate the effects of fisheries management action such as varying exploitation rates and enhancement of spawning success by use of spawning channels and manipulation of juvenile carrying capacities.

The program itself is relatively easy to use. Altering parameters to investigate response can produce quick results. The program requires approximately 30 seconds to complete a 30 year scenario on a 20mhz 80386 system with an 80387 math coprocessor. The difficult and lengthy process is the actual building of the data to input into the model.

The model was developed using the Adaptive Environmental Assessment Process (AEA). whereby a participant group of scientists and managers work with a modelling team to produce a working simulation model of the target system or problem (Holling 1978; Walters 1986) Together this group worked out the values for all the different variables required to produce a model that would take into account the many ecological and physical processes that affect fertilization response.

It is possible for this model to be applied to a completely different lake holding other populations of fish and plankton than Kootenay Lake. It is probable that the program would have to be altered to include new variables and exclude others Walters *et al..*, 1991).

System Requirements:

1.Quickbasic (Microsoft Corp. TM) program. Note: Quickbasic is only necessary for making modifications to the program.
2.IBM compatible PC with VGA graphics adapter.

Availability:

A copy of the model and data files may be obtained on 720K 3-1/2" disk from the authors: Fisheries Centre, University of British Columbia, 2204 Main Mall, Vancouver, B.C. V6T 1Z4. Phone (604) 660-1812. Fax (604) 660-1849.

Reference:

1. Holling, C.S. (ed). 1978. Adaptive environmental assessment and mangement. John Wiley, N.Y. 377p.

2. Walters, C.J. 1986. Adaptive management of renewable resources. McMillan Pub. Co., N.Y. 374p.

2. Walters, C., J. DiGisi, J. Post, J. Sawada. 1991. Kootenay Lake fertilization response model. Fisheries Management Report No. 98, British Columbia Ministry of Environment.

2.5 Annotated Bibliography of Great Lakes Modelling Accounts

The Great Lakes, because of their ecological and economic importance, have received more specialized modelling attention than any other set of lakes. The level of sophistication and detail in many Great Lakes models are far greater than is available from other sources. An annotated bibliography is included here so that the references can be referred to as a source of measurements, coefficients, process descriptions and general approaches. None of these models could be applied directly to British Columbia lakes but they may provide a basis for assembly of other models or modification of existing ones.

1. Blumberg, A. F., and D.M. DiToro. 1990. Effects of climate warming on dissolved oxygen concentrations in Lake Erie. Transactions of the American Fisheries Society, 119:210-223.

This paper describes a coupled hydrodynamic and eutrophication model that was used to examine the response of DO concentrations to climate-related warming of the central basin of Lake Erie. The water quality model was made up of 15 mass balance equations that predicted distributions of phytoplankton biomass, nutrient concentration, and dissolved oxygen. This paper includes a description of 10 governing equations, 9 figures, 2 tables and 33 references.

2. Boyce, F.M. and P.F. Hamblin. 1975. A simple diffusion model of the mean-field distribution of soluble materials in the Great Lakes. Limnol. Oceanogr., 20(4):511-517.

This paper describes the development of a two-dimensional steady-state model used to predict the movement of a soluble contaminant in the Great Lakes after being introduced from shore. The model was applied to the central basin of Lake Erie where experimental data concerning the distribution of chloride already existed. This paper includes a description of the mathematical theory behind the model, as well as 3 figures, 1 table, and 6 references.

3. DiToro, D.M., N.A. Thomas, C.E. Herdendorf, R.P. Winfield, J.P. Connolly. 1987. A post-audit of a Lake Erie eutrophication model. J. Great Lakes Res., 13(4):801-825.

In this paper a eutrophication model, comprised of mass balance equations that quantify the mass transport of the biota and nutrients, and predict changes in levels of DO, is evaluated by comparison of model predictions to observed Lake Erie water quality data. This paper includes 17 figures, 2 tables, and 35 references.

4. Gobas, F.A.C.P. 1993. A model for predicting the biocaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario. Ecol. Modelling, 69:1-17.

This paper describes a steady-state model used to estimate the bioaccumulation of hydrophobic organic chemicals in organisms of aquatic food-webs from inputs of chemical concentrations in water and sediments. The model is made up of a series of sub-models that simulate chemical uptake, elimination and bioaccumulation in fish, aquatic macrophytes, benthos, and plankton. The model is considered relatively simple and easy-to-apply because it requires only basic data. Included are 3 figures, 2 tables, and 32 references.

5. Lam, D.C.L., and E.Halfon. 1978. Model of primary production, including circulation influences, in Lake Superior. Appl. Math. Modelling 2: 30-40.

This paper describes two models, a finite difference hydrodynamical model and a two-compartment phosphorus model, that were used together to simulate the observed temporal and spatial changes in the nutrient conditions and primary productivity. Included are 15 figures, 5 tables, and 27 references.

6. Lam, D.C.L., and W.M. Schertzer. 1987. Lake Erie thermocline results: comparison with 1967-1982 data and relation to anoxic occurrences. J. Great Lakes Res. 13(4):757-769.

This paper presents and validates a one-dimensional thermocline model used to estimate daily vertical temperature distributions, thermal layer thicknesses, thermal interface depths, and vertical diffusion. Also included is a description of the model equations, 5 figures, 1 table, and 28 references.

7. Lam, D.C.L., W.M. Schertzer, and A.S. Fraser. 1987. A post-audit analysis of the NWRI nine-box water quality model for Lake Erie. J. Great Lakes Res. 13(4):782-800.

In this paper the National Water Research Institute's nine-box water quality model for Lake Erie is evaluated by comparison of calibration, verification, and post-audit data from 1967-1982 to observed Lake Erie water quality data. A description of the nine-box model is not included. The paper contains 13 figures, 1 table, and 20 references.

8. Murthy, C.R., T.J. Simons, and D.C.L. Lam. 1986. Simulation of pollutant transport in homogeneous coastal zones with application to Lake Ontario. J. Geophys. Res. 91(C8):9771-9779.

This paper describes the coupling of an empirical model for coastal currents with a pollutant transport model in order to simulate the transport of pollutants in the coastal zone. Included are 6 figures, 4 tables, and 19 references.

9. Scavia, D. 1980. An ecological model of Lake Ontario. Ecol. Modelling 8:49-78.

This paper describes a three-layer ecological model of Lake Ontario that includes several phytoplankton and zooplankton groups; cycles of phosphorus, nitrogen, carbon, and silicon, and sediment particulates and pore water nutrients. It is demonstrated that the model agrees with measurements made during the International Field Year for the Great Lakes (IFYGL). Included are 8 figures, 5 tables, and 86 references.

10. Schertzer, W.M. and D.C.L. Lam. 1989. Modeling Lake Erie water quality - a case study. In: Water quality modeling. Volume IV: decision support techniques for lakes and reservoirs. CRC Press, Inc., Boca Raton; Florida.

This chapter is a summary of the water quality modelling work already undertaken on Lake Erie. It includes a description of the Lake Erie basin, collected observations and data, three models: thermocline, nine-box, and phosphorus-oxygen sub-model, and the results from each model study. The chapter contains 21 figures, 6 tables, and 79 references.

3.0 Modelling the Water Quality of Rivers and Streams

3.1 General Simulation Models

3.1.1 CE-QUAL-RIV1

Type: A dynamic, one dimensional (longitudinal) water quality model for unsteady flows in rivers and streams. Computer simulation.

Description:

CE-QUAL-RIV1 consists of two modelling components, a hydrodynamic (RIV1H) part and a water quality (RIV1Q) part. Output from the hydrodynamic submodel is used to drive the water quality model .

The water quality variables include: temperature, dissolved oxygen, carbonaceous BOD, organic nitrogen, ammonia nitrogen, nitrate nitrogen, orthophosphate phosphorus, coliform bacteria, dissolved iron, and dissolved manganese. The effects of algae and macrophytes are also included.

The model allows the simulation of branched river systems with multiple hydraulic control structures, such as run-of-the-river dams, waterway locks and dams, and regulation dams. The model was developed to simulate the transient water quality conditions associated with highly unsteady flows that can occur on regulated streams.

Technical Support and Availability:

Contact Ms. Toni Schneider or Mr. Marc Dortch: USAE Waterways Experiment Station, P.O. Box 631, Vicksburg, MS 39180-0631. Phone: (601) 634-3670.

Reference:

1. Environmental Laboratory. 1990. CE-QUAL-RIV1: A dynamic, one-dimensional, (longitudinal) water quality model for streams: User's manual. Instruction Report E-90-1, US Army Engineer Waterways Experiment Station, Vicksburg, MS.

Note: This manual is available from the National Technical Information Service (NTIS) in either paper copy or microfiche form. Phone: (703) 487-4650.

3.1.2 QUAL2E and QUAL2E-UNCAS: Enhanced Stream Water Quality Models

Type: A comprehensive and versatile stream water quality model that can simulate up to 15 constituents in any combination desired by the user. Computer simulation.

Description:

Constituents which can be simulated are: DO, BOD, temperature, algae as chlorophyll *a*, organic nitrogen, ammonia, nitrite, nitrate, organic phosphorus, dissolved phosphorus, coliforms, arbitrary nonconservative constituent, and three conservative constituents.

The model is applicable to dendritic streams that are well mixed. It assumes that the major transport mechanisms, advection and dispersion, are significant only along the main direction of flow (longitudinal axis of the stream or canal). It allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow. It also has the capability to compute required dilution flows for flow augmentation to meet any prespecified DO level.

Hydraulically, QUAL2E is limited to the simulation of time periods during which both the stream flow in river basins and input waste loads are essentially constant. QUAL2E can operate either as a steady-state or a dynamic model. When operated as a steady-state model, it can be used to study the impact of waste loads (magnitude, quality and location) on instream water quality and also can be used in conjunction with a field sampling program to identify the magnitude and quality characteristics of nonpoint source waste loads. By operating the model dynamically, the user can study the effects of diurnal DO variations due to algal growth and respiration. However, the effects of dynamic forcing functions, such as headwater flows or point loads, cannot be modelled in QUAL2E.

QUAL2E-UNCAS is a recent enhancement to QUAL2E that allows the modeller to perform uncertainty analysis on the steady-state water quality simulations. Three uncertainty options are available: sensitivity analysis, first order error analysis, and monte carlo simulations. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts. Quantifications of the uncertainty in model forecasts will allow assessment of the risk (probability) of a water quality variable being above or below an acceptable level.

System Requirements:

QUAL2E is written in ANSI FORTRAN 77 and is compatible with mainframe and personal computer systems that support this language. QUAL2E typically requires 256K bytes of memory.

Availability:

QUAL2E and QUAL2E-UNCAS are available as one program (QUAL2EU) from the EPA's Center for Exposure Assessment Modeling. For ordering information see page 123.

Reference:

1. Brown, L.C. and T.O. Barnwell. 1987. The enhanced stream water quality models QUAL2E and QUAL2E-UNCAS: documentation and user's manual. EPA/600/3-87/007. United States Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

3.1.3 One-Dimensional Hydrodynamic and Water Quality Model

Type: A one-dimensional computer simulation program for unsteady flow in a complex river system.

Description:

The One-D model simulates one-dimensional unsteady flow in a network of branching and/or looping channels which may consist of bank or embayment storage areas, various hydraulic control structures, and tidal boundary conditions. The water quality sub-model can simulate salinity, temperature, BOD, dissolved oxygen, organic nitrogen, inorganic nitrogen, organic phosphate, phytoplankton, zooplankton, fecal coliform, decaying lignins, and conservative lignins .

System Requirements:

1. MS-DOS 3.1 or higher
2. BASIC interpreter
3. IBM Professional Fortran compiler or a Microsoft Fortran compiler

Comments:

The One-D model has been compared to the U.S. EPA's water quality model, QUAL2E. Briefly, the conclusions from that study determined that if modelling a steady-state system on micro-computer the QUAL2E program is recommended because it is simpler and faster to use. However, the One-D Model is capable of simulating water quality coupled with complex and dynamic hydraulic conditions such as flow variation, hydropower operation, and backwater conditions that are commonly found in Canadian river basins. The estimated running time for the One-D model on an IBM AT is 20 minutes for a simulation period of one day. (Using the Cray X-MP super computer the same simulation takes eight seconds). Also, the One-D model has been shown to be more sensitive to sediment oxygen demand (SOD) that QUAL2E, while QUAL2E is more sensitive to biochemical oxygen demand (BOD).

The water quality option of the model has been previously applied in the St. Lawrence River, St. Croix River, Prince Edward Island West River estuary, and St. John River water quality studies in Canada.

Future Developments:

Inclusion of sediment computations to derive total sediment load with or without mobile bed options. Model testing has been conducted on the Fraser and South Saskatchewan Rivers.

Inclusion of river ice parameters to simulate ice conditions throughout the ice-covered period. Computation of frasil ice, hanging ice, border ice, anchor ice and ice thickening are possible.

The model will be tested on the St. Lawrence, Niagra, and Nelson Rivers as well as the Peace-Athabasca and MacKenzie Deltas.

Availability:

The One-D computer program is available from:

Morriss Sydor: Water Systems Division, Water Habitat and Conservation Branch, Canadian Wildlife Service, Environment Canada, Place Vincent Massey, Ottawa, Ontario K1A 0H3.

A fee for disks and photocopying may be required.

Reference:

1. Cheng, H. and D. Lockerbie. 1994. Water quality modelling of the Upper Saint John River: A comparison study. Environment Canada Scientific Series No. 196. Environmental Conservation Service, Ottawa, Ontario.

Other Sources of Information:

1. Environment Canada. 1988. One-dimensional hydrodynamic model computer manual. Prepared by the Water Modelling Section, Water Planning and Management Branch, Inland Waters Directorate, Environment Canada.

2. Environment Canada. 1992. One-dimensional computer model: supplementary computer manual for water quality. Water Planning and Management Branch, Inland Waters Directorate, Environment Canada.

3.1.4 CHARIMA

Type: Numerical Simulation of Unsteady Mobile-Bed Hydrodynamics and Contaminant Transport In River Systems. Computer simulation.

Description:

CHARIMA is a general-purpose computer program for the simulation of steady or unsteady water, sediment, and contaminant movement in simple or complex systems of channels. Water movement (hydrodynamics) forms the core of a CHARIMA simulation; mobile-bed (sediment) and contaminant dynamics can be activated or deactivated.

Mobile-bed capabilities include bedload and/or suspended-load transport of mixtures of noncohesive or cohesive sediment, along with the associated short- or long-term bed-level changes (aggradation and degradation), bed-sediment sorting, and armouring. Subsurface layering, pre-existing or as the result of persistent deposition, is included.

Contaminant capabilities include transport and fate of any number of conservative contaminants, and heat. Transport of radionuclides and their selective sorption interaction with sediment size classes, including subsurface sediments, is currently under development. Other nonconservative and interacting constituents are easily introduced through implementation of the appropriate source/sink relations in the program.

Channel systems may comprise a single channel, branched systems, or looped networks of arbitrary connectivity and flow direction.

Data Requirements:

Hydrodynamic simulation requires essentially the same data as backwater circulation, i.e.: channel cross sections and roughnesses, plan-view connectivity, hydrographs of inflow at upstream boundary points (possibly steady flow), and stage hydrographs (or rating curves) at downstream boundary points.

Mobile-bed simulation additionally requires the initial distribution of bed sediments, as well as sediment inflow (rate and distribution) at upstream inflow points.

Contaminant simulation requires contaminant inflow rates at upstream inflow points. Initial suspended -sediment concentrations are useful but not required.

System Requirements:

CHARIMA is written exclusively in FORTRAN and thus requires a FORTRAN compiler. Modest applications can be performed in a 640K DOS environment. Larger models are effectively run in expanded DOS memory (with an appropriate compiler) or workstations (UNIX, Appolo-Domain, etc.) Input and output data sets are in formatted ASCII form. Graphical support must be provided by the user.

Applications:

Recent applications include:

- Thermal regime and hydrodynamics in the Chicago Sanitary and Ship Canal (Commonwealth Edison Company)
- Cohesive sediment and radionuclide transport and unsteady hydrodynamics in the Watts Barr Reservoir (Tennessee Valley Authority)
- Radioisotope transport and hydrodynamics in the Columbia River (Battelle Pacific Northwest Laboratories)
- Thermal regime and hydrodynamics in the Missouri River (IOWA Consortium of Electric Power Utilities)
- Mobile-bed dynamics in the Cho-Shui River (National Science Foundation)
- Mobile-bed dynamics in the Missouri River from Gavins Point Dam to Rulo (National Science Foundation)
- Mobile-bed dynamics in the Missouri River from Ft. Randall to Gavins Point Dam (Corps of Engineers)

Limitations:

Subcritical flow. Fully-mixed transport (one-dimensional). Fixed bank location and plan-view channel layout.

Availability:

CHARIMA is under continuous development and generalization, and therefore is not generally available to outside users. However the Institute has worked directly with users to effect code transfer and training in conjunction with specific user projects. The contact is: Iowa Institute of Hydraulic Research (IIHR), The University of Iowa, Iowa City, IA 52242 (Phone 319-335-5229; Fax 319-335-5238), Attn: Forrest M. Holly Jr.

3.1.5 DSSAMt -- Dynamic Stream and Simulation Model with Temperature

Type: A steady-state river flow model with dynamic representation of 14 water quality constituents. Computer simulation.

Description:

Constituents which can be simulated are: water temperature, organic and various inorganic fractions of nitrogen and phosphorus, BOD, DO, pH, alkalinity, CO_2, TDS, chloride, blue green and non-blue-green benthic algae, and coliform bacteria.

The following river processes are included in DSSAMt: equilibrium temperature and heat exchange; advection, biochemical and physical kinetics of all constituents modelled including variation over 24-hour-day; nutrient, spatial, and light limitation of benthic primary production; algal removal processes including respiration, erosion, and herbivory; shading by topography and riparian vegetation; light attenuation by water column; and temperature dependent rates.

System Requirements:

1. IBM PC with 640 RAM KB and 30MB space on hard drive
2. FORTRAN 77 compiler

Applications:

Successful applications include:

- Truckee River (Nevada): nutrient wasteload allocation studies, water quality standards evaluation, instream flow requirements
- Red Deer River (Alberta): water quality assessment of instream flow requirements including temperature

Limitations:

Steady-state, one-dimensional flow. Unbranched, unstratified flow and fixed channel geometry within each hydraulic reach. Not suitable to rapidly changing flow and hydraulic conditions. No direct calculation of error or uncertainty. Vascular macrophytes and phytoplankton not presently modelled.

Availability:

DSSAMt was developed by Craig L. Caupp, James T. Brock, and Henry M. Runke. The program is available from : Rapid Creek Research, Inc., P.O. Box 2616, Boise, Idaho 83701-2616 USA (Phone 208-322-8950; Fax 208-376-9557).

3.1.6 Dynamic River Basin Water Quality Model

Type: Computer simulation.

Description:

Analyzes the impact of point source wastes from industries and municipalities, non-point sources and water diversions upon the aquatic ecosystems of freely-flowing rivers, river-run reservoirs and stratified reservoirs. The model can simulate carbonaceous BOD, DO, algal biomass, organic nitrogen, ammonia nitrogen, nitrate, nitrite, organic phosphorus, orthophosphorus, temperature, coliform bacteria and two conservative constituents.

Availability:

The dynamic river basin computer program may be obtained free of charge (may be disk exchange) from:

John Yearsley, EPA Region 10, ESO98, 1200 6th Ave., Seattle, WA 98101. Phone: (206) 553-1532. Fax: (206) 553-0119.

Reference:

1. Yearsley, J. 1991. A dynamic river basin water quality model. EPA 910/9-91-019. Environmental Protection Agency, Region 10, Seattle Washington.

3.1.7 REGUSE -- Basin Regulation and Water Use Model

Type: Computer simulation.

Description:

The REGUSE model is a river basin regulation and water use computer model. It was developed as a water management tool to assist river basin managers in managing their water resources. In large and complex basins, a variety of water users can have conflicting lake and channel level requirements. The model's principle applications include planning studies and real-time simulations of river basins having complex flow and reservoir regulation policies.

The REGUSE model was designed so that it could be easily and quickly applied to any river basin. The PC version of REGUSE is completely operational. Although the computer program is not fully user interactive, REGUSE does use a simplified editorial method of data management and allows direct user interaction with its procedures.

Technical Support and Availability :

Contact either G. Brown, model developer: (819) 997-1953, Morriss Sydor, hydraulic technical advisor: (819) 953-1528, or W. Boutot, applications engineer: (819) 997-1235.

The program was developed by: The Ecosystems Modelling and Analysis Section, Economics and Conservation Branch, Environment Canada, Ottawa, Ontario.

3.1.8 STREAMDO IV -- Stream Dissolved Oxygen Model

Type: A spreadsheet-based, steady-state model for evaluating wasteload analyses of river reaches with respect to dissolved oxygen and unionized ammonia.

Description:

Values representing average conditions for the time period of interest are entered into the spreadsheet for the following variables: flow, velocity, slope, depth, temperature, DO, carbonaceous BOD, organic nitrogen, ammonium, nitrite, nitrate, pH, and sediment oxygen demand. The model can be used for simulations that include shallow run-of-the-river impoundments, although STREAMDO IV is not intended for reservoirs with extended residence times.

A separate model (WLANH3) is distributed with STREAMDO IV for steady-state analysis of un-ionized ammonia wasteload allocation in streams.

System Requirements:

1. IBM compatible 286 class microcomputer
2. 640 KB RAM
3. LOTUS 123 or equivalent software

Availability:

The STREAMDO IV program is available from: Bruce Zander and Jeb Love: Water Management Division, U.S. EPA; 8WM-SP, Suite 500, 999-18th Street, Denver, CO 80202-2405. Phone: (303) 293-1580. Fax: (303) 391-6957.

Reference:

1. Zander, B. and J. Love. 1990. STREAMDO IV and supplemental ammonia toxicity models. Water Management Division U.S. Environmental Protection Agency, Region VIII, Denver, Colorado. Unpublished Typescript. September 1990. Cited in: Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

3.1.9 HEC5Q -- Simulation of Flood Control and Conservation Systems (Including Water Quality Analysis)

Type: Computer simulation.

Description:

The model simulates the sequential operation of reservoir systems for flood control and conservation purposes. A separate water quality module is provided which may be linked by means of data files. Reservoir releases are determined by the program to meet at-site and downstream control point requirements. The model can be useful for sizing reservoir for flood control and conservation storage; selecting proper reservoir operational releases for hydropower, water supply and flood control; and for evaluating water quality in river-reservoir systems.

Two alternative water quality simulation options are provided: Option 1 simulates up to three conservative constituents and up to three non-conservative constituents, and DO. Option 1 requires that water temperature be simulated. Option 2 simulates water temperature, total dissolved solids, nitrate, phosphate, phytoplankton, carbonaceous BOD, ammonia, and DO.

Comments:

The model is similar to the WQRRS model (Section 3.1.10); however, HEC5Q emphasizes the flow and storage aspects while WQRRS attempts a much more sophisticated ecosystem model. The input data requirements are high, and the input files are considered large and complicated.

System Requirements:

IBM compatible 386 class microcomputer with 560 KB RAM and 6MB available extended memory.

Technical Support and Availability:

The program is available for an approximate fee of $200 from: Robert G. Willey: Hydrologic Engineering Center, 609 Second Street. Davis, CA 95616. Phone: (916) 756-1104.

Reference:

1. Gummer, Bill. 1991. Water quality modelling within the Souris River Basin. Prepared for Water Quality Branch, Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

3.1.10 WQRRS -- Water Quality for River-Reservoir Systems

Type: Comprehensive water quality computer simulation model for river systems including up to 10 reservoirs.

Description:

The model is comprised of three independent modules: reservoir, river flow and water quality. The modules may be run separately or linked by means of data files.

The water quality variables included in the model are: water temperature, three types of fish, aquatic insects (stream module only), benthic animals, zooplankton, two types of phytoplankton, benthic algae (stream module only), detritus, organic sediment (i.e., settled detritus), inorganic suspended solids (five types with different settling velocities), inorganic sediment, dissolved ammonia as nitrogen, and dissolved nitrites as nitrogen.

Comments:

The model is similar to the HEC5Q model (Section 3.1.9); however WQRRS attempts a much more sophisticated ecosystem model while HEC5Q emphasizes flow and storage aspects.

System Requirements:

1. IBM compatible 386 class microcomputer with 640 KB RAM (MS-DOS compatible)

Technical Support and Availability:

The WQRRS program is available for an approximate fee of $200 from: Robert G. Willey: Hydrologic Engineering Center, 609 Second Street, Davis, CA 95616. Phone (916) 756-1104.

Reference:

1. Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for the Water Quality Branch, Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

3.1.11 QUASAR -- Quality Simulation Along Rivers

Type: Computer simulation.

Description:

QUASAR is a dynamic flow and water quality model designed by the Institute of Hydrology in England. QUASAR simulates eight variables in addition to flow: nitrate, ionized and unionized ammonia, DO, BOD, pH, temperature, and any conservative or inert material in solution. The river system is modelled as a series of reaches, the reach boundaries being sited at locations of interest. The model performs a mass balance of flow and quality over each reach, taking into account inputs from the previous reach, tributaries, effluent discharges and abstractions. Within each reach allowances are made for chemical decay processes and biological behavior. The residence time of the water within each reach is allowed to vary with flow rate so that pollutants are transported along the river system at the correct velocity. The output from a reach provides the upstream input to the next reach.

Comments:

QUASAR is currently being used to predict estimates of water quality for the Great Ouse River in eastern England as part of the Great Ouse Automatic Monitoring Scheme (GOAMS). The QUASAR program is considered to be user-friendly as it provides a menu-driven system for inputting data and the outputs can be formatted to graphs and tables.

Reference:

1. Tester, D.J., P.A. Waldron, and R. Williams. 1992. The Great Ouse automatic quality monitoring network. J. IWEM, 6: 165-171.

3.1.12 SQRM -- Stochastic River Water Quality Model

SRQM consists of a series of three separate modules, DOSTOC, NUSTOC, and UNSTOC which are one-dimensional, steady-state stochastic simulations. They assume that longitudinal dispersion is neglected, velocity and rate coefficients are uniform for each river reach and mixing is instantaneous and complete.

Each module can be run independently of the others. The input requirements are considered small, relative to other river models, and are more than sufficient for the databases existing for many river systems. The graphical and tabular output facilitates interpretation of results.

I. DOSTOC: Dissolved Oxygen Stochastic Model

Type: A Dissolved oxygen model for rivers that performs steady-state stochastic analyses.

Description:

DOSTOC determines the dissolved oxygen concentration in a river, describing the interactions between sources and sinks of oxygen in river processes by three differential equations. The model is relevant to river systems where carbonaceous BOD processes are more important than nitrogen processes.

II. NUSTOC: River Nutrient Stochastic Model

Type: A nitrogen and phosphorus model for rivers that performs steady-state stochastic analyses.

Description:

NUSTOC predicts the organic and inorganic nitrogen, and dissolved and particulate phosphorus content of rivers. The anaerobic denitrification of nitrate to ammonia is not simulated.

III. UNSTOC: Unspecified Substance Stochastic Model

Type: A conservative or non-conservative variable model for rivers.

Description:

UNSTOC simulates any single conservative or nonconservative constituents affected by volatilization, biodegradation, or sedimentation.

Availability:

In order to request the user's manuals and diskettes for any of the three modules included in SRQM contact:

John Campbell: Water Evaluation Branch, Alberta Environmental Protection Water Resources Administration Division, 2nd floor, Oxbridge Place, 9820-106 Street, Edmonton, Alberta T5K 2J6. Phone: (403) 427-8985. Fax: (403) 422-3572.

References:

1. Alberta Environmental Protection Division Internal Document. Provided by John Campbell in November 1994. p. 20-21.

2. Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for the Water Quality Branch, Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

3.1.13 BLTM -- Branched Lagrangian Transport Model

Type: A one-dimensional Lagrangian dynamic transport model capable of mimicking QUAL2E kinetic structure. Up to 10 constituents can be modelled. Computer simulation.

Description:

The BLTM model was developed for simulation of a complex flow network with multiple branches, each with multiple cross-sections. The required inputs are: boundary conditions, kinetic rates, Fortan code for kinetics and flow field at fixed grid points, including discharge, cross-sectional area, top width, and tributary inflow.

Comments:

The model is limited to one-dimensional channels, unstratified flow and fixed channel geometry. A separate model is required to provide hydraulic computations. Examples of hydraulic models are provided in the BLTM user's manual. The model does not include a reservoir component, although a slow-moving, nonstratified reservoir could be modelled as a stream segment. The user must be able to program in Fortran in order to define the constituents and the constituent's reaction kinetics.

System Requirements:

1. IBM and DOS compatible 286 class microcomputer with 620KB RAM

Availability:

Contact: H.E. Jobson, Phone (703) 648-5224. The manuals may be obtained from: U.S. Geological Survey, Books and Open-File Reports, Federal Center, Building 810, Box 25425, Denver, Colorado 80225.

References:

1. Jobson, H.E. and D.H. Schoelhamer. 1987. Users manual for a branched Lagrangian transport model. U.S. Geological Survey, Reston, Virginia. Water Resources Investigations Report 87-4163, 73p. Cited in: Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for: Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

2. Schoelhamer, D.H. and H.E. Jobson. 1986. Programmers manual for a one dimensional Lagrangian transport model. U.S. Geological Survey Water Resources Report 86-4144, 101p. Cited in: Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for: Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

3. Schoelhamer, D.H. and H.E. Jobson. 1986. Users manual for a one-dimensional lagrangian transport model. U.S. Geological Survey Water Resources Investigation Report 86-4145, 95p. Cited in: Gummer, B. 1991. Water quality modelling within the Souris River Basin. Prepared for: Inland Waters Directorate, Environment Canada, Regina, Saskatchewan.

3.2 General Empirical and Mechanistic Models

3.2.1 Empirical Models for Estimating the Concentrations and Exports of Metals in Rural Rivers and Streams

Type: Empirical.

Description:

Concentrations of Al, Fe, Mn, Zn, and Cu were measured monthly at 24 sites in 21 rivers in Ontario and Quebec. Relationships between metal and suspended particulate matter (SPM), turbidity, color (g440), temperature and system hydrology were quantified, and used to derive empirical models for predicting metal concentrations. In a test of the models using an independanr data set, they explained a significant proportion of the variation in Al (90%), Fe (85%), and Mn (57%), but only 37% of the variation in riverine Zn concentrations. Metals concentrations are most strongly associated with SPM concentrations. The proportion of the total metal load associated with particulates (>0.45μm) is highly variable below 10ppm SPM, indicating that this concentration approximates the division between systems dominated by weathered (solution) versus eroded (particulate) inputs. Annual metal exports were calculated, and empirical models for predicting catchment exports were developed using system hydrology and average SPM concentrations. These simple models can be used to estimate metals concentrations and exports from routine water quality monitoring data, without requiring chemical analyses. They also serve to distinguish background levels from those indicating metal contamination, and will, therefore, be useful for water quality evaluation (Author's abstract).

Reference:

1. Cuthbert, I.D. and J. Kalff. 1993. Empirical models for estimating the concentrations and exports of metals in rural rivers and streams. Water, Air, and Soil Pollution 71: 205-230.

3.2.2 Streeter-Phelps Oxygen Sag Model

Type: Mechanistic.

Description:

The classic Streeter-Phelps model that is now considered the prototype river model is used to predict the oxygen deficit in a river resulting from the discharge of a waste. The model can be considered for steady-state and non-steady state conditions.

Reference:

1. Tchobanoglous, G. and E.D. Schroeder. 1985. Water Quality. Addison-Wesley Publishing Company, Inc., Don Mills, Ontario. p. 339.

Other Sources of Information:

1. Streeter, H.W., and E.B. Phelps, (1925), "A study of the pollution and natural purification of the Ohio River, III. Factors concerned in the phenomena of oxidation and reaeration," U.S. Public Health Service, Bulletin No. 146.

3.2.3 Biofilm Consumption Model

Type: Mechanistic.

Description:

The biofilm consumption model is an analytical model of the consumption of organic contaminants by bottom biofilm in river flow situations. An idealized biofilm of constant thickness and density is assumed. The model describes a diffusion type process in which the contaminant material is transported because of the existence of a concentration gradient. Once the substrate reaches the biofilm, its concentration is determined by a diffusion term and a reaction term. The biodegradation as well as sorption processes are all incorporated into these terms.

The solutions to the steady-state equation will vary depending upon the kinetics chosen for the rate of consumption and upon the boundary conditions. Three different modelling cases involving different kinetics are presented in Lau (1990): zero-order kinetics with full penetration of the biofilm by the contaminant, zero-order kinetics with partial penetration, and first-order kinetics.

Comments:

This model may require more testing before it can be applied with any significant amount of certainty. The author mentions that there has been little work done in this area and that there is no general agreement on the kinetics of the bottom biofilm of rivers.

Reference:

1. Lau, Y.L. 1990. Modelling the consumption of dissolved contaminants by biofilm periphyton in open-channel flow. Wat. Res., 24(10):1269-1274.

3.3 Models Developed for Specific River and Stream Applications

3.3.1 A Steady-State Stream Water Quality Model for Monument and Fountain Creeks, East-Central Colorado

Type: Computer simulation.

Description:

This model was developed using the EPA's QUAL2E model shell with the necessary modifications to model the water quality of both the Monument and Fountain Creeks of east-central Colorado. One reach of each of the streams was used to evaluate summer conditions, especially the depletion of dissolved oxygen. One reach on Fountain Creek was used to evaluate winter conditions, especially the concentrations of un-ionized ammonia. Other water quality constituents considered in the modelling analysis were total organic nitrogen, total ammonia, total nitrite and nitrate, 5-day carbonaceous BOD, and DO.

Reference:

1. Kuhn, G. 1991. Calibration, verification, and use of a steady-state stream water-quality model for Monument and Fountain Creeks, east-central Colorado. U.S. Geological Survey. Water Resources Investigations Report 91-4055. 149p.

3.3.2 Columbia River Water Quality Model

Type: Computer simulation.

Description:

The Columbia River water quality model was developed in order to estimate the concentrations of conservative substances (substances that do not decay or "drop out" from the flow") in the Columbia River just upstream of the U.S. border, resulting from releases into the river from the Cominco plant at Trail. Inputs include: river flow, distance downstream, river velocities, dispersion parameters, loading data, and load uncertainty factors.

The dispersion model contains three command selections: input of river characteristics and loading data, calculation of the entire worksheet, and display of either the loading data or the concentration results in graphical form. Each of the inputs for the velocities, dispersion parameters, load factors require three values: a low, probable and high estimate. The model computes confidence limits of the predicted concentrations and displays them graphically using these estimates. It is possible for this model to be altered so that rivers other than the Columbia River can be modelled.

System Requirements:

Lotus 1-2-3 worksheet program, 640KB RAM, expanded memory and math co-processor recommended.

Availability:

Adam LaRusec: Emergency Spills, Environmental Protection Branch, Environment Canada, 224 West Esplanade, North Vancouver, British Columbia V7M 3H7. Phone (604) 666-2165. Fax (604) 666-1140.

Reference:

1. Russell, S.O.D. 1989. Columbia River Water Quality Model. Department of Civil Engineering, University of British Columbia.

3.3.3 Empirical Regression Models for the Prediction of Nutrient Export - Specific to the Muskoka-Haliburton Area of Central Ontario

Type: Empirical.

Description:

In the Muskoka-Haliburton region of central Ontario, the ability to predict nutrient export from unmonitored forested stream catchments is necessary in order to help predict the impact of shoreline development on lake trophic status. Dillon and Molot (1990) present empirical regression models for prediction of annual NH_4^+, NO_3^-, total organic nitrogen, and total phosphorus export based on data collected from 32 central Ontario streams during the 8 year period 1976/77 to 1983/84.

Reference:

1. Dillon, P.J., and L.A. Molot, 1990. Prediction of annual nitrogen and phosphorus export from forested stream catchments in central Ontario. Prepared by the Dorset Research Centre for the Ontario Ministry of Environment.

3.3.4 Fraser-Thompson River Basin Ecosystem Model

Type: Computer simulation.

Description:

The Fraser-Thompson River Basin ecosystem model is a combined environmental fate and food-chain model designed to relate the emissions of dioxins and furans from pulp and paper mills in the Fraser-Thompson River Basin to resulting concentrations in water, sediment, air and various fish species in the Fraser and Thompson Rivers.

The environmental fate model represents the Fraser and Thompson Rivers as, respectively, 18 and 5 smaller interconnected compartments, varying in length between 15 and 60 km. Each river compartment consists of a water (including suspended solids) and a bed-sediment sub-compartment, which are assumed to be completely mixed. In each compartment the transport and transformation of dioxins and furans were considered to be the result of: inflow and outflow, volatilization, sorption to suspended sediments, diffusion between water and sediments, settling of suspended solids, resuspension of bed sediments, deposition (or burial), and degradation in water and sediments. The environmental fate model predicts two types of information: the relationship between released dioxins and furans and the resulting concentrations in the water and sediments at various locations in the Fraser-Thompson River Basin, and the time response of the water and sediment concentrations to changes in the amount of dioxins and furans released.

The food-chain model includes the processes of organisms that are considered to be the most important members of the local food-chain and those organisms on which sufficient data is already available. These organisms are: phytoplankton, zooplankton, emerging insects, salmonoid fry , and four resident fish species including Large Scale Sucker, Rocky Mountain White Fish, Dolly Varden, and Rainbow Trout. The food-chain model consists of a series of mathematical expressions to represent the uptake, elimination, and bioaccumulation of chemicals in these organisms. The food-chain model also predicts two types of information: the resulting concentrations of dioxins and furans in these organisms and the time response of the concentrations to changes in pulp mill emissions.

Reference:

1. Gobas, F.A.C.P., and J.P. Pasternak. 1993. The application of a computer simulation model for the management and regulation of dioxin and dibenzofuran emissions by pulp mills in the Fraser-Thompson River Basin: Regulation based on best available science. In: The Aquatic Resource Research Project: Towards environmental risk assessment and management of the Fraser River Basin. p.99-120. Simon Fraser University/ British Columbia Ministry of Environment.

Other Sources of Information:

1. Gobas, F.A.C.P., amd J.P. Pasternak. 1993. Chemical fate modelling in the Fraser River Basin: A literature review. In: Integrative environmental impact modelling: Application to organic chemical emissions from pulp and paper mills in the Fraser River basin. The British Columbia Science Council. p. 10-18.

2. Frank Gobas: School of Natural Resources and Environmental Management, Faculty of Applied Sciences, Simon Fraser University, Burnaby, British Columbia V5A 1S6.

3.3.5 Kapuskasing River Dual Model Approach - HSPF and DO Water Quality Model

Type: Computer simulation.

Description:

In order to effectively model the levels of DO of the lower Kapuskasing River, in northern Ontario, that result from the river's inherent physical and biochemical characteristics and operation of the Spruce Falls Pulp and Paper Mill, a dual-model approach has been undertaken. Both the U.S. EPA's HSPF hydrologic forecasting program and a dissolved oxygen water quality model have been implemented.

HSPF is used to generate a 20-day continuous forecast of the Kapuskasing stream flow and water temperature based on a concomitant forecast of prevailing meteorology. The DO model predicts DO concentrations along the river on a daily basis and predicts 20 days of future water quality in the river as a function of the HSPF outputs and predicted mill operation. The water quality model was developed by Beak Consultants Ltd.

Reference:

1. Holloran, M.F. and D.G. Wilson. 1990. A computer implemented protocol to maximize water quality in the Kapuskasing River downstream from Kapuskasing. (Journal unknown. See below for author's work address as of 1990.)

Other Sources of Information:

1. Beak Consultants Ltd., 14 Abacus Rd., Brampton, Ontario, L6K 3N6.

3.3.6 Optimization Model to Maximize Power and Maintain DO Criteria at Hydropower Stations

Type: Optimization.

Description:

In order to determine the spill flow requirements for 16 proposed hydropower projects in the Ohio River Basin an optimization model was adopted by the hydropower licensing commission. It consists of two model components: a piecewise linear model of power generation as a function of spill flow developed for each dam from records of historic flows and plant design criteria, and a DO model based on a Streeter-Phelps formulation. The DO criteria is included in the optimization model as a set of constraints. The DO concentration at each reach is estimated as a function of the spill flow rate at upstream dams and other model variables and parameters, such as the aeration rate at each dam.

Comments:

Although this model is considered a "simple model" that does not attempt to simulate all the biological processes that affect DO concentration, such as photosynthesis, non-point-source BOD and sediment BOD, and mixing zones it has been determined to be adequate for determining spill flow requirements by the Federal Energy Regulatory Commission in the U.S. For further discussion see Railsback and Sale (1990).

Reference:

1. Railsback, S.F., and M.J. Sale. 1990. Application of optimized water quality mitigation to hydropower development in the Ohio River Basin in: Water Resource Systems Application. S.P. Simonovic, I.C. Goulter, D.H. Burn, and B.J. Lence, ed., Dept. Civil Engineering, University of Manitoba. p. 413-422.

3.3.7 PRAM -- The Pigeon River Allocation Model

Type: Computer simulation.

Description:

This model was developed using the U.S. EPA's QUAL2E-UNCAS model shell in order to investigate the depressed DO concentrations that the Pigeon River, North Carolina, experiences during low flow periods in the summer. PRAM is a steady-state representation of the Pigeon River during late-summer low flow conditions. The model simulates river dynamics over a 20-mile area using 13 biological/ chemical state variables: DO, carbonaceous BOD, chlorophyll *a*, total nitrogen, organic nitrogen, ammonia, nitrate, nitrite, organic phosphorus, dissolved phosphorus, total phosphorus, chlorides, and temperature, and 6 physical state variables: streamflow, travel time, velocity, depth, stream width, and volume. The 20-mile stretch is modelled as 105 connected segments that are of equal length. The dominant biological and chemical mechanisms represented in the model structures include: microbial/chemical degradation and transformation, respiration, primary productivity, and chemical oxygen demand; while the major physical mechanisms include: advection, reaeration, deaeration, and mixing. PRAM was constructed and calibrated using data collected over a 24-hour period.

For a description of the specific mathematical relationships used to represent algal dynamics; BOD decay; nutrient transformations, uptake, and excretion; hydrodynamics; and transport in PRAM see Summers et al. (1991).

Reference:

1. Summers, J.K., P.F. Kazyak, and S.B. Weisberg. 1991. A water quality model for a river receiving paper mill effluents and conventional sewage. Ecol. Modelling, 58:25-54.

Other Sources of Information:

1. Brown, L.C. and Barnwell, T.O., 1987. The enhanced stream water quality models QUAL2E and QUAL2E-UNCAS, documentation and user manual. EPA-600-3-87-007. U.S. EPA, Environmental Research Laboratory,Athens, GA.

3.3.8 Whole Toxicity Model for Streams -- Naugatuck River

Description:

Determines the toxicity at any given location in the Naugatuk River, Conneticut using a toxic unit (TU) determined by using the Mount-Norberg *Ceriodaphnia dubia* toxicity assay. The model assumes the discharges, effluent from publicly owned treatment works (POTW), and industrial copper, act independently.

Comments:

The descriptive paper states that while this toxicity model obtains better agreement between observed and predicted values than a model which assumes additivity of the discharge effects, this model has consistently overestimated toxicity at the site that is farthest downstream.

Reference:

1. DiToro, D.M., J.A. Hallden, and J.L. Plafkin. 1991. Modeling *Ceriodaphnia* toxicity in the Naugatuck River II. Copper, hardness and effluent interactions. Env. Tox. and Chem., 10:261-274.

4.0 Modelling the Fate and Transport of Toxic Contaminants in Freshwater Environments

4.1 General Models

4.1.1 TOXMOD

Type: A framework that is designed to assess the impact of toxic organic compounds on lakes and impoundments. Computer simulation.

Description:

The modelling framework is implemented via a personal-computer oriented software package--Toxmod 1.0. It is designed for interactive implementation and is self-documented. Toxmod allows the user to rapidly generate and analyze scenarios. The software includes graphical displays and can be run on IBM-PC compatible microcomputers. It is presently designed for implementation with EGA color graphics.

Comments:

The author outlines the limitations of Toxmod in the user's manual. Chapra warns that the model has not been thoroughly "beta tested," a process whereby users, other than the original developer, test the model by running it for new applications. As well, the computer program does not contain an efficient "error trapping" system. In other words, the program will attempt to process all the data that the user inputs, even if the data represents an unrealistic scenario. Due to these weaknesses in the Toxmod program users should be aware of how to apply the model properly and minimize the model's shortcomings.

Availability:

The Toxmod program is available through the North American Lake Management Society (NALMS). For ordering information contact:

NALMS, 1 Progress Boulevard, Box 27, Alachua, Florida 32615. Phone: (904) 462-2554; Fax: (904) 462-2568.

Reference:

1. Chapra, S.C. 1991. TOXMOD 1.0. Software to model long-term trends of toxic organics in lakes. CADWES Working Paper No. 13.

Other Sources of Information:

1. Chapra, S.C. 1991. Toxicant loading concept for organic contaminants in lakes. J. Environ. Eng. 117(5).

2. Steven C. Chapra: CADWES, Campus Box 428, University of Colorado, Boulder, CO 80309-0428. Phone: (303) 492-3972.

4.1.2 WASP5 -- Version 5.10 Water Quality Analysis Simulation Program

Type: WASP5 is a generalized framework for modelling contaminant fate and transport in surface waters. WASP5 can be applied in one, two, or three dimensions.

Description:

Two WASP models are provided with WASP5: TOXI5 is a toxics model. It predicts the dissolved and sorbed chemical concentrations in the sediment bed and overlying waters; EUTRO5 is a oxygen/eutrophication model. It predicts dissolved oxygen and phytoplankton dynamics affected by nutrients and organic material. The WASP5 package also includes DYNHYD5, a hydrodynamic model that is capable of simulating tidal cycles, wind, and unsteady inflows.

Problems that have been studied using the WASP framework include biochemical oxygen demand and dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and organic chemical and heavy metal contamination.

Water quality constituents include, but are not limited to organic nitrogen, ammonia nitrogen, nitrite nitrogen, nitrate nitrogen, organic phosphorus, orthophosphate, ultimate carbonaceous biochemical oxygen demand, conservative materials, coliform bacteria, nonconservative constituents, algae as carbon and chlorophyll, dissolved oxygen, up to 17 specific organic chemicals and other environmental variables.

Availability:

The WASP5 package is available from the U.S. EPA's Center for Exposure Assessment Modeling. See ordering information on page 123.

Reference:

1. Bouchard, D.C., R.B. Ambrose Jr., T.O. Barnwell, Jr., Disney, D.W. Environmental software available at the U.S. Environmental Protection Agency Center for Exposure Assessment Modeling. *Computer Supported Desk Management*. In press.

Other Sources of Information:

1. Culp, J.M., and P.A. Chambers. 1993. Proceedings of a workshop on water quality modelling for the North River Basins Study, March 22-23, 1993. North River Basins Study Project Report No. 37. ISBN 0-662-22366-7. Pages 4.14-4.29.

This report includes a section on the WASP framework as it has been applied in Alberta. As well, it examines the potential applicability of the program in the North River Basins Study (NRBS). Table 4.1 contains a summary of the advantages and disadvantages of applying the EUTRO sub-model to the Athabasca and Peace Rivers of the NRBS.

4.1.3 EXAMS II -- Exposure Analysis Modelling System

Type: Computer simulation of the probable aquatic fate of synthetic organic chemicals.

Description:

EXAMS II is an interactive modelling system that allows a user to specify and store the properties of chemicals and ecosystems, modify either via simple commands, and conduct rapid evaluations and error analyses of the probable aquatic fate of synthetic organic chemicals (1). The program produces output tables and simple graphics describing chemical exposure, fate and persistence (2).

Availability:

EXAMS II is available from the U.S. EPA's Center for Exposure Assesment Modeling. See ordering information on page 123

References:

1. Burns, L.A. 1990. Exposure analysis modeling system: User's guide for EXAMS II Version 2.94. EPA/600/3-89/084. U.S. EPA, Athens, GA, 30605.

2. Bouchard, D.C., R.B. Ambrose Jr., T.O. Barnwell Jr. 1994. Environmental software available at the U.S. Environmental Protection Agency's Center for Exposure Assessment Modeling. Computer Supported Desk Management. In press.

4.1.4 FGETS -- Food and Gill Exchange of Toxic Substances

Type: Computer simulation.

Description:

FGETS is a FORTRAN simulation model that predicts temporal dynamics of a fish's whole body concentration of nonionic, nonmetabolized, organic chemicals that are bioaccumulated from either: (a) water only - which is the predominant route of exchange during acute exposures, or (b) water and food jointly - which is more characteristic of chronic exposures (1) FGETS also calculates the time to reach the chemical's lethal activity by assuming that the chemical elicits its pharmacological response through a narcotic mode of action (2).

Availability:

FGETS is available from the U.S. EPA's Exposure Assessment Laboratory. See ordering information on page 123.

References:

1. Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1988. Modeling bioconcentration of nonpolar organic pollutants by fish. Environ. Toxicol. Chem. 7: 545-558.

2. Bouchard, D.C., R.B. Ambrose Jr., T.O. Barnwell, Jr., D.W. Disney. 1994. Environmental software available at the U.S. Environmental Protection Agency's Center for Exposure Assessment Modeling. Computer Supported Desk management. In press.

4.1.5 QWASI -- Quantitative Air Water Sediment Interaction Fugacity Model

The QWASI models are based on the concept of fugacity, a thermodynamic quantity related to chemical potential or activity that characterizes the escaping tendency from a phase (1). Fugacities have units of pressure (Pa). All rates in QWASI are expressed as a products of a fugacity (f) and a transport or transformation parameter (2). The QWASI model for lakes has been converted to a computer simulation program.

I. QWASI for Lakes

Description:

The QWASI model for lakes describes the fate of chemicals in any well-mixed water body for which the hydraulic and particle flows are defined (3). Processes included in the model are advective flow, volatilization, sediment deposition, resuspension and burial, sediment-water diffusion, wet and dry atmospheric deposition, and transformation reactions. The lake system modelled consists of water, bottom and suspended sediments, and air.

Availability:

Send a self-addressed, stamped disk mailer to :

Donald Mackay: University of Toronto, Department of Chemical Engineering and Applied Chemistry, Toronto, Ontario, M5S 1A4. Phone:(416) 978-4019. Fax:(416) 978-8605.

II. QWASI for Rivers

Description:

The QWASI model for rivers describes the fate of chemicals in a river in which the sediment and water are well-mixed or homogeneous (2). The transport and transformation processes included in the model are advective flow (in solution and in association with suspended particles), reaction in sediment and water, sediment deposition, resuspension and burial, and air-water exchange processes of volatilization, adsorption, and wet and dry deposition with particulate matter.

Solutions can be obtained for steady-state and unsteady-state conditions using either an analytical or sectioning approach. The analytical approach involves describing the composition of water and sediment continuously with flow-time or flow-distance. The sectioning approach simulates the river as a series of homogeneous connected lakes.

Availability:

Contact Don Mackay at address above.

References:

1. Mackay, D. and S. Paterson. 1982. Fugacity revisited. The fugacity approach to environmental transport. Environ. Sci. Techno. 16(12): 654A-660A.

2. Mackay, D., S. Paterson, and M. Joy. 1983. A quantitative water, air, sediment interaction (QWASI) fugacity model for describing the fate of chemicals in rivers. Chemosphere 12(9/10): 1193-1208.

3. Mackay, D., and M. Diamond. 1989. Application of the QWASI (Quantitative Water Air Sediment Interaction) Fugacity Model to the dynamics of organic and inorganic chemicals in lakes. Chemosphere. 18(7/8): 1343-1365.

Other Sources of Information:

1. Ling, H., M. Diamond, and Mackay, D. 1993. Application of the QWASI Fugacity/Aquivalence Model to assessing sources and fate of contaminants in Hamilton Harbour. J. Great Lakes Res. 19(3): 582-602.

2. Mackay, D., S. Paterson, and M. Joy. 1983. A quantitative water, air, sediment interaction (QWASI) fugacity model for describing the fate of chemicals in lakes. Chemosphere. 12(7/8): 981-997.

3. Mackay, D. 1991. Multimedia environmental models: the fugacity approach. Lewis Publishers, Inc., Boca Raton, Florida.

4.1.6 A Pollutant Transport Model for a Complex River System

Type: A dynamic model for simulation of unsteady flow and nonpoint source pollutant flow from watershed runoff. Computer simulation.

Description:

The models consists of three sub-models: an unsteady flow sub-model, a stream water quality sub-model, and a nonpoint source pollution transport model. The model combines the theory of the CHARIMA and HSPF models as well as basic stream water quality theory. The descriptive paper describes the application of the model to the Ta-Han River in Taiwan.

Comments:

The author's compare this model to other nonpoint source pollutant simulation models such as HSPF. The main difference in this model is the ability to model the dynamic effect of water flow that occurs during flood waves. The descriptive paper does not state what the computer requirements are for this program or if it is available for application in Canada.

Reference:

1. Yang, J,C., H.P. Lee, and J,H, Chang. 1992. Pollutant transport modelling for a complex river system. Computer techniques and applications. Hydraulic engineering software IV. Computational Mechanics Publications, Southhampton, England, and Elsevier Applied Science , London, England. p. 49-60.

4.1.7 Models for Predicting the Fate of Synthetic Chemicals in Aquatic Ecosystems

Type: Mechanistic

Description:

Burns (1985) discusses models for each of the transformation and transport processes involved in the distribution of chemicals in aquatic environments: ionization, sorption, volatilization across the air/water interface, hydrodynamic motion, exchanges across the benthic boundary layer, transport in infiltrating flows and movements of the sediment bed, hydrolysis, photochemical reactions, photolysis and oxidation, and microbial biotransformation. The paper also includes an introduction to the concept of aquatic fate computer codes. EXAMS, an EPA-supported program, is presented as an example.

Reference:

1. Burns, L.A. 1985. Models for predicting the fate of synthetic chemical in aquatic ecosystems. In: Validation and predictability of laboratory methods for assessing then fate and effects of contaminants in aquatic ecosystems. ASTM STP 865. T.P. Boyle, Ed., American Society for Testing and Materials, Philadelphia. pp. 176-190.

4.2 Annotated Bibliography of Fate and Transport-Related Modelling Accounts

1. Halfon, E., T.J. Simons, and W.M. Schertzer. Modeling the spatial distribution of seven halohydrocarbons in Lake St. Clair in June 1984 using the TOXFATE model. J. Great Lakes Res. 16(1):90-112.

Describes the use of two models, TOXFATE and a hydrodynamic model, to predict the fate of seven volatile halocarbons in Lake St. Clair. The paper contains a description of both models and their original sources. 11 figures, 8 tables and 27 references are included.

2. Halfon, E. and B.G. Oliver. 1990. Simulation and data analysis of four chlorobenzenes in a large lake system (Lake Ontario) with TOXFATE, a contaminant fate model. In: Jorgenson, S.E. (Ed.) 1990. Modeling in ecotoxocology. Published in Elsevier, Amsterdam. p. 197-213.

Describes the problem of toxic contaminants in Lake Ontario and an application of TOXFATE to Lake Ontario. Also presented is the theory and mathematical equations that TOXFATE is based on. Includes 2 figures, 4 tables, and 12 references.

3. Lam, D.C.L., R.C. McCrimmon, J.H. Carey, and C.R. Murthy. 1988. Modelling the transport and pathways of tetrachlorophenol in the Fraser River. Water Poll. Research J. Canada. 23(1): 141-159.

Describes a mathematical model that was developed to simulate the advection, sorption, photolysis and sedimentation of 2,3,4,6-tetrachlorophenol in the Fraser River Estuary. Efforts were made to produce a model that was simple yet adequate for the modelling purposes. The model is one-dimensional and only includes those chemical and biological processes that are known to contribute most significantly to the changes as manifested in the data. The authors cite a need for more detailed loading and hydrodynamic data in order to enhance the current model. 11 figures, 1 table and 7 references are included.

4. Lang, G.A., and T.D. Fontaine. 1990. Modeling the fate and transport of organic contaminants in Lake St. Clair. J. Great Lakes Res. 16(2):216-232.

Describes the development, calibration, and application of a multisegment, contaminant mass balance model to improve general understanding of the processes and parameters that are important for accurate simulation of contaminant fate and transport in Lake St. Clair. 10 figures, 3 tables and 33 references are included.

5. McCorquodale, J.A. and E.M. Yuen. 1990. Modelling the toxic contaminants in the St. Mary's River. In: Water resource systems application. Ed. S.P. Simonovic, I.C. Goulter, D.H, Burn, and B.J. Lence. Department of Civil Engineering, University of Manitoba.

Describes the combined use of KETOX, a two-dimensional fate and transport model, and TOXI4 on St. Mary's River. The models are compared. 8 figures and 15 references are included.

6. Mackay, D. and A.I. Hughes. Three-parameter equation describing the uptake of organic compounds by fish. Environ. Sci. Technol. 18(6):439-445.

An equation for describing the uptake of organic compounds by fish is derived and discussed. The equation is derived using the fugacity concept. Includes 5 figures and 1 table.

7. Murthy, C.R., T.J. Simons, and D.C.L. Lam. 1986. Dynamic and transport modelling of the Niagra River Plume in Lake Ontario. Rapp. P.-v. Reun. Cons. int. Explor. Mer. 186:150-164.

Describes the use of temperature and velocity observations of the Niagra River Plume in Lake Ontario to develop simulation models of its flow and diffusion characteristics. Using computed currents, a transport model is used to simulate the dispersion of contaminants. 6 figures, 1 table and 3 references are included.

8. Rodgers, P.W., T.A.D. Slawecki, J.V. DePinto, and W. Booty. 1991. LTI TOXICS MODEL application: PCB's in Lake Ontario, an exploratory application.

A comprehensive report on the use of the LTI TOXICS MODEL for Lake Ontario. Includes 12 figures, 8 tables and 83 references.

9. Stepian, I., D.C.L. Lam, C.R. Murthy, M.E. Fox, and J. Carey. 1987. Modelling of toxic contaminants in the Niagra River Plume of Lake Ontario. J. Great Lakes Res. 13(3):250-263.

A two-dimensional model that can be used for the purposes of near-shore and short-time prediction of fate and transport of toxic chemicals in the coastal zone is described as it is applied to simulate the transport and compartmental distribution of chlorinated benzenes in the Niagra River bar area. 12 figures, 1 table and 25 references are included.

10. Stronarch, J.A., C.R. Murthy, and T.S. Murty. 1990. Pollutant transport modelling in large river plumes. In: Estuarine and Coastal Modeling. American Society of Civil Engineers, New York. p.759-770.

Describes the combined use of hydrodynamic models for the Fraser River and the Niagra River plume in Lake Ontario with a generalized pollutant transport model to simulate the horizontal distributions of pollutants. Recommendations for improving the model based on applications to both rivers are discussed. Includes 6 figures and 14 references.

5.0 Other Models

5.1 General Models

5.1.1 CORMIX -- Cornell Mixing Zone Expert System

Type: A series of software subsystems for the analysis, prediction, and design of aqueous toxic or conventional pollutant discharges into diverse water bodies. Computer simulation.

Description:

The major emphasis of CORMIX is on the prediction of plume geometry and dilution characteristics within a receiving water's initial mixing zone so that compliance with regulatory constraints may be judged. The system also predicts the behavior of the discharge plume at larger distances. The highly user-interactive CORMIX system is implemented on microcomputers (IBM-PC, or compatible), and consists of three subsystems. These are: (a) CORMIX1 for the analysis of submerged single port discharges, (b) CORMIX2 for the analysis of submerged multiport diffuser discharges and (c) CORMIX3 for the analysis of buoyant surface discharges. Without specialized training in hydrodynamics, users can make detailed predictions of mixing zone conditions, check compliance with regulations and readily investigate the performance of alternative outfall designs.

System Requirements:

1. IBM-PC/XT compatible microcomputer
2. 582Kb of available RAM memory (minimum)
3. a math co-processor
4. approx. 1Mb of hard disk space per installed subsystem
5. DOS 3.3 or higher operating system

Comments:

The user's guide gives a comprehensive and uniform description of all three CORMIX subsystems; it provides guidance for the assembly and preparation of required input data; it delineates ranges of applicability of the three subsystems; it provides guidance for interpretation and graphical display of system output; and it illustrates practical system application through three case studies.

Distribution:

CORMIX is distributed by the U.S. EPA's Center for Exposure Assessment Modeling. See ordering information on page 123.

Reference:

1. National Council of the Paper Industry for Air and Stream Improvement. 1992. User's guide for the Cornell Mixing Zone Expert System (CORMIX). Technical Bulletin No. 624.

Other Sources of Information:

1. Distante, D., R. O'Neill, G.A. Apicella, H. Tipping. 1994. CORMIX model nearfiled dilution evaluations for 12 water pollution control plant discharges. In: Proceedings of the Water Environment Federation 67th Annual Conference and Exposition. Surface Water Quality and Ecology. Volume 1V. ISBN -- 1-881369-68-4. p. 135-145.

This paper discusses the results of an application of CORMIX to the discharge of 12 water pollution control plants. Capabilities and limitations of CORMIX are discussed as they relate to tidal waters. Includes 5 figures, 2 tables, and 13 references.

5.1.2 PLUMES

Type: Computer simulation.

Description:

Pollution control authorities often use buoyant plume models to simulate expected concentrations of effluent contaminants in ambient receiving waters. Applications have also included industrial wastes, drilling fluids from offshore oil exploration and development projects, and effluent discharge into freshwater systems (1).

The PLUMES program is intended for use with plumes discharged to marine and freshwater bodies. Both buoyant and dense plumes, single sources, and multiple diffuser outfall configurations can be modelled (2).

PLUMES is a computer implementation for preparing input data and controlling two initial dilution plume models: RSB and UM. It also contains two far-field algorithms, which are auomatically initiated beyond the zone of initial dilution. PLUMES incorporates the EPA's CORMIX model flow classification scheme with recommendations for model usage, thereby providing a link between the two EPA models (2).

System Requirements:

PLUMES is designed to be used on IBM compatible PC's running under DOS. No graphics are displayed although a color monitor is required. The PLUMES memory requirement is at most 200K (1).

Comments:

The full report (1) gives a detailed description of both buoyant plume models in technical terms. It includes a discussion on the general aspects of dilution modelling and a user's guide to PLUMES. The report is intended to be used by readers who are familiar with the terminology of buoyant plume mechanics, either as applied in regulatory practice or in fluid mechanics generally.

Tables V and VI (1) are given below so that the reader can get an idea of what type of situations these models are recommended to operate in. The EPA mixing zone model, CORMIX, is included in the table for comparison purposes.

Conditions / Effluent Types	Stratification			Current		Other Sources, Decay	BCs	Intrusion	VSW
	none	1,2	3+	2-D	3-D				
Buoyant discharge: sewage, industrial waste especially to saline waters	*I* U	*C* U	U	*C* U	*C* u	*C* (decay) U	*C* u	*C* u	u
Slightly buoyant discharges, signif. momentum: thermal discharges	*C* U	*C* U	U	*C* U	*C* u	*C* (decay) U	*C* u	*C* u	u
Dense discharges: light brine, R.O. discharge, industrial waste	*C* U	*C* U	U	*C* U	*C* u	*C* (decay) U	*C* u	*C* u	u
Discharges with nascent or non-linear density effects: thermal discharge to cold water	U	U	U	U	u	U	u	u	u

Table V. Single port discharge model recommendations. C = CORMIX, U,u = UM BCs = boundary conditions, VSW = very shallow water.

Conditions / Effluent Types	Stratification			Current		Merging		Other Sources, Decay	BCs	Intrusion	Stage
	none	1,2	3+	cross	para'l	part	full				
Buoyant discharges: sewage, industrial waste especially to saline waters	C R U	C R U	R U	C R U	C R	R U	C R U	C(decay) U	C u	C R u	C
Slightly buoyant discharges, signif. momentum: thermal discharges	C r U	C r U	r U	C R U	C R	C R U	C R U	C(decay) U	C u	C R u	C
Dense discharges: light brine, R.O. discharge, industrial waste	C R U	C R U	r u	C r U	C r	C R U	C R U	C(decay) U	C u	C R U	C
Discharges with nascent or non-linear density effects: thermal discharge to cold water	U	U	U	U	u	U	U	U	u	u	

Table VI. Multiport outfall model recommendations. C = CORMIX, U,u = UM R,r = RSB, BCs = boundary conditions. The term "R.O. discharge" refers to brine plumes created by a reverse osmosis desalination process.

Table V specifies the applicability of the CORMIX1 (single port CORMIX) and UM models to single port submerged discharge problems. Multiport discharge model recommendations are given in Table VI. Uppercase letters are used in the tables to indicate that a model is "well suited" for the specified application, while lowercase letters are used to indicated that a model is "less suitable." The full report should be consulted as to the full implications of these tables and other recommendations.

Availability:

PLUMES is distributed by the U.S. EPA's Center for Exposure Assessment Modeling. See ordering information on page 123.

References:

1. Baumgartner, D.J., W.E. Frick, P.J.W. Roberts. 1994. Dilution models for effluent discharges. EPA/600/R-94/086

2. Bouchard, D.C., R.B. Ambrose, Jr., T.O. Barnwell, Jr., D.W. Disney. Environmental software available at the U.S. Environmental Protection Agency's Center For Exposure Assessment Modeling. Computer Supported Desk Management. In press.

2. Booty, W.G., D.C.L. Lam, A.G. Bobba, I. Wong, D. Kay, J.P. Kerby, G.S. Bowen. 1992. An expert system for water quality modelling. Environmental Monitoring and Assessment. 23: 1-18.

3. Booty, W.G., D.C.L. Lam, I. Wong, D. Kay, J. Kerby, and G. Bowen. A preliminary study of impact assessment procedures for mine effluents. Rivers Research Branch, National Water Research Branch, Burlington, Ontario.

5.1.4 MINTEQA2

Type: Computer simulation of metal speciation in aqueous systems.

Description:

MINTEQA2 is a geochemical equilibrium speciation model for dilute aqueous systems (1). MINTEQA2 can be used to calculate the equilbrium concentration of dilute solutions in the laboratory or in natural aquatic systems. It can be used to calculate the mass distribution between dissolved, adsorbed, and multiple solid phases under a variety of conditions.

MINTEQA2 is accompanied by an interactive program PRODEFAC2, which is used to create MINTEQA2 input files. With PRODEFAC2, the user can both (1) access the species available in the MINTEQA2 thermodynamic database and (2) define other aqueous, solid, and/or adsorption species not present in the database. The MINTEQA2 user should have a scientific or engineering background with at least one year of introductory chemistry. Additional experience with thermodynamics is helpful.

In general, the data needed to run MINTEQA2 consist of a chemical analysis of the water sample to be modelled giving total dissolved concentrations for the components of interest, and other relevant measurements for the system like the pH, pE, and/or the partial pressure of one or more gases.

It is appropriate to use MINTEQA2 only if the assumption can be made that the chemical system is at or will reach equilibrium. This equilibrium assumption is important to remember because natural systems can be kinetically constrained. The equations used in MINTEQA2 apply only to aqueous systems with ionic strengths less than 0.5M. MINTEQA2 is designed to perform best at 25°C; however, corrections to perform calculations between 0°C and 100°C are incorporated in the model. A major assumption in the application of MINTEQA2 is that the thermodynamic database is complete, internally consistent, and accurate. Additional assumptions pertain to specialized submodels for adsorption and organic matter.

Availability:

MINTEQA2 is available from the U.S. EPA's Center for Exposure Assessment Modeling. See ordering information on page 123.

References:

1. Allison, D.J., D.S. Brown, and K.J. Novo-Gradac. 1991. MINTEQA2/PRODEF2, a geochemical assessment model for environmental systems: Version 3.0 User's Manual. EPA 600/3-91/021, U.S. EPA, Athens, GA, 30605.

2. Felmy, A.R., D.C. Girvin, and E.A. Jeanne. 1984. MINTEQ--A computer program for calculating aqueous eqilibria. EPA 600/3-84-032, U.S. EPA, Athens, GA, 30605.

3. Bouchard, D.C., R.B. Ambrose Jr., T.O. Barnwell, Jr., D.W. Disney. 1994. Environmental software available at the U.S. Environmental Protection Agency's Center for Exposure Assessment Modeling. Computer Supported Desk management. In press.

5.2 National Council of the Paper Industry for Air and Stream Improvement (NCASI) Surface Water Modelling Program Software Products for PC's

Ordering information for Sections 5.2.1 - 5.2.4 is on page 121

5.2.1 Dispersion Models for Rivers

PSY Plume Model

The PSY plume model is a steady state two-dimensional river plume model that can be applied to far-field mixing analyses in shallow rivers. PSY assumes that the plume is attached to either the shore or the river bottom. NCASI has modified the program from its original code so that it is now written in BASIC and is suitable for use on an IBM PC or compatible.

MOBEN Plume Model

The MOBEN plume model is a depth-averaged two-dimensional surface plume model. MOBEN assumes that the plume is free from the shore or river bottom. MOBEN is valid for low ambient currrents and low buoyant discharge. NCASI has modified the program from its original code so that it is now written in BASIC and is suitable for use on an IBM PC or compatible.

Turbulent Jet Model

The turbulent jet model is a generalized jet dispersion model that applies to discharges to unmoving water and streams with flows perpendicular to the outfall. The turbulent jet model is designed for near-field dispersion studies. No mention is made in the technical bulletin about the system requirements of the turbulent jet model.

Reference:

1. "Initial review of some outfall dispersion models and an asymptotic jet dispersion model for use in river systems." NCASI Technical Bulletin No. 486 (March 1986).

5.2.2 Dual First Order Long Term BOD Model

Type: Computer simulation.

Description:

In 1982 the National Council for Air and Stream Improvement, NCASI, tested several mathematical models to determine which best described the exertion of carbonaceous BOD with time for biologically treated effluent samples from paper industry facilities. The results of this work determined that the long-term de-oxygenation attributed to carbonaceous BOD of treated effluents was best represented by a dual first order model.

Equation [1] $$y = L_1 (1 - e^{-k_1 t}) + L_2 (1 - e^{-k_2 t})$$

The parameters k_1 and k_2 represent the de-oxygenation rates of carbonaceous BOD while L_1 and L_2 represent the magnitude of the ultimate carbonaceous BOD for the liable and refractory components of the waste. Typically, one fraction of carbonaceous BOD is exerted at a different rate from the other; hence the need for a treated effluent model with two different rates of de-oxygenation.

The model requires the estimation of the forementioned parameters. In order to do this NCASI has developed a computerized non-linear least squares algorithm. This program is considered easy-to-use and reliable although it is recommended that users routinely check program results for reasonableness.

Reference:

1. "A computerized non-linear least squares algorithm for estimating the parameters of the dual first order long term BOD model (NLS-DFO)," NCASI Technical Bulletin No. 633 (June, 1992).

5.2.3 RES -- Reaeration Expert System

Type: Computer simulation.

Description:

A self-documented program to estimate oxygen reaeration rates in rivers based on an extensive self-contained empirical database or user-supplied field data. In the main menu of the reaeration Expert System, there are four basic options available: (a) "Consult Samples" to enter data about the river in question, and search the sample data base for similar rivers in order to estimate a coefficient (K2); results are to be presented as a statistical plot. (b) "Consult Models" to enter data about the river in question and search the model database for a suitable equation which would provide an estimate of K2. (c) "See Info on Samples" to see some statistical information on the number of samples for which valid measurements are available, minimum and maxiumum values for that parameter, the average for that parameter, and the standard deviation for each sample database parameter)K@, depth, slope, flow, and velocity). (d) "See Info on Models" to review a description of the models and a graphic describing their forms.

Reference:

1. Hinton, S. 1994. Personal commmunication by electronic mail.

5.2.4 RIVER and FISH

Type: Computer simulation.

Description:

The model RIVER allows the user to estimate the concentration of dioxin in the receiving water on every day for which stream records are available. Dioxin is partitioned between aqueous and solid phases within river reaches designated by the user. Information from the river model is then used in the food chain model FISH to estimate the concentrations od dioxin throughout the aquatic food chain for trophic levels and aquatic species specified by the user. The programs require the user to provide supply flow and suspended solids records for river and effluents, dioxin concentrations in effluents, organic carbon fraction in riverine solids and information regarding the chain existing in each river reach. The model has been developed for riverine environments but not for lakes or estuaries.

Reference:

1. Hinton, S. 1994. Personal communication by electronic mail.

Availability:

For regulatory agencies and universities these programs may be obtained free of charge from: Dr. Hinton , NCASI Northeast Regional Center, Tufts University, Department of Civil and Environmental Engineering, Medford, Massachusetts 02155. Phone: (617) 627-3254; E-mail: SHINTON@pearl.tufts.edu

Requests for programs should include a floppy disk and be made in writing. NCASI does not support model studies not conducted by their membership.

5.3 Annotated Bibliography of Other Water Quality Modelling Accounts

1. Stevens, C., G. Lawrence, C. Rogers, and P. Hamblin. 1994. Modelling the thermal stratification of water-filled mine pits. Environment Canada Pacific and Yukon Regional Report MS 94-01.

This report details a current study that Environment Canada has undertaken to examine the hydrodynamic mixing of open pit mine waters. The study is determined necessary in order to evaluate the potential contamination of surrounding water resources in the event that the mines should flood. The contamination concern stems from the fact that many open-pit mines contain high heavy metals concentrations. The report describes the Brenda Mines pit site, the parameters that influence hydrodynamic mixing, and the mixed layer modelling that has been completed. In addition to the 12-page report are 11 figures and 6 appendices.

2. Piedrahita, R.H. 1990. Calibration and validation of TAP, an aquaculture pond water quality model. <u>Aquacultural Engineering AQEND</u> 6. 9(2): 75-96.

A computer model of water quality in aquaculture ponds (The Aquaculture Pond model, TAP) is described as it is calibrated and validated. Includes 8 figures, 3 tables, and 19 references.

6.0 Software Product and Information Request Form

Center for Exposure Assessment Modeling (CEAM)
U.S. Environmental Protection Agency (U.S. EPA)
Office of Research and Development (ORD)
Environmental Research Laboratory (ERL)
960 College Station Road
Athens, Georgia 30605-2700

706-546-3549

Type or print the information requested on this form. Date:____/____/____

CEAM Information to be sent to:

Circle One: Dr. Mr. Ms. Mrs.

Requester's Name: ______________________ Phone No ________

Organization: ______________________

Complete Address: ______________________

____

____

City, State: ______________________

Country/

Postal Code: ______________________

E-Mail Address: ______________________

There are no fees for CEAM software product distribution. CEAM has a diskette exchange Policy. CEAM must receive diskettes before shipping software products. Send appropriate number (see back or second sheet) of 3.5 high density (1.44 MB) disks to :

Model Distribution Coordinator
(at the above address)

Domestic requests are sent Fourth Class. Delivery time is approximately 10 days to 2 weeks from the date sent. Requests are processed on a first come, first serve basis by CEAM.

Foreign Requests are sent Air Mail. Estimated time of delivery varies greatly. Requests are processed first come, first serve basis by CEAM.

Note: CEAM does not send information via FAX

Software Product Acronym	Version Number	Release Date	Number of 3.5" HD Diskettes to send	Check ✓ This Column for Ordering	Documentation Status
ANNIE-IDE	1.14	Sept. 1991	1		NTIS
CEAMINFO	3.10	June 1991	1		* *
CLC Database	2.01	April 1992	1		* *
CORMIX	2.10	Oct. 1993	5		* * *
DBAPE	1.05	Oct. 1990	2		NTIS
EXAMSII	2.94	Jan. 1990	1		* * *
FEMWATER /LEWASTE	1.00	July 1993	1		* * *
FGETS	3.0.18	Sept. 1994	1		* * *
HSPF	10.10	Dec. 1993	6		* * *
MINTEQA2/ PRODEFAC2	3.11	Dec. 1991	2		* * *
MULTIMED	1.01	June 1991	4		* * *
OFFSPACE	1.61	Sept. 1991	1		* *
PATRIOT	1.10	April 1993	4		* * *
PLUMES	2.00	June 1993	1		* * *
PRZM2	1.02	Feb. 1993	2		* * *
QUAL2EU	3.20	Mar. 1994	2		NTIS
SYMPTOX3	2.01	Feb. 1993	1		* * *
SWMM	4.30	May 1994	2		NTIS
WASP	5.10	Sept. 1993	3		* * *

Software Product Acronym	Version Number	Release Date	Number of 5.25" DS/DD Diskettes to Send	Check ✓ This Column for Ordering	Documentation Status
GCSOLAR	1.10	Feb. 1988	1		* * *
LC50	1.00	Dec. 1986	1		* * *

* * No documentation, * * * Documentation contained on product diskette, NTIS = order from National Technical Information Service (information will be provided)