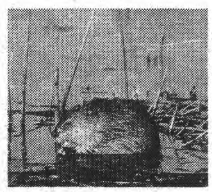
Canada Alberta Northwest Territories

Northern River Basins Study



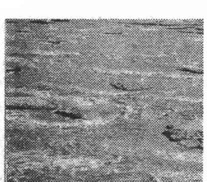


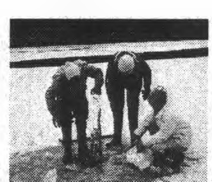





NORTHERN RIVER BASINS STUDY PROJECT REPORT NO. 82

A REVIEW AND EVALUATION OF WATER QUALITY AND QUANTITY MODELS USED BY THE NORTHERN RIVER BASINS STUDY







DATE DUE

Prepared for the
Northern River Basins Study
under Project 5327-D1

by

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Published by the
Northern River Basins Study
Edmonton, Alberta
March, 1997

CANADIAN CATALOGUING IN PUBLICATION DATA

McCauley, Edward, 1953-

A review and evaluation of water quality and
quantity models used by the Northern River
Basins Study

(Northern River Basins Study project report,
ISSN 1192-3571 ; no. 82)
Includes bibliographical references.
ISBN 0-662-24829-5
Cat. no. R71-49/3-82E

1. Water quality -- Models -- Alberta -- Athabasca River
Watershed.
2. Water quality -- Models -- Peace River Watershed
(B.C. and Alta.)
3. Water quality -- Models -- Slave River (Alta. and N.W.T.)
I. Northern River Basins Study (Canada)
II. Title.
III. Series.

TD387.A43M32 1997 628.1'61'0113 C96-980284-6

PREFACE:

The Northern River Basins Study was initiated through the "Canada-Alberta-Northwest Territories Agreement Respecting the Peace-Athabasca-Slave River Basin Study, Phase II - Technical Studies" which was signed September 27, 1991. The purpose of the Study is to understand and characterize the cumulative effects of development on the water and aquatic environment of the Study Area by coordinating with existing programs and undertaking appropriate new technical studies.

This publication reports the method and findings of particular work conducted as part of the Northern River Basins Study. As such, the work was governed by a specific terms of reference and is expected to contribute information about the Study Area within the context of the overall study as described by the Study Final Report. This report has been reviewed by the Study Science Advisory Committee in regards to scientific content and has been approved by the Study Board of Directors for public release.

It is explicit in the objectives of the Study to report the results of technical work regularly to the public. This objective is served by distributing project reports to an extensive network of libraries, agencies, organizations and interested individuals and by granting universal permission to reproduce the material.

NORTHERN RIVER BASINS STUDY
PROJECT REPORT RELEASE FORM

This publication may be cited as:

McCauley, Edward, Ecology Division, University of Calgary. 1997. ***Northern River Basins Study Project Report No. 82, A Review and Evaluation of Water Quality and Quantity Models Used By the Northern River Basins Study,*** **Northern River Basins Study, Edmonton, Alberta.**

Whereas the above publication is the result of a project conducted under the Northern River Basins Study and the terms of reference for that project are deemed to be fulfilled,
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F. J. Wrona — 11 Jan 96
(Dr. Fred J. Wrona, Science Director) — (Date)

Whereas it is an explicit term of reference of the Science Advisory Committee "to review, for scientific content, material for publication by the Board",
IT IS HERE ADVISED BY THE SCIENCE ADVISORY COMMITTEE THAT;
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P. A. Larkin — 11 Jan/96
(Dr. P. A. Larkin, Ph.D., Chair) — (Date)

Whereas the Study Board is satisfied that this publication has been reviewed for scientific content and for immediate health implications,
IT IS HERE APPROVED BY THE BOARD OF DIRECTORS THAT;
this publication be released to the public, and that this publication be designated for: **[ ] STANDARD AVAILABILITY [ ] EXPANDED AVAILABILITY**

Lucille Partington — 11/01/96
(Lucille Partington, Co-chair) — (Date)

Robert McLeod. — 11/01/96
(Robert McLeod, Co-chair) — (Date)

A REVIEW AND EVALUATION OF WATER QUALITY AND QUANTITY MODELS USED BY THE NORTHERN RIVER BASINS STUDY

STUDY PERSPECTIVE

Environments are constantly changing; that the aquatic environments contained within the Northern River Basins Study (NRBS) area were being changed as a result of development was not challenged. However, the ability to describe and predict those changes likely to arise from development continued to be a challenge to resource managers at the onset of the Study.

> ***Related Study Questions***
>
> *13a)* *What predictive tools are required to determine the cumulative effects of man made discharges on the water and aquatic environment?*
>
> *14)* *What long term monitoring programs and predictive models are required to provide an ongoing assessment of the state of the aquatic ecosystems. These programs must ensure that all stake holders hove the opportunity for input.*

Typically, the change that occurs within the environment like those found in the Peace, Athabasca and Slave rivers, take place over an extended period of time. Although not as evident or dramatic, the change and its effects can be just as substantive as those occurring within a shorter time frame; the changes are so subtle as to go unnoticed. A major difficulty for aquatic scientists working with these large aquatic systems is the lack of documented information covering a long period of time. The monitoring that was underway or done prior to the onset of the NRBS Study was disparate and information gaps existed.

For large, complex aquatic ecosystems like the Peace, Athabasca and Slave rivers, subjected to significant seasonal variation, scientists use tools like models to help them assess the consequence of changing one or many parameters. Models offer researchers and managers with the capability of being better able to understand and predict changes arising from development.

NRBS involved numerous researchers who applied a variety of tools to better understand processes taking place within the aquatic environment of the Peace, Athabasca and Slave rivers. As a multi-faceted study it was important to integrate the efforts and finds of the various researchers in an attempt to understand the cumulative effects of development on these rivers. This report presents a compilation and discussion of the models employed by NRBS researchers and how they could be applied to understand cumulative effects and improve the capability to predict future changes. Besides scoping the difficulties of water quality in the northern river basins and the shortcomings of developing working models that reliably simulate changes, the report describes and assesses models used by NRBS. General recommendations for future work are provided. The report concludes that; predictive transport models are significant tools to better handling of future progress in understanding and predicting cumulative effects; multi-disciplinary teams need to be established to address the difficultly of devising models to meet this challenge.

Information from this project was used to assist in the preparation of the NRBS Synthesis Report, *Cumulative Impacts within the Northern River Basins*" (NRBS Synthesis Report No. 11).

REPORT SUMMARY

Modelling water quality in the Peace, Athabasca, and Slave River Systems represents some fundamental challenges. These are large complex systems that are relatively oligotrophic, located at relatively high latitudes, and experience highly seasonal environmental fluctuations. This report summarizes the major modelling projects undertaken by the NRBS, provides a critical summary of major results, and makes recommendations for future work. Section 1.0 describes the scope of the problem of model water quality in the Northern River Basins and provides a summary of the models used by NRBS to predict key water quality variables. Section 2.0 provides a general overview of the utility and shortcomings of models of water quality with the goal of establishing key criteria for assessing the successes or failures of models developed by NRBS. Section 3.0 summarizes the key findings of NRBS models and evaluates the modelling results against the criteria outlined in Section 2.0. Section 4.0 presents a series of recommendations along with strategic suggestions for future work in the modelling of water quality in the Northern River Basins.

In Section 4.0, specific recommendations for modelling dissolved oxygen, transport and fate of contaminants, and distribution of contaminants in the food chain are summarized. General recommendations for future work include: 1) The development of predictive transport models for the Northern Rivers is of paramount importance for future progress. 2) Models need to be developed to predict the impact on the biota of changes in water quality. 3) A process-oriented database needs to be created and maintained for the modelling efforts in the Northern Rivers. 4) Management objectives with regard to scale of prediction need to be clarified, and these goals have to be carefully evaluated with respect to data availability. 5) More emphasis has to be placed on models of water quality that can be adapted to evaluate changes in water quality brought about by changes in the process technology of the pulp and paper industry. 6) Modelling teams need to be established, drawing experts from government, industry, and universities, to tackle the difficult interdisciplinary problems associated with the development of predictive water quality models.

ACKNOWLEDGMENTS

I would like to thank Dr. F.J. Wrona for his valuable suggestions and advice in the preparation of this report. Drs. Patricia Chambers, Terry Prowse, and Brian Brownlee provided extensive comments and suggestions. Tammy Rosner provided excellent technical support and offered constructive criticism for several modelling sections.

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1.0 <u>GENERAL INTRODUCTION</u>

1.1 Major Objectives and Questions

The aquatic ecosystems in the Northern Rivers Basin Study represent large, complex, and highly seasonal systems. NRBS is charged with gathering information on the water quality of Athabasca, Peace, and Slave River Basins. Development within the Basins is on-going, and one result of this development is the discharge of materials into the Northern Rivers by industries and municipalities. What is the effect of these discharges on water quality in the Northern Rivers? How can we assess the cumulative impacts of present and future development on water quality? These are the overarching questions addressed by NRBS, and work on Synthesis/Modelling has complemented and extended the extensive empirical results obtained by NRBS to answer these two important questions.

1.2 Challenges For NRBS

Modelling water quality in the Peace, Athabasca, and Slave River Systems represents some fundamental challenges. These are large complex systems that are relatively oligotrophic, located at relatively high latitudes, and experience highly seasonal environmental fluctuations. The vast extent of the rivers, covering 1000's of kilometers, implies extensive spatial heterogeneity in flow regimes, substrates, extent of vertical and horizontal structure, geological and landscape influences, and point source inputs from tributaries and streams. The complexity arising from spatial heterogeneity is magnified by the highly seasonal environmental variation that produces distinct hydrological periods in the Athabasca and Wapiti-Smoky Rivers (e.g. the winter period of ice-cover featuring low turbidity and potentially low dissolved oxygen concentrations, the spring/early summer period of rising hydrograph with high turbidity, and the late-summer autumn period of falling hydrograph and high water clarity). This spatial and temporal heterogeneity can have profound effects on the fate and impact of industrial discharges on the diverse biotic communities found in these rivers. It is easy to appreciate how the vast spatial extent and highly dynamic environments of these rivers bedevils our ability to model water quality.

Much of the effort in modelling water quality has been focused on smaller, more eutrophic rivers in more southerly latitudes with much less seasonality (e.g. ice-cover) (see Appendix 1). Can models developed for southern rivers be simply transferred to our Northern Systems? River systems, in general, clearly share a variety of properties and processes, but what are the major problems associated with effecting this transfer? For example, can model coefficients or parameters be simply scaled to take into account the dramatic differences in average temperature or seasonal variance in important input variables found in our Northern Rivers? Are there any anticipated changes in model structures that need to be invoked, when models are transferred to these large northern rivers? Second, the amount of biological, chemical, and physical information on basic processes in these Northern Rivers is limited compared with more southern counterparts. The availability of data on the composition and seasonal dynamics of the biotic communities, feeding relationships, patterns of movement for mobile species, limits of productivity etc. affects both model formulation and parameterization. A major question for the Synthesis/Modelling Component is whether sufficient information, data, and models exist to predict and assess the impact of development on water quality in the Northern Rivers. The effects of point-source discharges have to be distinguished from the natural spatial and temporal variability in the composition of communities and the dynamics of aquatic populations.

A final important question considers the spatial scale for predicting the effects of industrial and municipal discharges on water quality. At a first glance, the answer to this question might appear to be obvious. We are considering the effects of point-source discharges from industrial or municipal operations. Predicting local changes in water quality and the biotic communities would seem paramount. But, how can we objectively identify a spatial scale for these "local" effects in these large flowing systems and how can we objectively distinguish impacts caused by point-source effluents from natural variation in the structure or composition of the biotic communities or the influence of non-point source inputs? Life-stages of some fish species are highly mobile in the Northern Rivers. During their sojourns, these fish are "integrating" over potentially large spatial scales, and a model that does not take into account this integration of exposure to a variety of environments could severely underestimate or overestimate potential responses. Over what spatial and temporal scales can we average responses to understand and assess the impact on biotic communities?

These introductory paragraphs simply raise some key issues associated with modelling water quality in the Northern Rivers. To some extent, NRBS is breaking new ground in that it is one of the first integrated studies designed to assess the impact of a broad range of industrial and municipal discharges on the water quality of large, northern rivers. It is important to recognize from the outset that model formulation and parameterization has occurred in parallel with the gathering of basic empirical information on physical, chemical, and biological features of the Northern Rivers. The paucity of data severely restricts the level and scale of predictive power that we can expect from our water quality models.

This Synthesis Report will briefly summarize the modelling approaches and rationale used in NRBS (Section I), discuss the general issues concerning utility and short-comings of modelling water quality (Section II), summarize the strategic results of models developed by NRBS (Section III), and evaluate the progress made in the modelling components, and look to the future regarding further developments and requirements to achieve the goal of understanding and predicting the impact of discharges on water quality in the Northern Rivers (Section IV). The NRBS modelling results, which form the basis for this synthesis report, are drawn from Technical Reports available as of 1 November, 1995.

1.3 Water Quality Modelling

Man-made discharges contain a variety of compounds and materials that could have an impact on the aquatic environment. Our ability to assess the effects of these discharges, and to distinguish these effects from natural influences, is greatly enhanced by using models that can: (1) predict the changes to the environment brought about by the industrial discharges and (2) predict how these environmental changes affect the growth, reproduction, mortality, and dispersal of aquatic species. The first-stage models predict the distribution and fate of industrially discharged materials or compounds. They consider, for example, how concentrations of discharged organic contaminants are affected by processes such as physical transport, or chemical and biological transformations. These transport/fate models can predict environmental concentrations of contaminants that can be used to assess the exposure of various organisms in the rivers to the contaminants. In addition, these models can be used to predict how discharged materials modify the physical/chemical environment (i.e. concentrations of nutrients or dissolved oxygen) that directly influence water quality for various aquatic species by either stimulating productivity or creating adverse environmental conditions. The accurate prediction of how man-made discharges affect environmental concentrations of contaminants or key water quality variables is essential for both predicting potential impacts on the biota and establishing a causal link between the discharges and changes in the aquatic ecosystem.

Predicting the response of the biota to changes in environmental factors (stage 2) produced by discharges requires the identification of appropriate endpoints and models to predict effects on these endpoints. Man-made discharges contain materials and compounds that could alter the quality of the environment for all major biotic components (e.g. benthic flora and fauna, fish species, planktonic algae and invertebrates). NRBS has investigated the biological responses of various components of the river systems (e.g. potential effects of enrichment and/or exposure to contaminants on benthic primary and secondary production , effects of dissolved oxygen concentration on survivorship of bull trout and mountain whitefish). However, the response of fish species has been identified as one key endpoint for assessing the impact of changes in water quality. This choice does not ignore the potential effects on the other food-chain constituents, but it simply emphasizes that the well-being or state of the fish populations provides an obvious important indicator of water quality for the residents of the Northern River Basins (Synthesis/Modelling Report 8.1).

To evaluate the cumulative effects of man-made discharges on the aquatic environment, NRBS collected extensive empirical information on physical, chemical, and biological features of the Northern Rivers (Synthesis Reports I-VII). These data are essential for understanding the state of these aquatic systems, and they provide valuable observations for the development of environmental models to predict the potential effects of man-made discharges. Modelling efforts focused on three major topics:

1) Modelling Dissolved Oxygen Concentrations

2) Modelling the Transport and Distribution of Organic Contaminants
3) Modelling the Fate of Organic Contaminants in Aquatic Food-Chains.

These modelling efforts reflect some of the most important concerns related to industrial discharges of organic materials: 1) potential reduction of dissolved oxygen concentrations via the biological oxidation of organic matter that could influence the survival of fish populations, and 2) contamination of aquatic biota (including potential biomagnification by fish) by toxic organic compounds including dioxin/furans and other organochlorines. All natural waters receive a variety of contaminants from erosion, leeching, and weathering processes. An important goal of developing sound, reliable, predictive models of water quality is to assess the relative impact of industrial discharges compared with natural sources.

Besides these major modelling efforts, work progressed on the development of a hydraulic model for the Northern Rivers (Synthesis Report VI), as well as the completion of a simple Spill-Response Model that could be used by water managers in the case of an accidental point-source spill along the river. In addition, benchmark experiments were performed to assess the potential role of nutrient enrichment in limiting productivity in Northern Rivers (Synthesis Report III), and these data provide valuable observations for future modelling efforts on the potential effects of nutrient discharges from industrial and municipal sources on water quality.

1.4 Specific Models in NRBS

This section summarizes the models employed or developed by NRBS to predict key water quality variables. The primary description of each model and their detailed results can be found in Technical Reports (**1.** Chambers et al. 1995, **2.** Golder Associates 1995, **3.** CanTox Inc. 1995, **4.** Hicks et al. 1994) and NRBS Synthesis Reports (I, III, and VI).

1.4.1 Modelling Dissolved Oxygen

Dissolved oxygen was modelled with one of the simplest possible analytical approaches based on the original Streeter-Phelps equations, which assume that rates of consumption and production of oxygen can, in essence, be modelled as first-order reactions (i.e. rates proportional to concentrations of reactants). The model DOSTOC, originally developed for Alberta Environment (HydroQual Consultants Inc and Gore & Storrie Ltd; Zielinski 1988), was used to predict average water column levels of oxygen for under-ice periods in the Athabasca River. A basic description of the major assumptions of the model is shown in Table 1.1. This model considers how rates of oxygen production and consumption in the water column are influenced by biological oxygen demand (BOD), respiration, photosynthesis, sediment oxygen demand (SOD), and reaeration. It assumes that mixing of effluent and input from tributaries is complete and instantaneous (i.e. the turbulence is sufficient to allow the concentration of BOD and dissolved oxygen to be uniform throughout the cross-section of the river and longitudinally within a reach). In essence, the model "follows" a volume of water as it moves down the river, through a series of reaches. The travel time for each reach is determined using Leopold-Maddox relationships for velocity, depth, and river width versus flow for a given reach. Along this sojourn, oxygen is consumed by biological oxygen demand, respiration, and sediment oxygen demand. The biological oxygen demand in the water column is calculated as the balance of inputs and outputs (sedimentation, adsorption, and decay). In the application of DOSTOC to the Athabasca River, consumption of oxygen via the conversion of ammonia to nitrate is considered unimportant, and the stochastic capabilities of the model are exploited to determine confidence limits for predictions by considering uncertainty in model inputs and parameters.

A major virtue of this model is that the input data requirements are relatively small compared with other approaches (see Appendix 1). Table 1.2 from Technical Report 1 summarizes the sources of data used for the application of DOSTOC in the Athabasca River. It is important to note that there are no "free" fitting parameters in the analysis. This is not to say that some assumptions were not needed to be made in assigning parameter values (e.g. assumptions concerning reaeration under-ice, temperature correction of kinetic rates, conversion of areal estimates of sediment oxygen demand to volumetric rates). An attempt was made to provide best estimates of parameters <u>prior</u> to predicting changes in dissolved oxygen concentration, and these parameters were not changed in subsequent model runs. This approach enables a direct interpretation of model successes and failures. [Please note: parameterization methods and subsequent limitations on interpretation are discussed in Section 2 of this Synthesis Report.]

Table 1.1. Summary of major features and assumptions of DOSTOC model

	Description	**Comments**
Physical Representation	-river represented as one-dimensional system -river length subdivided into series of connected segments - one tributary is modelled the others are considered inputs	- reaches assumed to be homogeneously mixed - no dispersion between reaches - first reach after an industrial inflow assumed to be ice free
Hydraulic Configuration	- average discharge for the modelled time period for each year is used - water column velocities and depth are calculated using Leopold-Maddox method	- discharge data was collected -velocity is uniform for each reach
Processes	- decay and sedimentation of BOD modelled as first-order rates - SOD and respiration are constant amounts independent of do concentration - NOD not considered - reaeration depends on velocity and temperature for ice-free reaches and is constant for ice covered reaches -statistical moments for predictions (mean, variance, etc) determined explicitly based on Zielinski (1988)	- BOD decay estimated from BOD_5 and are temperature adjusted -Rate constants and parameters are uniform for each reach - Decay rate changes in a reach with an input source. The new rate is that of the effluent of the new input - BOD is temperature corrected - reaeration calculated from reference flow and temperature -stochasticity incorporated by considering processes as being stochastic - initial conditions regarded as random variables, random variability associated with reaction rate coefficients

Table 1.2. Sources of Data for Parameter Estimates for DOSTOC (Chambers et al. 1995)

Parameter	Source of data
Atmospheric reaeration	0.001 day^{-1} at reference temperature of 20^0C and reference flow of 50 m^2/s (after Macdonald *et al.* 1989)
BOD decay rate	Mean annual decay rates for mill effluent obtained from each pulp mill. Decay rates set to 0.026 day^{-1} for sewage effluent and O.026 day^{-1} for tributaries and headwater.
BOD sedimentation rate	Sedimentation was calculated using Krisnappen *et al.* (1995) transport rates from below Hinton. In the absence of data for settling rates below other mills on the Athabasca River, the Hinton values were applied to all other mills.
BOD_5	Industrial, sewage, headwater and tributary data (expressed as mg/L) collected during the Alberta Environment winter water quality surveys.
BOD_u:BOD_5	Mill effluent rations obtained from the pulp mills. Ratio set to 7.80 for sewage and to 8.03 for tributaries and headwater at reference temperature of 20^0C.
Diffuse Loading	No data; set to 0 tonnes/km/day
DO	Collected during the Alberta Environment winter water quality surveys (expressed as mg/L)
Nitrogenous oxygen demand (NOD)	No data; set to 0 mg/L/day.
Effluent discharge	Obtained from the industries and sewage facilities (expressed as m^3/s).
River discharge	Obtained from Technical Services Division, Alberta Environment and Water Survey of Canada (expressed as m^3/s).
Sediment oxygen demand (SOD)	SOD ($g/m^2/day$) was measured *in situ* during the 1989, 1990, 1992,1993,1994, and 1995 winters (Casey & Noton 19989; Casey 1990; Monenco Inc. 1992; HBT Agra Ltd. 1993a,b; HBT Agra Ltd. 1994; Noton 1995). Mean SOD ($g/m^2/day$) from these years were plotted and values chosen at the midway point of each modelled reach. Areal SOD ($g/m^2/day$) was converted to volumetric SOD (mg/L/d) by multiplying by the average water depth. Since SOD was measured *in situ* at 0^0C all values were temperature corrected to 20^0C to fit the model requirements.
Time of travel	The Athabasca River was divided into nine hydraulic reaches (Macdonald & Hamilton 1989) and Leopold-Maddock coefficients were derived for each reach from HEC-2 simulations using under-ice time-of-travel and river cross-sections measured by Andres *et al.* (1989) and Haufe & Croome (1980). The Leopold-Maddock coefficients were then used to estimate reach-average travel time (days) and reach average depth (m).

In addition to the application of DOSTOC, statistical models were developed that describe how oxygen concentration declines in relation to distance along the Athabasca River from Hinton to Grand Rapids and from Grand Rapids to Lake Athabasca, for the years 1988-1993. The slopes of these regression relationships can be used to characterize rates of change of oxygen concentration with distance over large scales, and rates obtained for the Athabasca River were compared with rates observed in other ice-covered rivers receiving industrial effluent. The applicability of these statistical models for predicting changes in oxygen concentration is discussed in Section 2 and Section 3.

1.4.2 Modelling Contaminant Fate

The fate and transport of organic chemicals was modelled for the Athabasca and Wapiti/Smoky Rivers (Synthesis Report I and Technical Report 2) using the Water

Quality Analysis Simulation Program (WASP) developed by the U.S. Environmental Protection Agency. This is a highly complex simulation model, which allows the flexibility of employing different features or levels of complexity depending on the availability of data to describe accurately habitat structure, inputs, transport/fate processes, and parameters.

This study focused on seven selected organic chemicals in the Athabasca River and the Wapiti/Smoky Rivers:
1) 2,3,7,8 tetrachlorodibenzofuran (2,3,7,8,-TCDF)
2) dehydroabietic acid (DHA)
3) 12,14 dichlorodehydroabietic acid (12,14-dichloro-DHA)
4) 3,4,5 trichlorocatechol (3,4,5-TCC)
5) 3,4,5 trichloroguaiacol (3,4,5-TCG)
6) 3,4,5 trichlorovertrole (3,4,5-TCV)
7) Phenanthrene.

To predict the transport and fate of these contaminants, WASP combines three components: 1) a physical representation of the river system 2) algorithms describing the transport of water and material and 3) a structure for describing the transformations of organic compounds and their transfer between media or phases. In other words, the model provides a quantitative description of transport through the system, reactions within the system, and transfers of contaminants from one environmental phase to another. The major assumptions of the model as implemented for the Northern Rivers (Athabasca and Wapiti/Smoky) are summarized in Table 1.3.

The Northern Rivers were represented as one-dimensional systems (i.e. river completely mixed vertically and laterally). The length of the river was subdivided into a series of segments ranging from 4-7 kilometers in length. Each river segment is further represented by two interconnected compartments (a sediment bed and its overlying water). Bed sediments were composed of two solids: an inert coarse sediment that does not affect sorption of organic chemicals and a fine sediment that can both sorb organic chemicals and be transported. River flows were dynamic on a daily time-scale. To accommodate the effects of flow variation, the velocity, depth, and width of the river were calculated at each time step (Technical Report 2). For this purpose, the Athabasca and Smoky/Wapiti Rivers were divided into 15 and 4 hydraulic reaches, respectively, and Leopold-Maddox coefficients assigned for each hydraulic reach based on winter (under-ice) conditions.

In modelling the Athabasca River, the length of the river (~1160 km) was subdivided into 210 segments consisting of a water column segment overlying a corresponding bed segment. The length of the segments was chosen to arrive at segments with similar travel times. The physical representation of the Athabasca also included inputs from tributaries and industrial discharges. One major tributary (the Lesser Slave River) was treated explicitly and schematized in a similar manner as the Athabasca River (i.e. river divided into 12 segments and concentrations simulated). The physical representation of the

Wapiti/Smoky Rivers followed the same governing principles and the ~250 km river was subdivided into 95 segments.

A variety of fates was described for the organic contaminants (Table 1.3), which were treated as neutral species (i.e. no ionization was permissible). These fates include: sorption of contaminants to dissolved organic carbon in the water column and porewater; sorption to organic carbon in suspended and bed sediments; volatilization (except under ice-cover); hydrolysis and oxidation; and biodegradation in both water column and bed sediments. This implementation of WASP only considers chemical factors that transform contaminants (e.g. hydrolysis, oxidation/reduction) or influence their distribution in various phases that may be subject to differential transport (e.g. sorption processes). Biologically mediated transfers and transformations (e.g. metabolism by microorganisms, assimilation and excretion by various taxonomic groups) are considered separately in a Food Chain Model (see below).

Because this is a dynamic model, the input conditions are extensive (e.g. time-series of water flows, sodium concentrations, total suspended solids, and organic chemicals for upstream boundary conditions and tributaries where appropriate). In addition, the equilibrium partitioning assumption, used to describe the distribution of contaminants between dissolved chemical, DOC-bound chemical, and solids-sorbed chemical, requires that the dissolved organic carbon (DOC) and the fraction of organic carbon (FOC) in fine solids be specified for each river segment. The sources of data for the extensive input conditions, along with details of necessary calculations and interpolations caused by limited observations, are presented in Technical Report 2.

The model analysis proceeded by calibrating the model using 2 years worth of data for both the Athabasca River (1992 and 1993) and the Wapiti/Smoky Rivers (1990 and 1991). To confirm the mass balance of the model, each river was calibrated using changes in sodium concentration (a conservative substance). The dynamics of total suspended solids (TSS) were calibrated by inputting a time-series of settling rates. Following these two steps, WASP was then calibrated for the seven organic chemicals. Initial parameter estimates for chemical processes were drawn from the literature and the rationale/justification for parameter choices is provided in Synthesis Report I. It is important to note here the fundamental dichotomy in approaches between modelling dissolved oxygen and modelling the transport and fate of contaminants. In modelling dissolved oxygen, all parameters were derived from best estimates using data that originated largely within the Northern Rivers. Once parameterized using the independent data, the dissolved oxygen model was tested against observed changes in dissolved oxygen in the Athabasca River. Because of the paucity of data and the large difference in complexity between WASP (a dynamic model possessing many compartments with diverse chemical species and processes) and DOSTOC (a steady-state, "parameter sparse" model), this approach was not feasible for modelling the fate of chemical species. All of the existing data (both from internal and external sources) was needed to either estimate parameters or refine literature values for the Northern Rivers. Thus, the initial model construction "consumed" all of the available data, and there are no independent data available to test either the predictions of the model or the modified parameter values needed to calibrate the model. The general issues associated with this problem will be discussed in Section 2 and recommendations for future work will be presented in Section 4.

Table 1.3. Summary of Major Assumptions for the Implementation of WASP in the Athabasca River and the Wapiti/Smoky System

	DESCRIPTION	COMMENTS
PHYSICAL REPRESENTATION	◆ RIVER REPRESENTED AS ONE-DIMENSIONAL SYSTEM ◆ RIVER LENGTH SUBDIVIDED INTO SERIES OF CONNECTED SEGMENTS ◆ EACH RIVER SEGMENT SUBDIVIDED INTO TWO COMPARTMENTS: SEDIMENT BED AND OVERLYING WATER ◆ VOLUME OF SEDIMENT CELL VARIABLE ◆ BED SEDIMENTS REPRESENTED BY TWO SOLID TYPES (FINE AND COARSE)	➪ LENGTHS RANGED FROM 4-7 KM AND DETERMINED BY EQUALIZING HYDRAULIC RESIDENCE TIME DURING LOW FLOWS ➪ RIVER WATER ASSUMED TO BE COMPLETELY MIXED VERTICALLY AND LATERALLY WITHIN A SEGMENT
HYDRAULIC CONFIGURATION	◆ DAILY FLOWS USED ◆ DYNAMIC FLOW ROUTING NOT IMPLEMENTED ◆ WATER COLUMN VELOCITIES, CELL VOLUMES, AND MASS EXCHANGE AREAS UPDATED USING THE LEOPOLD-MADDOX METHOD ◆ BED CELL AREAS REMAIN CONSTANT, VOLUMES VARY IN RESPONSE TO DESCRIBED PATTERNS OF DEPOSITION AND EROSION	➪ SUITABLE FOR GRADUALLY VARYING FLOWS ➪ LEOPOLD-MADDOX COEFFICIENTS ESTIMATED FOR EACH HYDRAULIC REACH OF THE ATHABASCA AND WAPITI/SMOKY RIVERS ➪ COEFFICIENTS BASED ON FLOWS DURING WINTER ➪ RESIDENCE TIME IN BED CELLS >> WATER COLUMN
CHEMICAL PROCESSES	◆ CHEMICALS MODELLED AS NEUTRAL SPECIES ◆ SORPTION TO ORGANIC CARBON IN SUSPENDED AND BED SEDIMENTS ◆ SORPTION TO DISSOLVED ORGANIC CARBON IN WATER COLUMN AND PORE WATER IN SEDIMENTS ◆ VOLATILIZATION POSSIBLE DURING ICE-FREE SEASONS ◆ HYDROLYSIS AND OXIDATION IMPLEMENTED AS FIRST-ORDER KINETIC PROCESSES ◆ PHOTOLYSIS NOT INCLUDED ◆ BIODEGRADATION CONSIDERED TO BE A FIRST-ORDER KINETIC PROCESS	➪ IONIZATION NOT CONSIDERED ➪ ORGANIC CARBON PARTITION COEFFICIENT (K_{oc}) USED TO DESCRIBE PARTITIONING BETWEEN DISSOLVED PHASE, SEDIMENT ORGANIC CARBON, AND DISSOLVED ORGANIC CARBON ➪ TWO-LAYER RESISTANCE MODEL USED FOR VOLATILIZATION ➪ TEMPERATURE CORRECTIONS FOR RATE PROCESSES

1.4.3 Modelling the Distribution of Contaminants in the Food Chain

A primary objective of the previous model is to predict the distribution and fate of a variety of organic contaminants in the environment (i.e. predict concentrations of contaminants expected in different environmental compartments such as water column, bed sediments etc.). A major question is whether these predicted concentrations can be used to predict the distribution of contaminants through the food chains in the Northern Rivers.

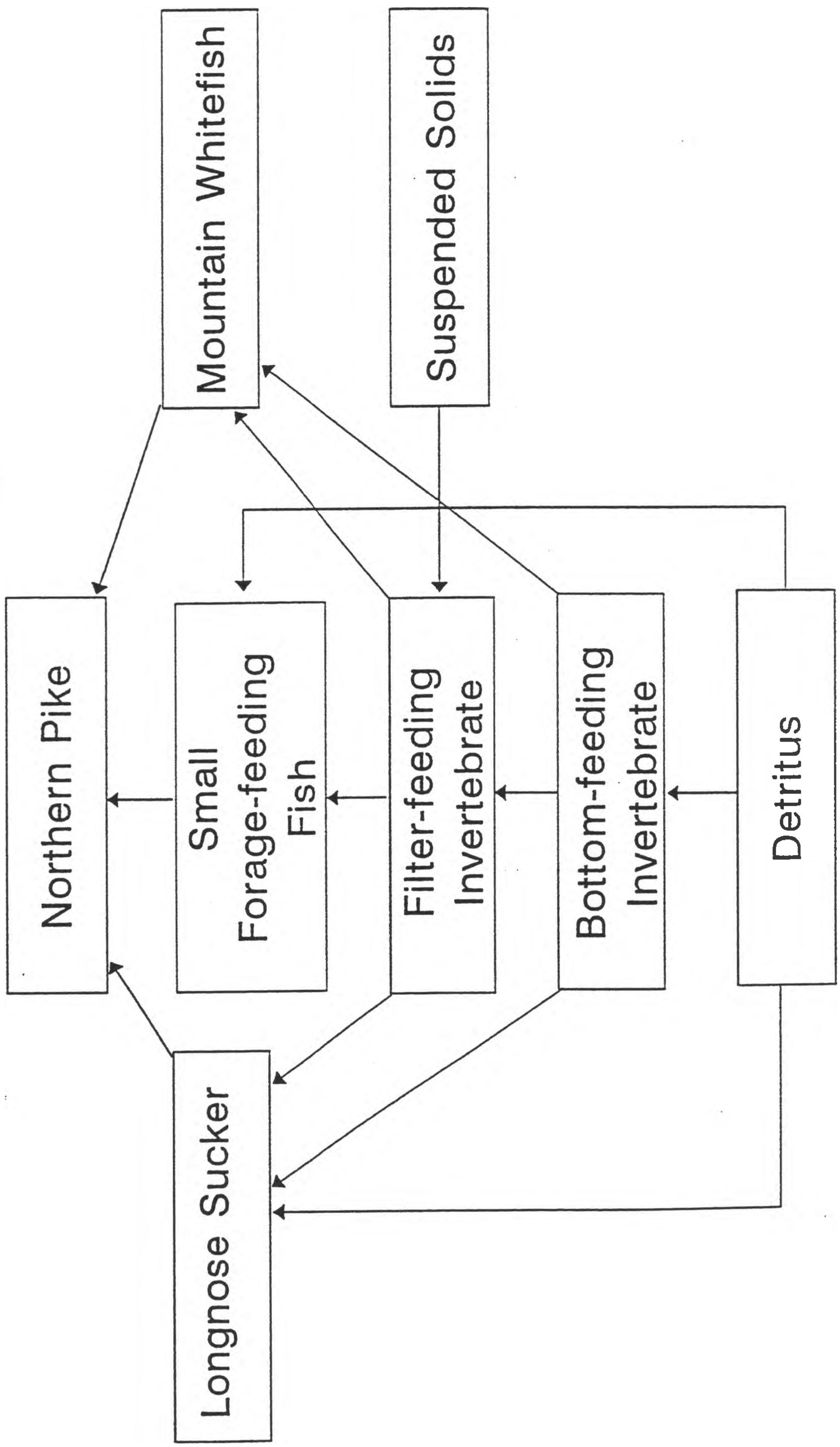
A food-chain model for the Northern Rivers was developed based on a bioenergetic model (Technical Report 3). Unlike the contaminant fate model (WASP), the food-chain model is a steady-state model designed to simulate the uptake and bioaccumulation of 6 of 7 organic contaminants modelled with WASP (2,3,7,8 tetrachlorodibenzofuran (TCDF), dehydroabietic acid (DHA), 12,14 dichlorodehydroabietic acid (12,14-dichloro-DHA), 3,4,5 trichlorocatechol (3,4,5-TCC), 3,4,5 trichloroguaiacol (3,4,5-TCG), and 3,4,5 trichloroveratrole (3,4,5-TCV)). The lack of information on spatial and temporal dynamics of the biota (including age-specific diet shifts etc.) precludes the formulation of a dynamic model.

Model formulation requires three types of information: 1) a description of feeding interactions for major species in the Northern Rivers; 2) mechanisms of uptake via non-feeding routes; and 3) excretion rates of organic contaminants. Information on feeding interactions is crucial for understanding exposure routes in the Northern Rivers. A simple food-web was constructed for the Athabasca River (Figure 1.1) based on observations drawn from the Northern Rivers (including data from the Athabasca River and the Wapiti/Smoky Rivers). Gut content analysis provided the basis for the food-web configuration. These predator-prey relationships describe distinct exposure pathways for the three species of fish considered in the model (mountain whitefish, longnose sucker, and northern pike). By considering the relative consumption rates of fish on benthic invertebrates or filter-feeding invertebrates and uptake from media, the model can calculate expected levels of organic contaminants resulting from exposure to constant concentrations of organic contaminants in abiotic media (i.e. water column dissolved, porewater dissolved, suspended-sediment adsorbed, and detritus adsorbed chemical concentrations). Thus, the distribution of contaminants through the food-chain can be predicted by inputting the observed concentration of the organic contaminants in the abiotic media, and using information from feeding pathways and rates of uptake and excretion by species.

The Thomann-Connolly (1981, 1984) approach models the concentration of contaminant for each constituent species of the food-chain. The rate of change of tissue concentration is determined from the balance of input rates (uptake via direct exposure and uptake via diet) and outputs (excretion rates from the organism and dilution of tissue concentrations due to growth). Uptake via direct exposure is a first-order process dependent upon contaminant exposure concentrations. Uptake via prey ingested is based on two components: 1) a calculated daily consumption rate of prey based on a consideration of

Figure 1.1

Feeding Interactions Modelled for Athabasca River Ecosystem



From CANTOX (1995)

the individual achieving an intake sufficient to grow at a specified rate given inefficiencies in assimilation and losses due to respiration, and 2) the assimilation efficiency of the organic contaminant under consideration. Weight-specific bioenergetics are central to the calculation of the "uptake via prey ingested" term in the equation. Finally, the loss rate is composed of two components: 1) loss due to excretion of the organic contaminant by the individual, and 2) dilution of tissue concentration via growth of the individual.

Biological parameters for the bioenergetics model were based either on data collected directly in the Northern Rivers (e.g. %lipid composition, growth rates etc.) or derived from general bioenergetic relationships drawn from the literature (e.g. allometric relationships for respiration rates or growth rates). Chemical parameters relating to the assimilation efficiencies of organic contaminants or excretion of these contaminants were determined from studies performed by NRBS and drawn from literature observations (Technical Report 3). Parameter estimates for TCDF were judged the most reliable, and there were considerable gaps in the data for the other classes of organic contaminants (i.e. resin acids and chlorinated phenolics).

Model predictions were derived for sites in the Athabasca River using observed input concentrations in the abiotic media and estimates of parameter values, and then compared with the observed distribution of contaminants in the food chain. Suspect parameters were subsequently adjusted to calibrate the model against the existing data for benthic feeding invertebrates, filter-feeding invertebrates, mountain whitefish, longnose sucker, and northern pike. Model predictions do not consider errors in parameter estimates (i.e. point estimates are predicted without any estimate of reliability). The major goals were to predict the distribution of the different organic contaminants in the food chain and to identify the primary exposure pathway for the different contaminants via sensitivity analysis.

1.4.4 Hydraulic Model of the Peace River (The final version of all sections on Hydraulic Modelling in this Synthesis Report will be completed with input from Dr. Terry Prowse, National Hydrology Research Institute, and the major discussion of the models and empirical foundation for this topic is presented in Synthesis Report VI. A brief presentation of the models is provided in this Synthesis Report because of the relevance for predicting water quality).

From the perspective of predicting water quality, hydraulic models provide both understanding and predictions of water levels, velocities, and discharges occurring at any point along the river and as a function of time. As described above in the contaminant/fate model, these quantities represent important inputs for calculating transport of materials and the volumetric or areal rates of processes that affect the creation or destruction of key water quality variables. A hydraulic flood routing model was developed for NRBS (Hick et al. 1994) for the Peace River from ~28 km downstream of the Bennett Dam to Peace Point in Wood Buffalo National Park (~1,000 km distance).

A major objective was to develop the input database for river geometry for the hydraulic model (based on data from topographic maps) and hydrologic data (i.e. tributary inflows). The geometric database consisted of channel distances, effective bed profile, channel widths, and channel resistance. Channel resistance (as estimated by Mannings n) was the only calibration parameter. Only a fraction of the streams entering the Peace River are gauged, and for consistency, the tributary inflows used in the hydraulic flood routing model were identical to the hydrologic flood routing model used by Alberta Environmental Protection (Hicks et al. 1994).

A one-dimensional model was developed based on the St. Vennant equations adapted for the situation in which a rectangular cross section of varying widths was assumed. For numerical analysis, the model uses a Petrov-Galerkin finite element method.

Two test scenarios were identified to evaluate model performance (the 1980 spring run-off event and the 1987 summer flood event). The decision to use these relatively simple scenarios, involving diffusive waves, was based on the relative availability of hydrologic data for the Peace River. Thus, this test provides a critical evaluation of the underlying hydraulic model for "moderate" events, with the view of future tests being conducted on the models capability to handle highly dynamic flood events, such as those associated with dam break floods or surges resulting from ice-jam releases (Hicks et al. 1994).

Before summarizing the results of the models in NRBS, it is important to discuss the utility and shortcomings of models. This discussion will assist in the objective evaluation of the successes and failures of the NRBS modelling programme.

2.0 UTILITY AND SHORTCOMINGS OF MODELS

2.1 Goal

To predict changes in water quality or ecosystem health, we need to predict the spatial and temporal dynamics of key water-quality variables, such as dissolved oxygen, contaminants, and nutrients, that potentially affect biotic components of the river systems (e.g. fish, benthic invertebrates, algae). There are two coupled modelling enterprises hidden in this simple statement. First, we need models to predict how inputs to rivers (e.g. effluents from pulp mills or sewage treatment plants, year-to-year variation in headwater inputs or discharges) alter or modify levels of environmental variables that are expected to affect the state of the system. Second, we need models to link the level of these variables to biological responses of species, where the principle effects on the biota are measured or perceived. For example, we require models to predict the dynamics of dissolved oxygen concentration in rivers (stage 1) in order to predict potential impacts (stage 2) on fish populations that are sensitive to low dissolved oxygen concentrations at particular points in their life-cycle. Similarly, we need models to predict the fate of contaminants (e.g. organic chemicals) added to the river and how the concentration of these contaminants become distributed throughout the food chain. The second modelling stage then considers the effects of these contaminant concentrations on the biota, including humans that are exposed to the contaminants via consumption of fish from the rivers. Thus, modelling efforts can be separated logically into modelling the fate of inputs to the rivers and the subsequent effects that changes caused by these inputs have on the biota.

It is fair to say that many members of the public and the scientific community have a healthy "skepticism" for the utility of mathematical models in predicting changes in environmental quality or ecosystem health. This skepticism ranges from mild apathy to scathing ridicule. Its sources are easy to understand. In the last three decades, we have been inundated with dire predictions from environmental models concerning global warming, acid rain, effects of toxic chemicals, and ozone depletion. Predictions from these models are often contradictory or disagree, and change from one period of time to another! We have also witnessed the disastrous outcomes that often accompany the development of policy based on these mathematical models (e.g. collapse of the cod fishery). Finally, there are two very popular perceptions that, at first glance, may seem contradictory but are really just views from different vantage points. Many scientists see models as being too simplistic to be able to capture real responses of natural systems to perturbations (i.e. natural systems are so complex that the process of simplification required to construct models renders them useless). In contrast, other scientists and many members of the public see these environmental models as being so complex that they can provide any desired prediction merely by "tweaking knobs" to get the "right" answer.

It is obviously important to be skeptical about the utility of mathematical models; we need tools for prediction that we can rely on to assist in making decisions or formulating environmental policies to manage the aquatic environments in the Northern River Basins. But, it is also important to put this skepticism into a realistic perspective of the existing knowledge and data concerning processes affecting water quality in the Northern Rivers. Our modelling effort is simply one part of a much larger scientific enterprise addressing the Study Questions posed in NRBS. Models have a variety of uses and it is crucial to discuss their utility and shortcomings in the context of NRBS.

2.2 Uses of Models

Mathematical models play a central role in environmental assessment, hazard or risk assessment, and decision making. In environmental assessments, we use predictive models to evaluate how potential inputs to the river systems might influence water quality. These models improve our ability to anticipate changes in water quality caused by perturbations from inputs, and also to evaluate the possibility that the observed changes in water quality simply reflect natural variation that is independent of the changes to the inputs to the river system. Helping to establish, or possibly eliminating, the causal link between inputs from development and water quality changes is a central concern in the decision-making or regulatory process. In risk assessment, models play an essential role in calculating levels of exposure for target organisms or groups by understanding the fate of contaminants, once these hazardous compounds have been identified, and determining the effects of exposure levels on the biota. In both of these cases, we are asking models to predict how inputs to the system under consideration affect state variables that have been identified as being key indicators of ecosystem health or endpoints of particular concern (e.g. health of both aquatic organisms and terrestrial wildlife that may be exposed to stressors) (see Synthesis Report 8-1). Ultimately, many agencies depend on models to organize, understand, and utilize the information available for regulatory decision making (e.g. Suter et al. 1993).

In the context of NRBS, models have a variety of uses and these are of direct importance to answering almost all of the Study Questions. First, models provide a compact, economical description of dynamics of key water-quality variables (e.g. dissolved O_2 concentration, tissue concentrations of contaminants in fish, quality of drinking water etc.). In developing predictive models, we have to describe quantitatively the relationship between important state variables and the processes causing changes in their temporal and spatial levels. Scientists use models to examine ideas about the causal interactions that give rise to phenomena. This process helps scientists to evaluate their understanding of the processes affecting water quality, and can point to areas of particular ignorance that need to be investigated. Second, models play an invaluable role in helping to organize and synthesize data concerning processes that affect water quality. As mentioned in Section I, the Northern Rivers are complex systems and prior to NRBS, our quantitative database on important state variables (e.g. concentration of contaminants, nutrient levels, etc.) and processes (e.g. sediment transport, biodegradation of organic compounds, bioconcentration, etc.) was relatively limited. When scientists attempt to construct a model to predict changes in water quality, data are required to parameterize functions describing processes associated with the creation, destruction, transformation, or transport of substances. The process of model parameterization typically involves a synthesis of existing data and a comparison of parameter estimates from previous studies. Very often, this systematic evaluation reveals that process-oriented data for key functions (e.g. temperature dependence of rate constants for kinetic reactions) are missing, and this stimulates empirical work, monitoring, or experiments to provide the missing quantitative information. It could be argued that the model building process itself provides the environmental scientist with the most crucial information: it exposes our ignorance of processes governing the dynamics of water-quality variables.

However, the existence of a mathematical model in no way implies that we have successfully produced a predictive tool that can be used in the decision-making process. The virtue of models is that they provide a crystal clear assessment of our ability to predict changes in water quality.

2.3 Sources of Uncertainty

Our ability to predict changes in ecosystem health or water quality depends critically on two sources of uncertainty inherent in the model building process. One source of uncertainty comes from our incomplete knowledge of processes, and this affects model formulation or our choice of how much physical, chemical, and biological complexity can be incorporated into our models. Our knowledge of the processes (i.e. causal relationships) operating in the Peace, Athabasca, and Slave Rivers is limited by our knowledge of both riverine processes in general, and how these general processes might be affected by the particular environmental circumstances presented by the Northern Rivers. For example, we have considerable empirical knowledge of how eutrophication influences water quality in large rivers in relatively warm climates (e.g. rivers in Europe, southern Canada, and the continental U.S.). How much of this knowledge can be transferred directly to the Northern Rivers with their highly seasonal flow-rates, ice-cover, and lower average temperatures? The successful application of a model (Summers et al. 1991) to predict how dissolved oxygen is affected by pulp mills and sewage inputs in the Pigeon River (North Carolina) does not guarantee in any way its successful application in the Northern Rivers. In particular, we have limited knowledge of the biotic communities in the Northern Rivers, food-chain interactions, large and small scale patterns of movement of major fish species (e.g. rocky mountain whitefish, longnose suckers, or northern pike), and their foraging habits. This poses crucial problems for understanding exposure to contaminants via food-chain processes. In addition, our knowledge of how processes governing the dynamics of complex organic compounds from effluents scale with temperature is quite limited. Thus NRBS represents, to some extent, a benchmark study in that it is breaking new ground in the development or application of a variety of water quality models to Northern Rivers.

The second major source of uncertainty comes from the quantification of processes (i.e. estimating parameters of functions that describe the rate of change or transport of materials or substances) and inputs. As discussed in Section I, there is not a shortage of water-quality models or models for the fate of organic contaminants from which to choose. The Northern Rivers are vast ecosystems covering many kilometers with different flow regimes, biotic communities, and sources of disturbance. Our ability to apply models successfully (i.e. to provide predictions on the appropriate spatial and temporal scale) in NRBS depends on the availability of process-oriented data to parameterize objectively the dynamics represented in the various models and an accurate characterization of inputs. For example, it makes little sense to use a highly non-linear, three-dimensional spatially-explicit representation for modelling the fate and transport of compounds when there are insufficient data to parameterize even the simplest one-dimensional model. Again it is important to recognize that, perhaps with the exception of models for dissolved oxygen, very little process-oriented data existed on the Northern Rivers prior to NRBS. Even the most ardent skeptic will accept that it is not fair to expect the successful development of a predictive model without providing the resources to adequately parameterize even the simplest model. The development of models in NRBS has occurred in parallel with the accumulation of empirical knowledge on the functioning of these systems, and in some cases crucial data for parameterizing models are only now becoming available as a result of the NRBS (see Section IV)

2.4 The Use of Predictive Models in the Face of Uncertainty

To combat this uncertainty and to assess objectively the predictive role of environmental models, scientists embark on what appears at first glance rather time-consuming and cautious process of model formulation, validation, and testing (Table 2.1 -after Dickson et al. 1982; Halfon 1990; Jorgensen 1994). [Please note: it is assumed that by this stage the problem under consideration has been sufficiently defined (i.e. scope and scale of predictions) and major modelling approaches have been chosen based on the problem to be solved (i.e. dynamic versus equilibrium approaches etc.)]. The models employed in NRBS are outlined in Section I and for the most part, the formulation of models was limited to adapting or applying existing models to the Northern Rivers. Model selection was based on a consideration of both the objectives of the study and our existing knowledge of processes in the Northern Rivers.

TABLE 2.1: Model Building Processes

Steps	Brief Description
Formulation	• identification of pertinent biological, physical, and chemical processes governing the transport, transformation, and accumulation of key substances or materials • identification of input variables and environmental forcing functions • identification of appropriate spatial and temporal scales • identification of subsystems and linkages among subsystems • parameterize functions using data from the systems under study, observations from other systems or laboratory experiments
Calibration	• "estimate" or "tune" parameters by comparing model output with previously measured values of the same state variables • determine the relative reliability of input data for parameter adjustment • compare parameter estimates and tuned parameter estimates against literature values • determine using a sensitivity analysis which parameters are most important
Verification or Validation	• test the model against an independent set of data to observe how well the model captures the observations • assess the prediction uncertainty (uncertainty or error analysis methods - e.g. Summers et al. 1994, Wang et al. 1994) • perform tests on independent data for cases in which input conditions differ considerably from those used during calibration (e.g. different flow regimes or loading rates)
Application	• use the model to predict dynamics of water quality and to determine whether water quality will be impacted by expected changes in inputs

By following this systematic approach, scientists attempt to address many of the criticisms raised by skeptics. For example, the criticism that "tweaking" complex models to obtain the right answer does not apply as long as the model is verified using an independent data set following the calibration stage. A major question that will be addressed in Section III and IV of this Synthesis Report is how far along in this sequence has modelling water-quality progressed as a result of NRBS?

2.5 How can we assess the utility of our predictive tools?

Once we have constructed our environmental models, how can we assess their reliability? Several authors have recently noted that while we have a clear idea of the processes related to model building (i.e. model development), we have very little objective guidance for verifying these models in a statistically rigorous manner (e.g. Little & Stevens 1990; Summers et al. 1993; Reckhow 1994). Often, we are only left with subjective assessments of how well model predictions compare with observed dynamics based on graphical comparisons judged by "experts" (e.g. Mayer & Butler 1993).

Model verification refers to the process of testing a mathematical model in a predictive scenario with the aim of providing a quantitative statement that the model adequately describes observed behaviour so that it will be a useful predictive method (e.g. Reckhow et al. 1990). Most often, we arrive at an estimate of reliability by performing some sort of statistical test that compares the agreement between model predictions and independent observations from the real system under consideration (i.e. determining the model "goodness-of-fit") (e.g. Mayer & Butler 1993). At this point, we have to introduce the use of statistical models for "goodness-of-fit" and we introduce new assumptions and problems that are not simply esoteric concerns for NRBS.

Techniques for the statistical evaluation of water quality models have been recently reviewed by Reckhow et al. (1990), Power (1993), Summers et al. (1993), and Smith & Rose (1995). There are basically four related techniques for assessing model goodness-of-fit as summarized by Smith & Rose (1995): (1) linear regression of observed versus predicted values, (2) the sum of squared prediction errors, (3) reliability indices that assess whether predictions are within a factor K_s from observed values, and (4) correlation-like measures that normalize the sum of squared prediction error to be between zero and one. The most common approach is to compare plots of predicted versus observed values. One then uses some sort of regression or correlation technique to assess goodness-of-fit. While this approach seems straightforward, it is fraught with difficulties. When we use regression or correlation techniques we introduce all of the assumptions associated with regression analysis into our problem (e.g. normality, homoscedasticity, independence of observations, etc.), and this creates particular difficulties for assessing the predictive ability of dynamical models. These problems are not just esoteric "statistical" concerns; they can severely hamper our ability to provide an objective estimate of the reliability of models. For example in testing dynamical predictions, independence of observations in either space or time becomes an important issue because lack of independence (i.e. presence of autocorrelation or serial correlation) can bias the estimate of the residual mean square term in the regression between predicted and observed values. In river systems, the observed values of state variables often show spatial or temporal autocorrelation. This autocorrelation implies a lack of independence, which in turn affects our estimates of the residual mean square, and unfortunately underestimates the residual mean square which could lead us to conclude that the model is performing better than it actually is.

An additional problem concerns multivariate assessment. In many cases, our water quality models output the dynamics of more than one state variable (i.e. predict multiple output variables). Determining the reliability of our models needs to be based on quantitative statements about how well all of the model prediction variables agree with observed data (Smith & Rose 1995). Several of the techniques advocated for univariate tests can be extended to the multivariate case, and here we need some judgment as to which of the many state variables will be used to judge the reliability of predictions.

By and large these statistical techniques for assessing model reliability are designed to provide an overall assessment of model performance. In NRBS, however, there are important issues related to the ability of our models to predict dynamics of water quality variables at various relevant spatial and temporal scales. One of the major objectives of NRBS is to predict the impact of discharges from pulp mills and sewage treatment plants. These impacts may be felt at both a large spatial scale (i.e. on the overall average value of a variable when calculated over a spatial scale of 100 km) and/or a small spatial scale (i.e. immediately downstream from a point source discharge). It is difficult to say *a priori* which of these scales (or some intermediate) is most pertinent. If "near-discharge" scales are considered most important (i.e. neighborhood effects), then in evaluating the success of water quality models we would need to somehow "weight" our points on the predicted versus observed curve to adjust for this goal. The overall predicted versus observed curve gives an indication of how well the total variation associated with the variable can be "explained" by the model, not whether the particular variation near point-source inputs is adequately explained by the model. A similar argument can be made for temporal patterns (i.e. model predictions may be more germane during certain part of the year when organisms may be particularly sensitive to environmental perturbations).

These issues concerning model reliability will be re-visited in Section III and IV where the successes and failures of NRBS modelling efforts will be evaluated.

2.6 What are the alternatives?

Most environmental models are mechanistic. They attempt to describe causal relationships between variables and use functions that quantify these relationships to predict future values given measured inputs. They are often formulated in terms of difference or differential equations and include some algebraic expressions along with parameters (e.g. Jorgensen 1994). With all of the drawbacks and problems associated with the use of mechanistic models (summarized above), some attempts have been made to explore alternative approaches.

For example, statistical models attempt to derive generalizations by using regression, principle component analysis, and other statistical techniques to summarize experimental or observational data (e.g. Klove et al. 1993; Suter 1993; Tsanis 1993; Landis et al. 1994). The simple goal here is to "explain" the observed variation in key water-quality variables through variation in independent variables (e.g. predicting variation in dissolved oxygen concentration from variation in flow rates, water temperature, levels of particulate carbon etc.). These techniques do not make any assumptions about causality in processes or relationships between variables, but instead introduce a whole series of alternative assumptions regarding drawing inferences based on existing empirical observations.

The major limitation in applying statistical models to answer the questions regarding water quality in NRBS is the lack of existing long-term data on the key variables of interest. We have incomplete knowledge of the natural levels of stochasticity present in the system, and thus our ability to distinguish an environmental impact from natural variation is severely hampered. In addition, the northern rivers are fairly pristine, thus the models must predict small changes from natural conditions. There are many general empirical relationships that have been developed, for example to relate nutrient loads to algal biomass, using observations from other aquatic systems throughout the world (e.g. Culp & Chambers 1993). These empirical relationships may be applied to the Northern Rivers, but predictions may be inaccurate because of the relative under-representation of observations from rivers in northern latitudes in the database used to construct the empirical relationships, and their prediction intervals may be too large to be useful in a regulatory or decision making process.

The paucity of long-term data for the Northern Rivers also limits the applicability of other alternatives, such as the use the of expert systems or artificial intelligence methods (Guerrin 1991; Varis 1994) and GIS methods (e.g. Engel et al. 1993; Clifford et al. 1995). These approaches are often limited by the same problem that we face in constructing mechanistic models for the system concerning how much knowledge of processes (or rules) from other river systems can be applied to the Northern Rivers. Of course, these modelling approaches are not mutually exclusive. Modellers developing mechanistic models may use expert systems (Bauffaut et al. 1990; Barnwell et al. 1989) or a variety of statistical models to estimate parameters.

The topic of alternatives for modelling water quality will be re-visited in Section IV dealing with Future Directions of Modelling Approaches.

3.0 KEY FINDINGS OF NRBS MODELS

3.1 Modelling Dissolved Oxygen

The major results are summarized in Figure 3.1-3.6 drawn from Technical Report 1 (Chambers et al. 1995). The model successfully predicted the "large-scale" trends in average oxygen concentrations, as indicated by the coefficient of determination for predicted versus observed relationships, for years in which reliable input data were available (e.g. 1990-1993). Successful model prediction appears to be correlated with higher discharge rates among years. The model failed to capture accurately the "local" or "small-scale" oxygen sags downstream from mills during the 1988-1989 period, and these failures are hypothesized to be the result of large and erratic BOD loadings from Millar Western Pulp Ltd, or limited data on tributary and sewage treatment plants (Chambers et al. 1995).

Stochastic solutions, based on observed variance for inputs and parameters, reinforce the general result that the model successfully predicts large-scale trends for the 1990-1993 period, but also suggest that the "small-scale" changes associated with oxygen sags fall, for the most part, within the 90% confidence limits for 1990-1993 period. Incorporating uncertainty associated with inputs and parameter estimates does little to improve model success for the 1988-1989 observations. This is especially troublesome because oxygen levels reach quite low values at some reaches during the 1988-1989 period, and the model fails to capture these significant oxygen lows in the Athabasca River.

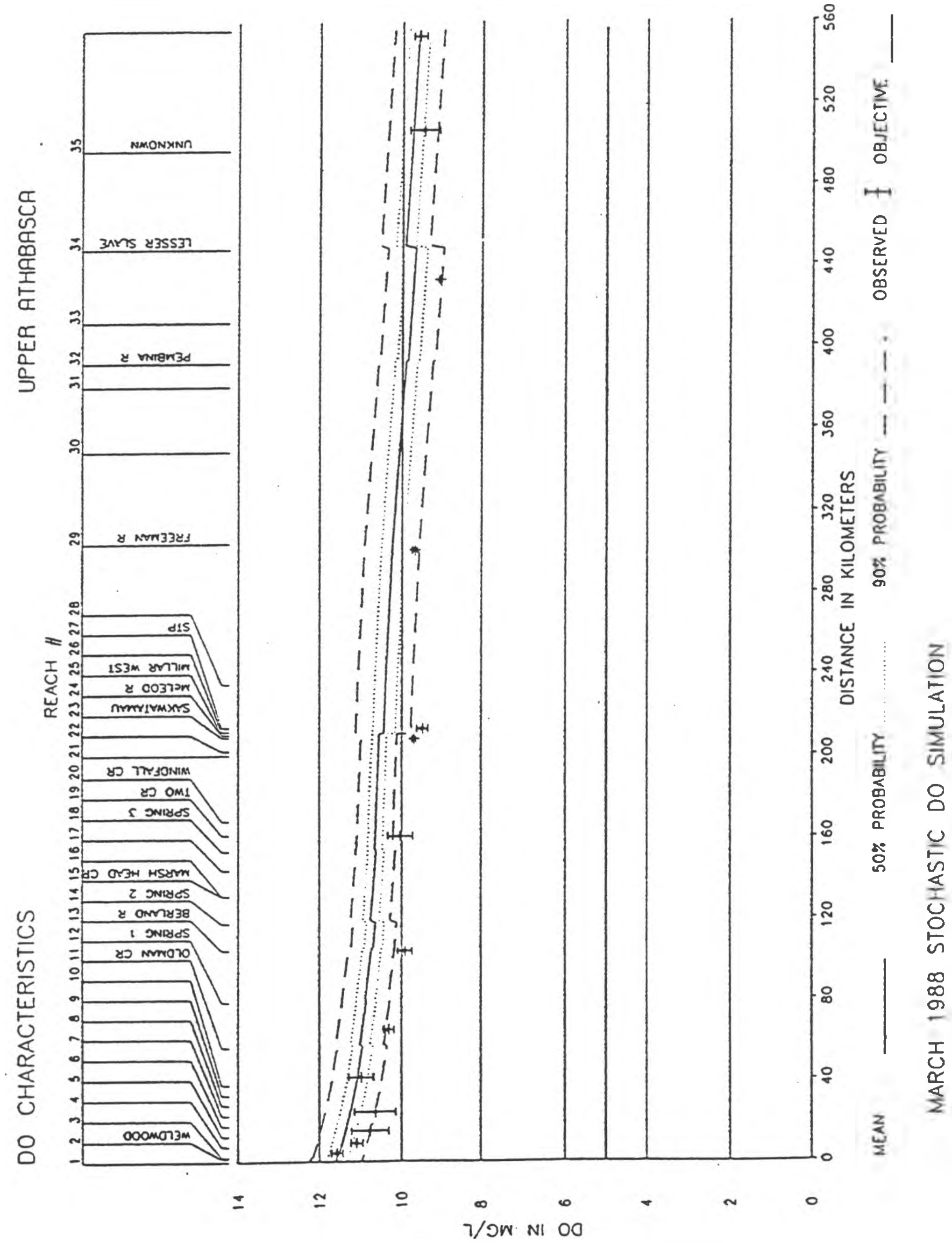
Chambers et al. (1995) also present the results of statistical models that describe changes on dissolved oxygen concentration with distance for various regions along the Athabasca River (i.e. Upstream of Hinton, Hinton to Grand Rapids, Downstream of Grand Rapids). This regression analysis yielded three major results: 1) slopes that describe the rate of decline of oxygen with distance differ significantly among river segments; 2) dissolved oxygen concentrations decrease linearly with distance in regions of the Athabasca River receiving pulp mill effluent; 3) slopes within major regions do not differ among years despite considerable variation in loading and flows.

In addition, a comparison of rates of decline in dissolved oxygen concentration with distance for ice-covered world rivers receiving effluent was performed. This among-river comparison suggests that the rate of change of dissolved oxygen concentration may be predicted from measurements of the effluent:river discharge ratio (a measure of the dilution of the effluent).

In summary, the dissolved oxygen models developed by NRBS are at the stage of model verification and application. This would include evaluating the ability of models to capture the changes in dissolved oxygen concentration with river distance for further independent observations (i.e. 1994-1995 data), and independently evaluating rates *in situ*.

Figure 3.1

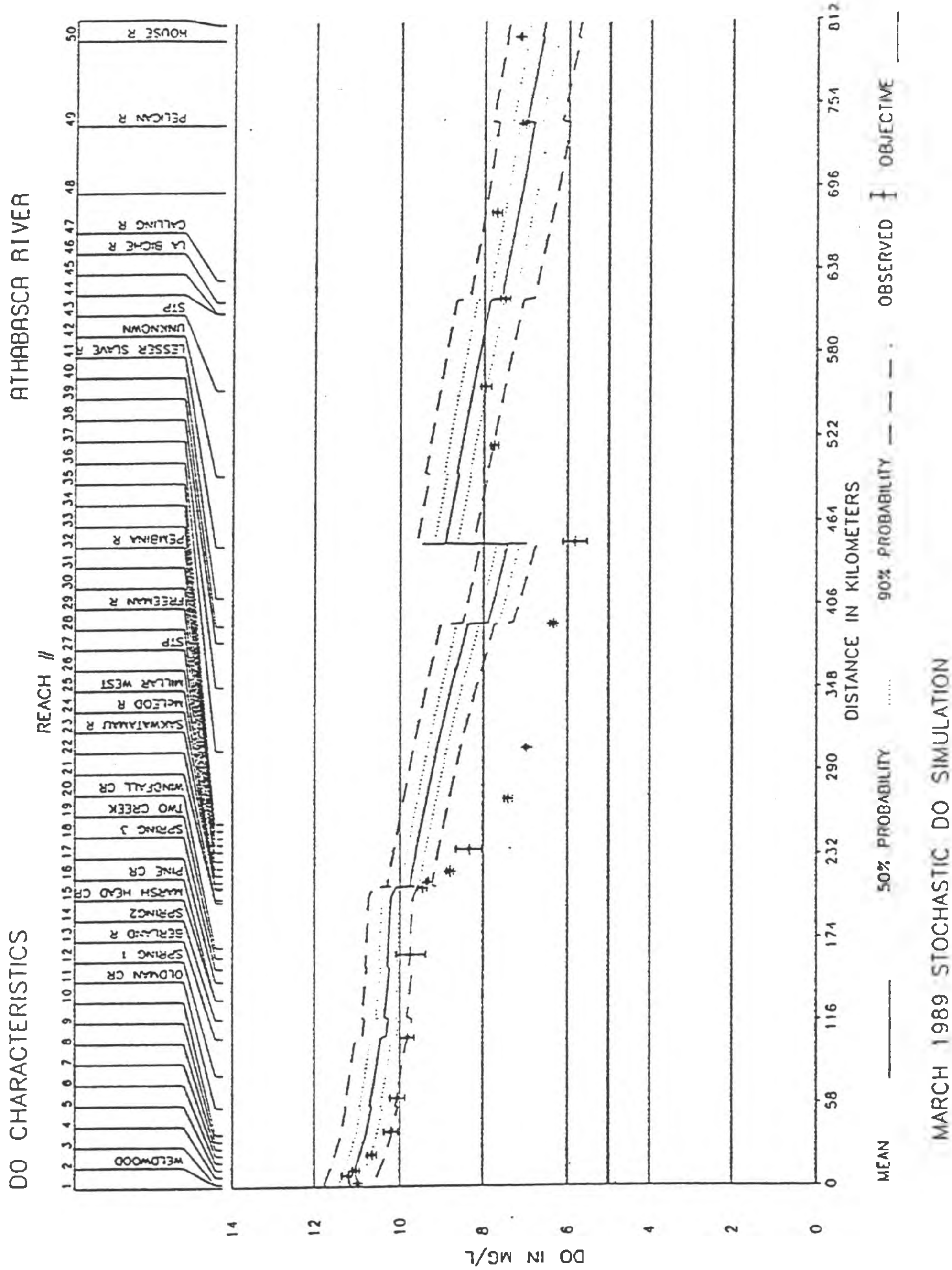
Dissolved oxygen (DO) concentrations predicted for the Athabasca River, AB for March 1988 using the simulation model DOSTOC run stochastically with best available estimates of standard deviation for BOD loadings and BOD and SOD decay rates.



From Chambers *et al.*(1995)

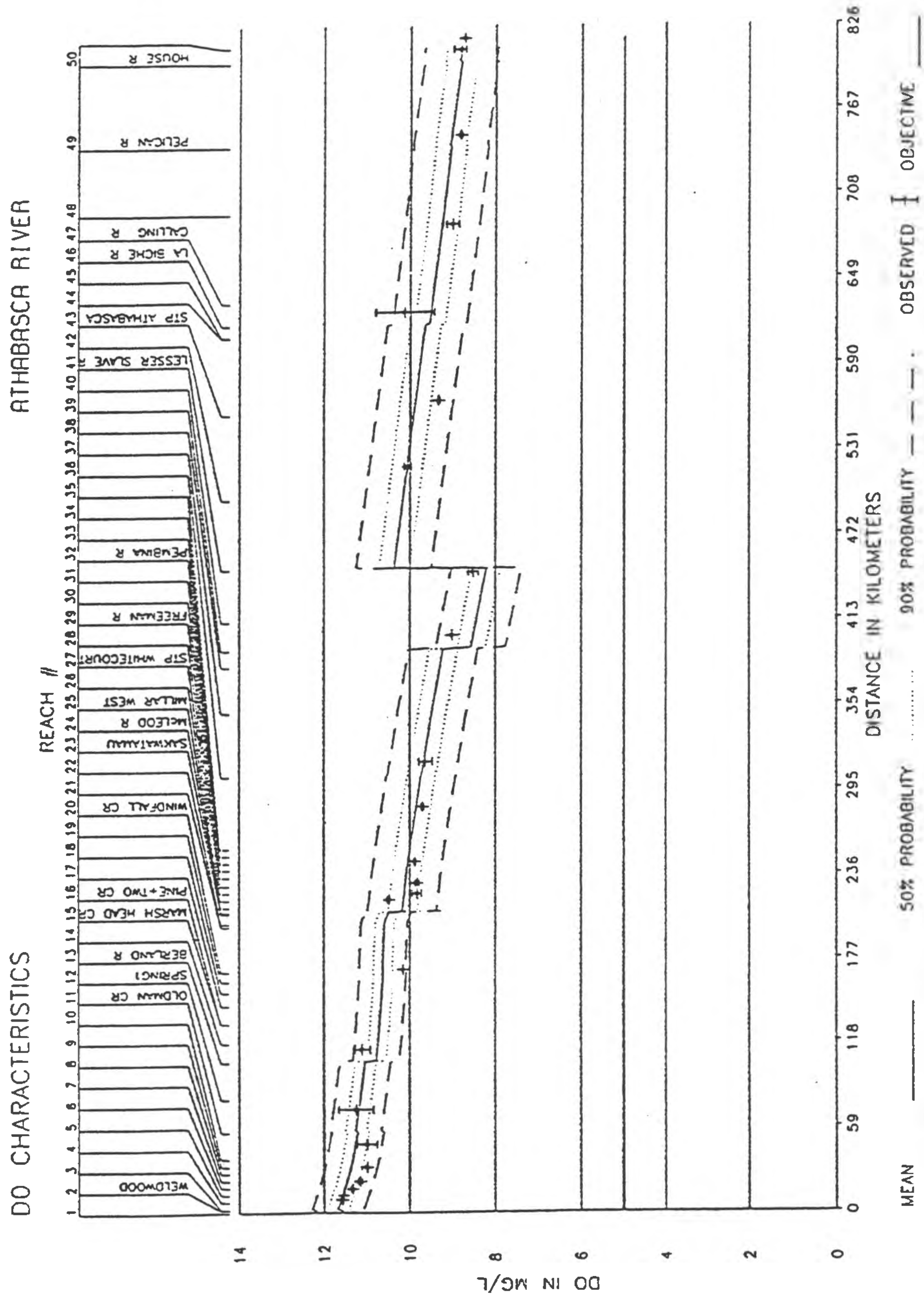
Figure 3.2

Dissolved oxygen (DO) concentrations predicted for the Athabasca River, AB for March 1989 using the simulation model DOSTOC run stochastically with best available estimates of standard deviation for BOD loadings and BOD and SOD decay rates.



From Chambers *et al.*(1995)

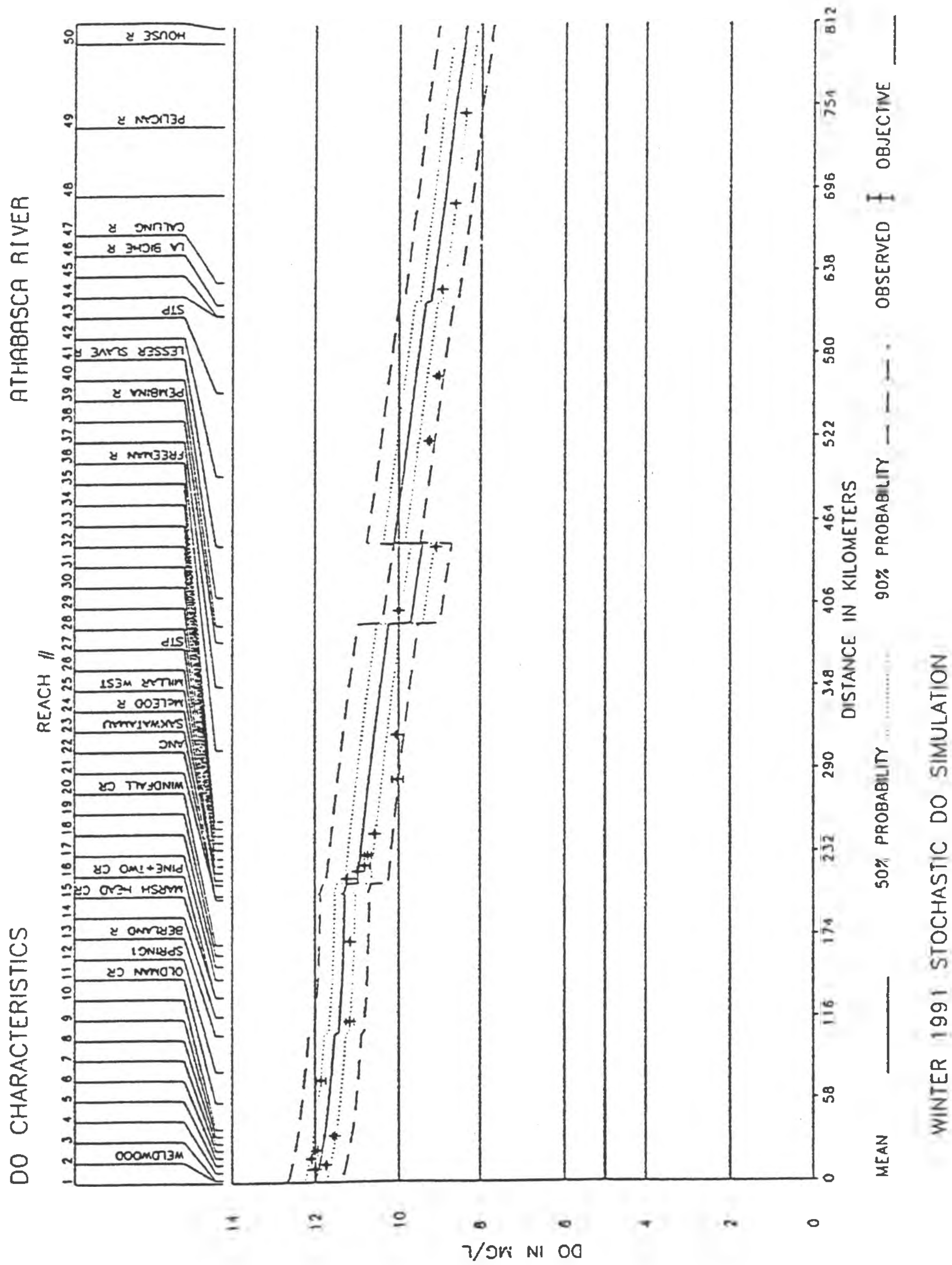
Dissolved oxygen (DO) concentrations predicted for the Athabasca River, AB for February - March 1990 using the simulation model DOSTOC run stochastically with best available estimates of standard deviation for BOD loadings and BOD and SOD decay rates.



From Chambers *et al.*(1995)

Figure 3.4

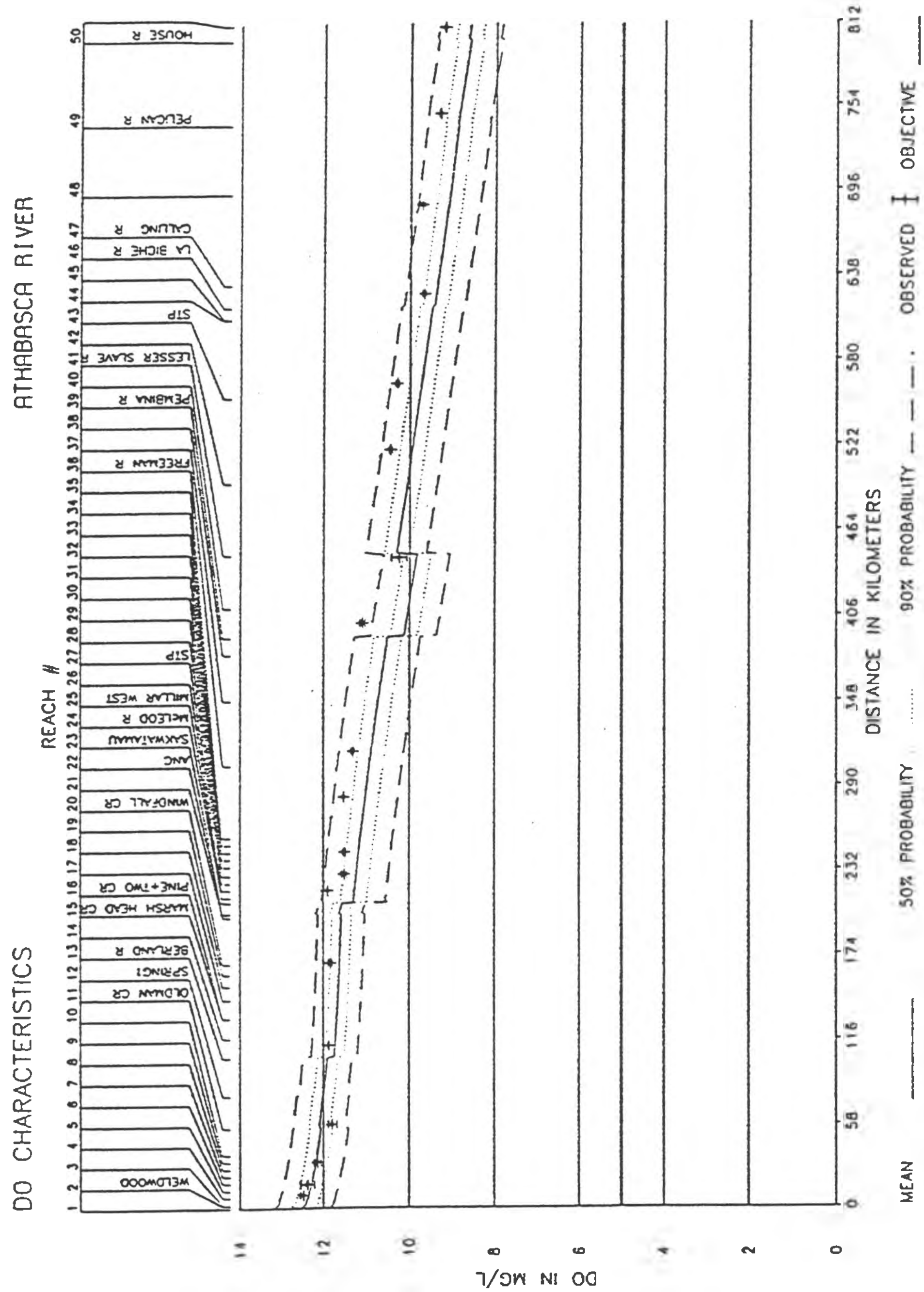
Dissolved oxygen (DO) concentrations predicted for the Athabasca River, AB for February - March 1991 using the simulation model DOSTOC run stochastically with best available estimates of standard deviation for BOD loadings and BOD and SOD decay rates.



From Chambers *et al.*(1995)

Figure 3.5

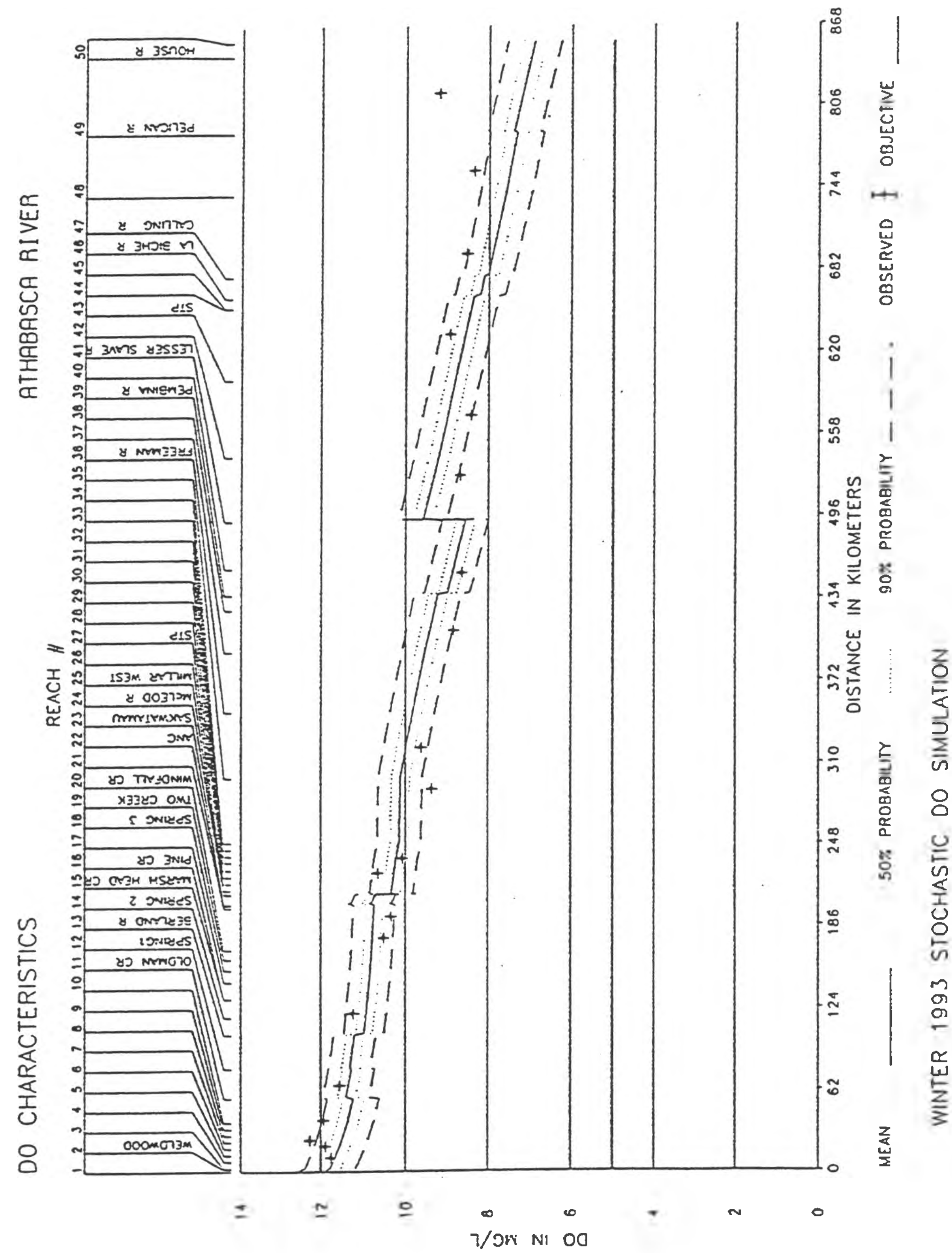
Dissolved oxygen (DO) concentrations predicted for the Athabasca River, AB for February - March 1992 using the simulation model DOSTOC run stochastically with best available estimates of standard deviation for BOD loadings and BOD and SOD decay rates.



From Chambers *et al.*(1995)

Figure 3.6

Dissolved oxygen (DO) concentrations predicted for the Athabasca River, AB for February - March 1993 using the simulation model DOSTOC run stochastically with best available estimates of standard deviation for BOD loadings and BOD and SOD decay rates.



From Chambers *et al.*(1995)

3.2 Modelling Contaminant Fate

Briefly summarizing the key results of modelling the transport and fate of contaminants using WASP is a daunting task. As discussed in Technical Report 2, the temporal and spatial output from this dynamic model is considerable and it is magnified by the fact that NRBS considered the fate of 7 organic chemical species. This section only attempts to summarize the strategic results based on conclusions provided in Technical Report 2 and provides some editorial comments on these conclusions.

Conclusion 1: Configuration and flow conditions adequately simulated for Athabasca and Wapiti/Smoky Systems.

Based on modelling sodium as a conservative substance, WASP provides a good representation of the hydraulics and mass balance for the Athabasca River and the Wapiti/Smoky Rivers. Unfortunately, this is only assessed in a subjective manner and a quantitative analysis of the strength of this result would be an asset. The sodium simulations point to the significance of variation in seasonal flows as being an important dilution factor in determining the realized concentration of organic contaminants, and hence exposure levels.

Conclusion 2: Descriptive simulations of total suspended solids (TSS) can capture changes in water column concentrations of TSS for both the Athabasca and Wapiti/Smoky Systems.

WASP does not predict settling and resuspension rates of solids based on hydraulic characteristics, thus the model must be provided with a time-series of settling and resuspension rates that can be cell specific. The correct prediction of total suspended solids is crucial because organic contaminants become sorbed to suspended solids and the transport of these solids represents an important component in predicting the fate of the contaminants. For the present application of WASP, calibration was achieved by adjusting the deposition rates only. Three zones were identified (a high settling rate zone directly below each pulp mill, a moderate settling-rate zone further downstream, and a background zone with extremely low settling rates). By adjusting deposition rates, the model is claimed to account adequately for both the magnitude of the concentrations observed and the seasonal pattern at a particular point in space for both the Athabasca and Wapiti/Smoky systems. A subjective evaluation suggests that the calibration was better for the Wapiti/Smoky Rivers than the Athabasca. The adjustment of deposition rates was able to capture two observations concerning the Wapiti/Smoky system: 1) runoff from non-point sources appear to be a dominant factor determining TSS in the Wapiti/Smoky Rivers and 2) the Smoky River carries more TSS than the Wapiti River.

Conclusion 3: For the one organic contaminant with well-defined environmental fate constants (2,3,7,8-TCDF), WASP was able to simulate adequately spatial and temporal variation in all media.

A good calibration was achieved for 2,3,7,8-TCDF for both the Athabasca River (e.g. Figure 3.7) and the Wapiti/Smoky Rivers (although data for the latter systems were sparse). It is important to note that this successful calibration was obtained without adjusting any of the chemical-specific fate constants. The model correctly accounted for the concentration differentials between the water column, suspended sediment, and bed sediment compartments.

Conclusion 4: WASP provides a reliable simulation of dissolved water column concentrations, in the Athabasca and Wapiti/Smoky systems, for all chemicals as long as the loads are adequately defined.

This conclusion could be a subject of considerable debate given the paucity of observations for most chemical species and the lack of a quantitative analysis to assess goodness-of-fit of the model simulations to the observed values. Simulation results suggest that fit could be improved by increasing the organic partition coefficients (K_{oc}) for some species beyond the defined range.

Conclusion 5: Simulated bed concentrations in the Wapiti/Smoky River system were overestimated for all chemicals except 2,3,7,8-TCDF.

"Simulations of bed sediment contaminant concentrations were limited by lack of adequate sediment transport routines and insufficient information to calibrate benthic biodegradation rates or sediment-water column diffusion" (Technical Report 2).

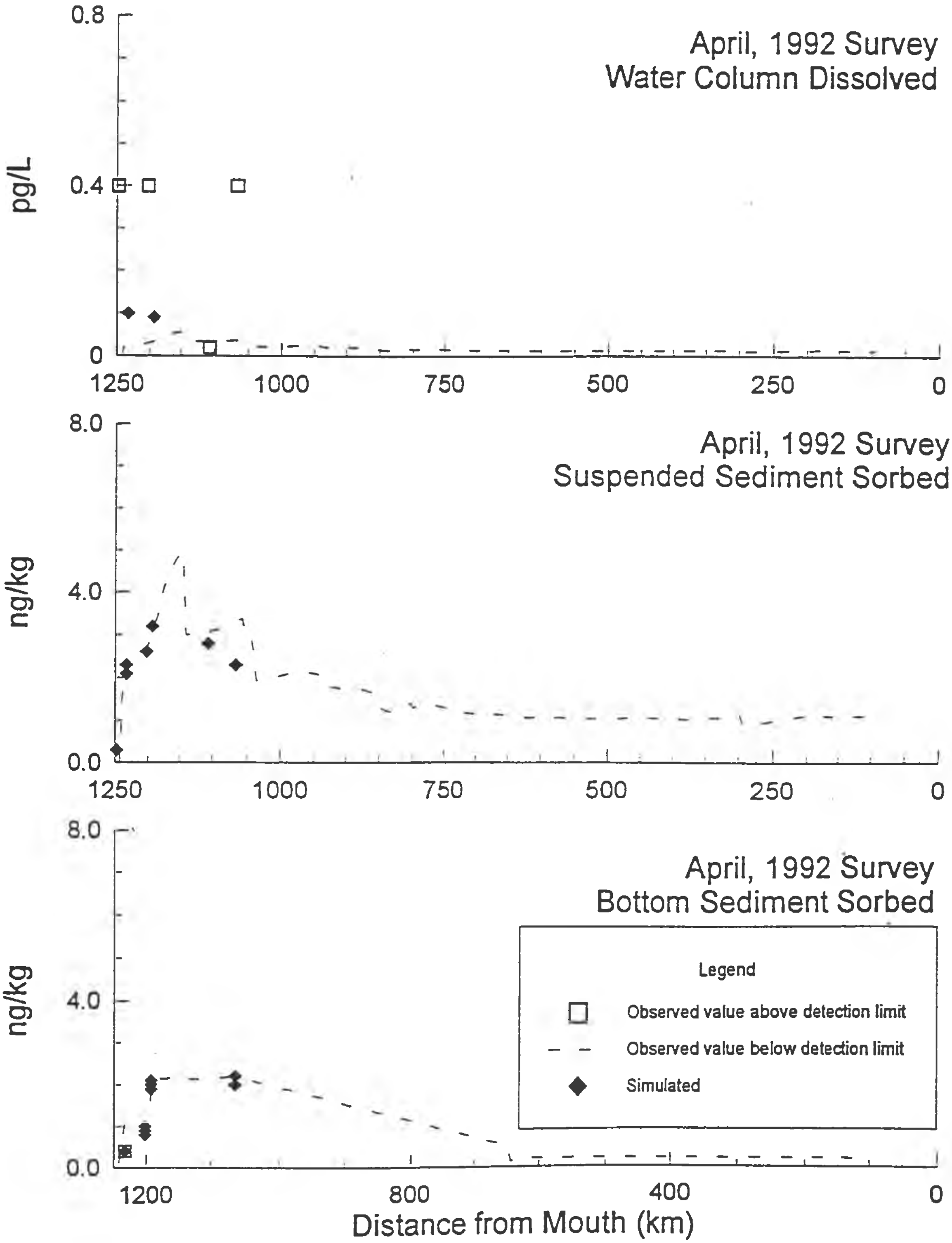
Conclusion 6: Calibration was not possible for DHA and dichloroDHA in suspended solids for the Athabasca River.

WASP was not capable of capturing the among year dynamics of DHA: "the simulated ratio of TSS sorbed to dissolve water column concentrations in 1992 is about twice as large as the observed ratio" (Technical Report 2). In addition, the results of the simulation suggest that bed sediment concentrations may not be completely reset each year.

Conclusion 6: For some chemical species (e.g. Phenanthrene) observed data are so sparse, or conflicting, that it is not possible to evaluate the calibration of WASP.

In summary, model development proceeded to the calibration stage for TSS and for at least one organic contaminant (TCDF), although a quantitative assessment of this calibration needs to be performed, as well as a quantitative assessment of the ability of the model to capture hydraulics and mass balance. As discussed in Section 4, progress is limited by availability of input data, observations on fate constants, and algorithms for sediment transport or resuspension.

Figure 3.7



Athabasca River, 2,3,7,8-TCDF Calibration, Synoptic Surveys

From Golder Associates (1995)

3.3 Modelling the Distribution of Contaminants in the Food Chain

Model predictions of the concentrations of organic contaminants expected throughout the food chain were derived for the Athabasca River. Two sets of model predictions were made considering alternative ways of calculating the biological concentration factor (BCF) (either from computation using the octanol-water partitioning coefficient (K_{ow}) and the fraction lipid for each species, or direct estimates of excretion rates). The best model predictions were found using the direct input of excretion rates. The success/failure of the model can best be appreciated by considering the case of TCDF for which the most reliable data are available.

Using best estimates of parameters, the food-chain model overestimates the concentration of TCDF in the biota by a factor of approximately 5-10 (figure 3.8- Technical Report 3 (figure 5)). The predicted versus observed relationship is improved if the input concentrations of TCDF are adjusted to take into account biofilm activity. Predicted values overestimate observed concentrations by ~2.5 fold. In the final calibration stage, the excretion rate parameter was adjusted to obtain a match between predicted and observed values for each biological species. Table 3.1 (Technical Report 3-Table 8) shows the comparison between original literature-based values and the adjusted values required for calibration. The modelling results support the hypothesis that preferential consumption of filter-feeding invertebrates feeding on suspended solids represents the primary exposure pathway of mountain whitefish to TCDF.

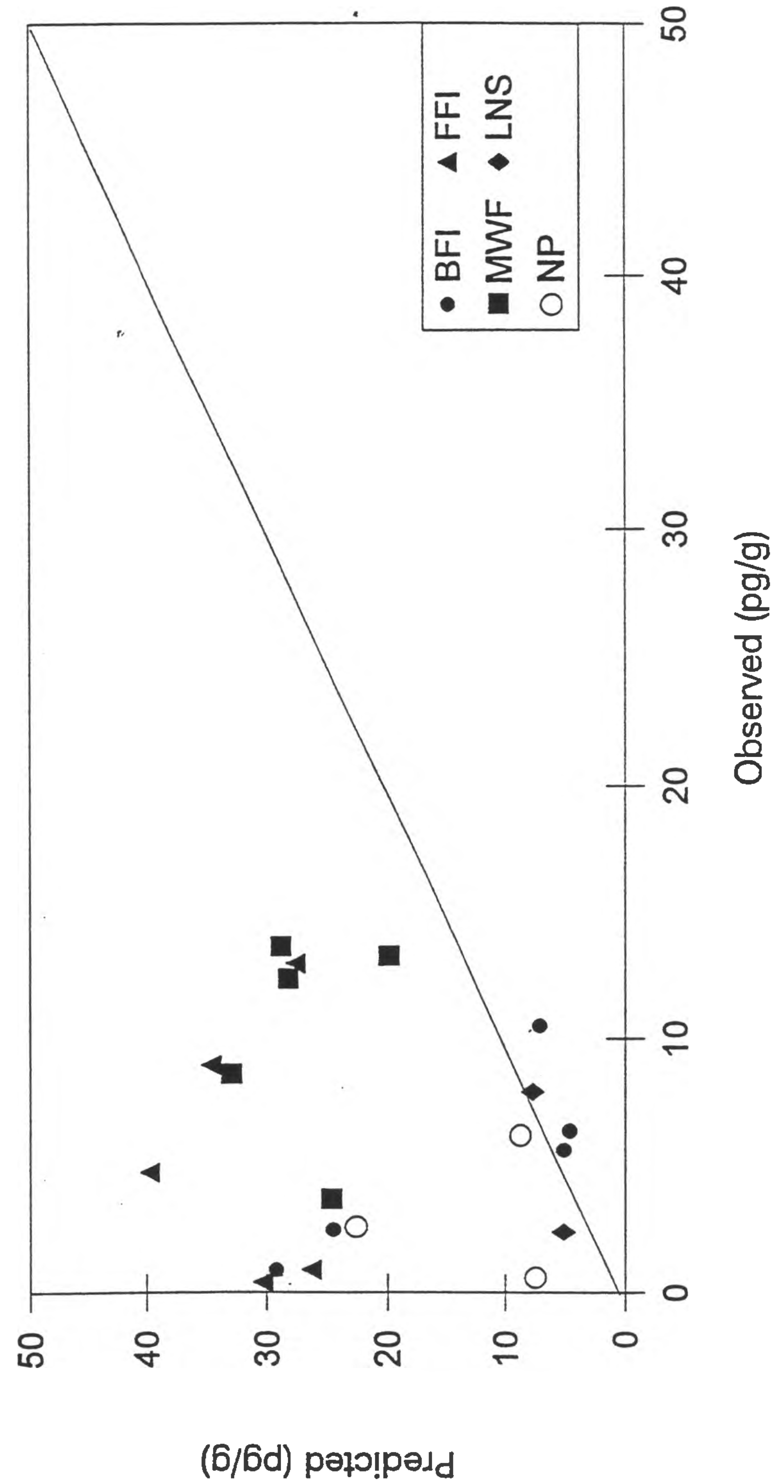
Table 3.1 Comparison of Literature based Excretion Rates *vs.* Adjusted Excretion Rates from CanTox (1995).

Species	Literature based Excretion Rate (d^{-1})	Adjusted Excretion Rate (d^{-1})
Bottom feeding invertebrate	0.014	0.003
Filter feeding invertebrate	0.014	0.052
Mountain whitefish	0.003	0.0025
Longnose sucker	0.003	0.025
Northern pike	0.003	0.0075
Brook stickleback	0.003	0.003

Because of the paucity of data on processes affecting the uptake and excretion of the resin acids (DHA and DCDHA) or the chlorinated phenolics, initial model predictions were not based solely on *a priori* estimates of parameters. Ranges of parameter values for chemical assimilation efficiency and BCF had to investigated. Resulting model outputs overestimated concentrations of these chemicals by roughly 2-10 fold even following calibration.

Figure 3.8

2,3,7,8-TCDF in Biota, Predicted *vs* Observed Using Biofilm, All Locations



From CANTOX (1995)

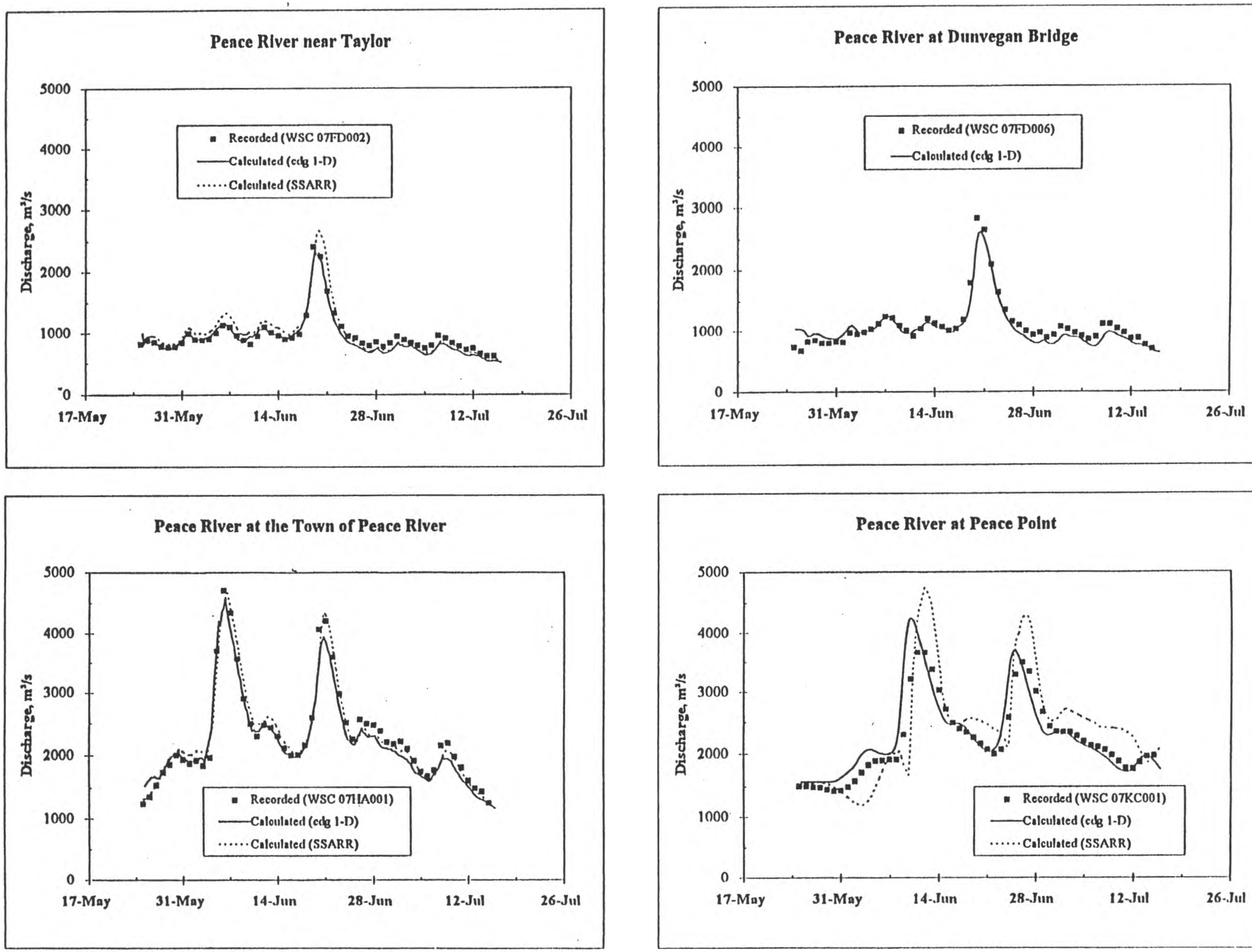
The significant lack of fit between predicted and observed values was primarily attributed to the lack of "steady-state" conditions probably present in the river systems rather than a structural failure of the food-chain model. This disequilibrium can come from two sources: 1) environmental variability in concentrations of the organic contaminants in the various environmental media (i.e. water column, suspended sediments, depositional sediments etc.), and 2) variation in biota within and among locations, including migratory movement of fishes. The non-equilibrium conditions would explain lower observed tissue concentrations than expected assuming steady-state conditions. However, it is extremely important to further investigate these two hypotheses concerning model failure (disequilibrium violating steady-state assumptions versus inadequate model formulation). In particular, the disequilibrium hypothesis can be investigated further by considering that the three major classes of organisms considered (benthic invertebrates, filter-feeding invertebrates, and fish) are operating on significantly different "time-scales", and the two invertebrate groups also experience different amounts of environmental variability in exposure concentrations of contaminants (e.g. temporal and spatial variance of TCDF in the water column and the sediment differ substantially). These observations could be exploited to perform a more rigorous quantitative analysis of model failure that might help to distinguish among these important alternatives.

In summary, model development for the distribution of contaminants in the food-chain proceeded to the calibration stage. However, the significant lack-of-fit between model output and observed values of contaminants for each of the major components of the food-chain indicates that considerable work needs to be done on evaluating the reasons for model failure before attempting any sort of verification.

3.4 Hydraulic Model of the Peace River

The hydraulic model was successful in capturing the dynamics of two separate diffusive wave scenarios (1980 Spring flood event and 1987 summer flood event) (Hicks et al. 1994). Model calibration only required one parameter (Mannings n values which were used to describe channel resistance), and initial values based on data from Kellerhals et al. (1972) were considered adequate given other uncertainties related to the lack of input data for tributaries. Figure 3.9 shows the model simulation of discharges for the 1980 event at 4 different sites along the Peace River. These sites were chosen to facilitate comparison with predictions from a hydrologic model developed by Alberta Environment Protection.

Figure 3.9



Comparisons of measured and computed discharge hydrographs (1980 event)

From Hick *et al.*(1994)

4.0 RECOMMENDATIONS AND FUTURE DIRECTIONS

NRBS has made considerable progress in the development of predictive tools in some areas, and laid a scientific foundation in other areas for future modelling efforts. This section will first summarize and comment on modelling recommendations made in specific technical reports, and then provide some pointed recommendations for future work.

Table 4.1 summarizes recommendations for modelling dissolved oxygen, transport and fate of contaminants, and distribution of contaminants in the food-chain. In general, these recommendations fall into 4 categories: 1) requirements for better data (i.e. more accurate or more spatially representative observations) on inputs from discharges and *in situ* concentrations of target variables (e.g. dissolved oxygen, chemical contaminants), 2) requirements for more data on rates that can be used either to provide better estimates of model parameters or to provide tests of existing model assumptions regarding spatial heterogeneity, temporal dynamics, or omitted processes (e.g. under-ice photosynthesis, species migrations), 3) requirements for experiments and *in situ* observations to test specific predictions or parameters derived from the model calibration procedure, 4) requirements for further modelling work involving models that are more complex (i.e. dynamic representation of processes) and consider more spatial dimensions. It is important to note that these calls for more data collection are not simply frivolous requests for monitoring; they are focused requirements based on either limitations impeding further development of predictive tools, or they are crucial for the evaluation of the reliability of model predictions. As mentioned previously, a virtue of these water quality models is to highlight existing gaps in our knowledge or understanding of these river systems, and to suggest key areas where research would be highly profitable for the development of predictive tools.

NRBS has made considerable progress in modelling dissolved oxygen. While the steady-state model does not provide the dynamic predictions that may be highly desirable from a management perspective, it does provide a simple framework that can be used to predict changes in under-ice concentrations over relatively large spatial scales and to evaluate our understanding of processes that influence the concentration of dissolved oxygen in the Northern Rivers. The model has no free-fitting parameters, and therefore it is at a stage where model predictions can be tested against *in situ* measurements of dissolved oxygen concentrations and model assumptions can be evaluated by targeted *in situ* measurements or experiments on specific rates (i.e. tests can be carried out to examine if the model is "getting it right" for the "right reasons"). The data from these *in situ* experiments can also be used to assist in the development of the next stage of model (i.e. a dynamic representation such as WASP). In particular, more work needs to be carried out to investigate why the steady-state model fails to capture the sags in oxygen concentration in the vicinity of mill discharges. Is this model failure related to our lack of understanding of sedimentation processes, sediment oxygen demand, or spatial heterogeneity? The existing model uses all of the available empirical information on rates, temperature dependencies, and conversion ratios. Many of these estimates would form an essential part of any further model development, and therefore much could be gained by verifying these estimates to test the existing model while at the same time ensuring a strong scientific foundation for future model development (specific rates, temperature dependencies, conversion ratios listed in Table 4.1). General points concerning future model development and limitations are presented below.

Table 4.1

MODEL	SPECIFIC RECOMMENDATIONS FROM INDIVIDUAL MODELLING REPORTS
DISSOLVED OXYGEN (Chambers et al.)	Measures of BOD decay rates for effluent from sewage treatment plants are required, along with a test of the estimate for the BOD_u:BOD_5 conversion ratio. In addition, more estimates of BOD decay rates at 0°C and 20°C for water from headwaters, effluents, and tributaries are needed.
	Sediment oxygen demand *in situ* needs to be evaluated in more detail, including cross-channel variability and the relationship between sedimentation and SOD in the vicinity of mill discharges and tributary inflows
	Sedimentation rates need to be measured below mills to determine if settling rates are the same for different effluent types
	Leopold-Maddox coefficients need to be re-evaluated and another under-ice time of travel study is required
	Under-ice photosynthetic rates need to be estimated in relation to snow-cover and evaluated as a potential source of oxygen in the model
	A dynamic model, such as WASP, could be implemented to address questions regarding temporal variability in the decrease in dissolved oxygen among months.
	A 2-dimensional simulation that includes cross-channel and longitudinal processes could be implemented to address concerns about dissolved oxygen concentrations in mixing zones
CONTAMINANT FATE (Golder Associates)	Model complexity should not be increased until the fate constants for the current model are better defined, sediment transport is modelled properly, and more information made available on the behaviour of the various chemical species
	Sediment transport routines should be incorporated based on the studies by Krishnappen et al. (1995) and Krishnappen and Stephens (1995)
	Experimental investigation of K_{oc} and benthic biodegradation values using Athabasca and Wapiti/Smoky River samples
	Monitoring of chemical concentrations in the bed sediment needs to be carried out to define seasonal and long-term patterns
	If phenanthrene is to be modelled adequately, data on TSS sorbed and dissolved concentrations are required for phenanthrene sources and in the river, along with better estimates of loading rates and sediment concentrations
FOOD CHAIN (CanToX)	Observations on the concentrations of resin acids (i.e. DHA and DCDHA) are required, along with laboratory experiments of the waterborne and chemical dietary uptake and excretion in invertebrates and fish species
	Pharmokinetic data are required for trichlorocatechol, trichloroguiacol, and trichloroveratrole in aquatic species, and BCF values need to be estimated independently to test model calibration
HYDRAULIC (Hicks et al. 1994)	More data on river geometry are required between the town of Peace River and Peace Point, unsurveyed reaches need to be evaluated

Modelling efforts for the transport and fate of contaminants had to contend with a much weaker initial database and uncertainties associated with inputs to the system. In addition, there was limited information available on the "behaviour" of many of the chemical species modelled under the environmental conditions in the Northern Rivers. Our knowledge of the partitioning and movement of the various chemical species was scarce, and as a result it was not possible to provide independent estimates of many parameters, as in the case of modelling dissolved oxygen. The paucity of data and information on the behaviour of chemicals, required that model development was restricted to the formulation and calibration stage (i.e. existing data had to be used to formulate the model and to adjust parameter values to obtain a calibration of model output and observed concentrations of contaminants in the various environmental compartments). Since all of the data were "consumed" in this process, there are no independent estimates available to test model predictions or evaluate parameter estimates required to calibrate the model output (data may be available from recent samples that are presently being analyzed by NRBS for the 1995 field season).

During model calibration, several parameters had to be adjusted (e.g. DOC binding effectiveness coefficients, biodegradation rates for water column and benthic compartments). It is important to either collect data or conduct experiments to evaluate the empirical basis for these parameter adjustments in the Northern Rivers. For example, the adjusted DOC binding effectiveness coefficients for the Wapiti/Smoky and the Athabasca River Systems differ by a factor of 3. What is the physical basis for this difference? Until independent information is provided that substantiates these parameter adjustments, the development of a <u>predictive</u> model is impeded. At this point, observations and experiments are needed on fate constants and parameters, along with improved estimates of inputs and chemical concentrations in the various environmental compartments. It is important to emphasize that NRBS made considerable progress in model development for the transport and fate of contaminants given the restricted database available at the onset of the study, knowledge of transport processes, and the diversity of organic contaminants that were identified as important chemical species to model (see Appendix 1 for comparison with other studies).

The food-chain model is closely linked to the contaminant fate model in developing predictions concerning the distribution of contaminants in the biota. The steady-state food-chain model considered the distribution of the three major classes of chemical species with very different physical-chemical and pharmacokinetic features (e.g. polychlorinated dibenzofurans, resin acids, and chlorinated phenolics) and there are very few comparable studies for river systems. The basis for the bioenergetic approach is an accurate description of the food-chain (or food-web) for the Northern Rivers. Considerable lumping of invertebrate families and orders into broad functional categories had to be undertaken (e.g. bottom feeding invertebrates and filter-feeding invertebrates), and it would be important to validate this classification scheme and examine whether the broad lumping of all species from particular orders is appropriate. Further experimentation is also required to evaluate the chemical assimilation efficiencies and excretion rates that were adopted in model calibration for the components of the food-chain.

As discussed in Section 3, there are several possible hypotheses that need to be examined to account for the significant discrepancy between model output and observed concentrations of contaminants in the various food-chain components. These hypotheses examine whether the inability of the model to capture variation in the distribution of contaminants throughout the food chain is related to a violation of the steady-state assumption, additional assumptions regarding model formulation and parameter estimation, and/or inappropriate input concentrations owing to high detection limits. For example, the model makes key assumptions about the exposure concentrations during growth of all food-chain components and these assumptions are sensitive to information regarding migratory movements of fish-species etc. Do mountain whitefish and long-nose suckers feed exclusively in mainstem rivers, or do they obtain a significant amount of their food during foraging bouts in tributaries with lower concentrations of organic contaminants? In other words, more information is required on the robustness of the food-web configuration and quantitative estimates of the spatial distribution of highly mobile fish species. It is crucial that these alternative explanations for the lack-of-fit in model calibrations be examined.

The hydraulic model of the Peace River provided an adequate prediction of water level and discharges for "moderate" flood events. Further model developments are limited by the availability of geometric data between Peace River and Peace Point, and a more complete characterization of tributary inflows.

4.1 General Recommendations for Future Work

1) The development of predictive transport models for the Northern Rivers is paramount for future progress. The rates of creation and destruction of materials at one point in space along the river may be well understood in some circumstances, but without a model to predict the transport of water, materials, and in some cases sediment, this knowledge cannot yield accurate predictions of water quality. Spatially-explicit models of water and sediment transport can then be used to assist our understanding of sedimentation processes, cross-channel variability, and mixing zone effects. A hydraulic model that is capable of handling dynamic flows would be highly desirable for the Athabasca River and the Smoky-Wapiti River System. At a minimum, time of travel studies should be conducted and Leopold-Maddox relationships revisited. At present, this is crucial for ensuring that the model predictions for dissolved oxygen are rigorously tested and for providing key information to evaluate the current calibration of WASP for the Northern River Systems. It is imperative that if WASP is going to be employed as the model of choice for the next level of complexity that the transport algorithms be critically assessed.

2) The modelling emphasis in NRBS was on predicting changes to the environment. This is only one-half of the story if the goal is to predict the impact on biota, including residents in the area. A crucial stage is the development of models to predict how

changes in the environment alter individual growth, reproduction, and probability of survival and how these changes affect population level phenomena, such as abundance, temporal and spatial dynamics, probability of local extinction etc. This is the "effects" side of the equation mentioned in Section 1, and it is the principle topic of Question 13b raised by the NRBS Study Board. Note, the "effects" side of the equation was not ignored by NRBS; predicting changes to the environment is a necessary precursor to predicting subsequent effects of these environmental changes on the biota as evidenced by the review of instream flow needs assessment (IFN methods) provided by Walder 1995 (Appendix 2). In NRBS, the principle focus on the effects side of the equation was to gather some of the pertinent empirical information needed to develop models on effects (e.g. effects of dissolved oxygen concentrations on development and survivorship of mountain whitefish eggs, migratory patterns of fish species in mainstem and tributaries etc.).

If modelling efforts in the Northern Rivers continue then more emphasis should be placed on the development of models that link environmental changes with expected changes in the biota. The stage is set to develop the quantitative link between changes in environmental variables and changes in the biota. There has been considerable progress made in the ecological and ecotoxicological literature on rigorous approaches that link changes in individual performance caused by environmental changes to population level phenomena. This link tightens the causal chain of reasoning, thereby improving our ability to distinguish impacts produced by industrial discharges from natural variability in the abundance of populations and community composition (in space and time). Predictions from models for changes in concentration of contaminants in water column, sediments, and biota, or changes in dissolved oxygen concentrations need to be coupled to expected changes in biota.

3) A "process oriented" database, which spans the diverse modelling efforts, needs to be created and maintained. The need for a monitoring database has been established in other Synthesis Reports. Please note, that the database referred to here is not the same as the monitoring database justified elsewhere in NRBS. The process-oriented database, consists of parameter values, the data underlying their estimation, data from any experiments used to estimate rates of creation or destruction of material (e.g. SOD measuring, algal growth rates, etc.), and spatial components of these measurements. This database could be implemented within a GIS framework, so that spatial location of measurements could be included as a descriptor. This database would enable investigators developing models for different water quality variables in the Northern Rivers to share and compare process-oriented data for common parameters, temperature dependencies, or conversion ratios. It would also allow for the efficient monitoring and comparison of published values generated from other studies on rivers throughout the world.

4) Management objectives need to be clarified with regard to scale of prediction (i.e. near-field far-field approaches, pre-impact and post-impact sites) and a corresponding hierarchy of models developed with realistic expectations. One has to break away from

the mindset that there is one (and only one) model that represents "the" solution. Models are simply tools to assist the scientific or management process. There is considerable merit in the approach of developing an array of models with varying degrees of complexity and scale of prediction, as witnessed by the work on modelling dissolved oxygen.

There has to be a critical evaluation of management goals and data availability. In some cases (e.g. modelling certain organic contaminants), there are more model equations than observations to derive parameter estimates! This obviously represents an absurd case, and it is unrealistic to expect the delivery of a modelling tool to assist in the management process under these circumstances. In other cases, the nature of the discharges from industry coupled with environmental variability dictate that more dynamic models are required to predict impacts on water quality. To evaluate the impact of these industrial discharges, we need a modelling framework that predicts both small scale effects and large-scale (and in some cases potentially long-term, i.e. among year changes) effects on water quality and ultimately the biota. There has to be a recognition that since this framework pertains to particular rivers, sufficient resources have to be applied to make the appropriate measurements on the appropriate spatial and temporal scales. To a large extent the model formulations exist, but their application in the Northern Rivers is limited by availability of input data and process-oriented data. An investment in data collection on the appropriate spatial and temporal scales and in conducting process-oriented rate measures is required to meet the predictive role expected of these models.

5) It is crucial that models developed in NRBS be flexible enough to deal with the evolution of the nature of industrial discharges. The pulp and paper industry has made strides in improving the water quality of discharges, and as a result of process changes the type and nature of contaminants released into the environment is changing over time. Any models that are developed need to be flexible enough to "evolve" with these changes. In NRBS the principle foci of water quality models were dissolved oxygen concentrations and organic contaminants. Given the empirical results obtained by NRBS on changes in nutrient limitation of primary producers along the length of the Northern Rivers, and the potential interaction between enrichment and response to contaminants, the development of water quality models concerning nutrient effects on the biota should be initiated. This could be accomplished using the WASP modelling framework, but the applicability of processes included in the eutrophication module of WASP should be critically evaluated.

The changing nature of discharges has one benefit that could be exploited from a modelling perspective in the testing of models developed by NRBS. The changing discharges imply reduced inputs for some key contaminants (e.g. polychlorinated dibenzofurans). This change in inputs represents a perturbation that could be used to test the ability of the contaminant fate models to predict responses under changing environmental input conditions. In other words, perhaps the changing nature of the discharges could be used as an experiment to test the ability of the contaminant fate model to capture longer-term changes in contaminant concentrations in sediment compartments.

6) Modelling of water quality and effects on biota could perhaps be achieved most economically and efficiently by the establishment of modelling teams. Please note, this is not a call for the creation of inefficient committees. Modelling water quality and impacts require state-of-the-art information and data from a variety of scientific disciplines (e.g. models for physical transport, behaviour of chemicals, dynamics of biota etc.). These teams could be composed of experts drawn from industry, government, and universities who would oversee modelling in a particular area. Each team would be led by an individual who is ultimately responsible for the modelling effort, and who would co-ordinate the work of consultants. Because of the interdisciplinary nature of the modelling problems, each team would be ideally composed at a minimum of a hydrologist, environmental chemist, and biologist, and ideally committees would share members. The team would be responsible for quality control and decisions regarding model structure or parameter estimation. In other words, the team would function as an "expert system" in making decisions regarding model formulation, parameterization, and evaluation.

Modelling teams could be established for each of the major modelling efforts. Each modeling team would be responsible for a particular aspect of water quality, and a modelling committee consisting of the team leaders of each of these separate groups could be established to synthesize results from disparate modelling efforts, co-ordinate the use of algorithms and parameter estimates, and deal with strategic problems of integrating scales and management objectives.

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NORTHERN RIVER BASINS STUDY

APPENDIX A - TERMS OF REFERENCE

**Project 5327-D1: SYNT; Modelling in the Northern River Basins Study
SYNTHESIS REPORT PREPARATION
(Peace-Slave Biophysical Description; IFN Modelling)**

I. BACKGROUND & OBJECTIVES

Examination of effects of flow regulation and instream flow needs is needed to address Northern River Basins Study (NRBS) Board Question #10, "how has and how could river flow regulation impact the aquatic ecosystem?". Development of models and/or analytical approaches for estimating instream flow needs and for evaluating effects of different flow regimes will also address parts of questions 13 and 14, which relate to predictive tools, cumulative effects assessments, and ecosystem condition assessment. Another Study Board question (Question #3) asks, in part, about the non-consumptive uses of water. This is related to the flow regulation issue because ecological uses of water and instream flow needs for environmental protection are part of the non-consumptive use of water.

The following NRBS projects are directly related to IFN analysis and are projects of the Other Uses Component:

1. Project 4103-C1 - Instream Flow Needs Workshop
2. Project 4131-D1 - Aquatic Habitat Mapping for Instream Flow Needs (Peace River)
3. Project 4133-D1 - Aquatic Habitat Assessment (Peace River) - flow model data collection
4. Project 4134-D1 - Riparian Wildlife Habitat Data Collection (Peace River)

Effects of regulation of flow in the Peace River on aquatic and riparian habitats and on the Peace-Athabasca and Slave deltas are also the subject of several other NRBS projects, which are led by the Hydrology/Hydraulics Component. These include:

1. Project 1321-D1 - Temporal Evolution of Channel Morphology and Riparian Vegetation (Peace River)
2. Project 1422-D1 - Hydrometeorlogical Conditions Controlling Ice Jam Floods on the Peace River
3. Project 1154-D1 - Peace/Slave River Flow Modelling
4. Project 1521-D1 - Regulation Effects on the Slave River Delta: Landform and Distributary Sensitivities to Changes in River Regime

5. Project 1512-D1 - Satellite Imagery of Flooding Extent - Peace Athabasca Delta

The results of all of the above studies will serve as source material for a synthesis report that will deal with effects of flow regulation on the Peace-Slave River system. Some of these studies will also provide information important for preparation of portions of synthesis reports planned by the Synthesis and Modelling Component and the Other Uses Component.

The purpose of this project is to undertake preparation of certain specified sections of the flow regulation synthesis report and a synthesis report on modelling.

II. REQUIREMENTS

1. Prepare a section for the Effects of Flow Regulation synthesis report that provides a detailed biophysical description of the Peace-Slave River system. Emphasis will be on aspects of the Peace-Slave River system potentially affected by flow regulation. This section will be based on previous publications and maps, relevant NRBS reports, and databases of relevant information. Approximate length is 15-20 pages. Following is a list of topics to be included.

    a) Landforms
    b) Climate
    c) River Geomorphology
    d) Basin Hydrology
    e) Vegetation Communities
    f) Fish Resources
    g) Wildlife

2. Prepare a report on modelling approaches that can be used to assess instream flow needs (IFN) in the Northern River Basins. This report will include a critical review and evaluation of existing numerically-based IFN models that have been used from a fisheries and a broader ecosystem health protection perspective. Approximate length of the report is 20 pages. The following topics will be covered:

    a) A critical evaluation of existing IFN modelling approaches. This section will build on the 1995 report prepared for Alberta Environmental Protection, Fish and Wildlife Services by EnviResource Consulting Ltd. This evaluation should clearly identify the data and parameterization requirements of each of the modelling approaches as well as the respective virtues and shortcomings in their ability to assess instream flow needs of fish populations and other aquatic biota.

    b) Evaluate the models reviewed in Section 2a in light of their applicability for use on the Peace, Athabasca, and Slave river systems.

    c) Make recommendations on future model development needs as pertains to the Athabasca, Peace and Slave river systems. This section should indicate what the current IFN-related data deficiencies are in these river systems and recommend what research and development is still necessary to implement an IFN-based modelling approach for fisheries and aquatic ecosystem protection and management.

III. REPORTING REQUIREMENTS

1. The Contractor is to provide draft and final report sections in the style and format outlined in the NRBS Style Manual. A copy of the Style Manual entitled "A Guide for the Preparation of Reports" will be supplied to the contractor by the NRBS.

2. Five copies of each draft report section, along with electronic disk copies, are to be submitted to the Project Leader/Certification Officer as indicated in the schedule below.

SCHEDULE FOR DELIVERY OF DRAFT REPORT SECTIONS

Item	Section Name	Delivery Date
1.	Biophysical Description of the Peace-Slave River System	August 15, 1995
2.	Modelling Approaches and Model Development Needs for Assessing Instream Flow Needs	September 15, 1995

Three weeks after the receipt of review comments on the draft report sections, the Contractor is to provide the Project Leader/Certification Officer with two unbound copies of each final report section along with electronic disk copies.

3. Text for the report should be set up in the following format:

   a) Times Roman 12 point (Pro) or New Times Roman (WPWIN60) font.
   b) Margins are 1" at top and bottom, 7/8" on left and right.
   c) Headings in the report body are labelled with hierarchical decimal Arabic numbers.
   d) Text is presented with full justification; that is, the text aligns on both left and right margins.
   e) Page numbers are Arabic numerals for the body of the report, centred at the bottom of each page and bold.

4. If photographs or digitized images are to be included in the report text they should be high contrast black and white unless colour is essential for communicating relevant information.

All tables and figures in the report should be clearly reproducible by a black and white photocopier.

5. Along with copies of the final report sections, the Contractor is to supply an electronic version of the report sections in Word Perfect 5.1 or Word Perfect for Windows Version 6.0 format.

   Electronic copies of tables, figures and data appendices are also to be submitted to the Project Leader/Certification Officer along with the final report sections. These should be submitted in a spreadsheet (Quattro Pro preferred, but also Excel or Lotus) or database (dBase IV) format. Where appropriate, data in tables, figures and appendices should be geo-referenced.

6. All figures and maps are to be delivered in both hard copy (paper) and digital formats. Acceptable formats include: DXF, uncompressed E00, VEC/VEH, Atlas and ISIF. All digital maps must be properly geo-referenced.

7. All sampling locations presented in report and electronic format should be geo-referenced. This is to include decimal latitudes and longitudes (to six decimal places) and UTM coordinates. The first field for decimal latitudes / longitudes should be latitudes (10 spaces wide). The second field should be longitude (11 spaces wide).

IV. CONTRACT ADMINISTRATION

The Scientific Authorities for this project are:

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for items of a scientific nature related to work of the Hydrology/Hydraulics Component; and

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for items of a scientific nature related to work of the Synthesis and Modelling Component.

The Project Leader/Certification Officer for this project is:

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Appendix B: Case Studies (E. McCauley and T. Rosner)

Introduction

The Case Studies described here are examples of models applied to real systems. Most of these studies include a description of the model used, the method of calibration, verification, and evaluation of the model. In addition several studies include an analysis of the expected results after changing some important features of the model which could have important implications for management decisions. NRBS is concerned with factors which are important to water quality and the effects of these factors on the organisms in the aquatic environment. Important features are such things as organic chemicals, pesticides, biological and chemical oxygen demand, nutrients, flow and habitat. The dynamics of these constituents as a function of ecosystem characteristics can give insight into health, management options and risks.

In this analysis of case studies, a general division is made between those models designed to describe the distribution of constituents in the environment (transport models) and those designed to describe the movement and concentration of constituents among organisms (food chain and bioconcentration models).

These studies were reviewed in order to understand the effects of chemicals on systems, however, they deal with the movement and concentrations of chemicals in the environments and organisms in a non-interactive way. That is, rates, food chain structure and thus the movement of the chemical, are not affected by the chemical concentration. This field of study includes understanding of how chemicals in the environment change ecosystems from an ecological, economic, and human health perspective. Risk assessment, expert systems, and dynamic models with feedback between constituent concentrations and ecosystem processes are necessary in order to make management decisions. Although these case studies have a more limited scope, the types of models used in them form the basis for understanding interactions between chemical movements and ecosystem processes. Some descriptions of a case studies include a table (Tables 1- 9) which describes the method of calibration of the model. Rates which need to be calibrated and the mechanism of calibration give the reader an idea of what features are more mechanistic and which are more empirical in each model. These tables also give an idea of how system specific parameters are estimated and the level of uncertainty expected in each investigation.

Transport Case Study 1

G. N. Van Orden and C. G. Uchrin. 1993. The study of dissolved oxygen dynamics in the Whippany River, New Jersey using the QUAL2E model. Ecological Modelling 70:1-17

The variables modelled were DO, CBOD, NBOD, SOD, daily averaged algal photosynthesis and respiration, and reaeration. There were nine reaches with 0.2 km long computational elements within them (completely mixed cells). Each reach has constant hydrogeological characteristics and reaction constants. Each computational element is assumed to be homogeneously mixed.
The single constituent mass balance model equation numerically iterated by QUAL2E w.r.t. both distance and time is:

$$\frac{\partial C}{\partial t} = \frac{\delta}{A_x \delta x}\left[A_x D_x \frac{\delta C}{\delta x}\right] - \frac{1}{A_x}\frac{1}{\delta x}\left(A_x \bar{u} C\right) + \frac{dC}{dt} + \frac{s}{V}$$

C- concentration
$\bar{u}$ - mean velocity in the unit
V- incremental volumes
Ax- cross sectional area
S- internal sources and sinks
Dx- longitudinal dispersion coefficient
$\frac{dC}{dt}$ - refers to constituent change w.r.t. growth and decay

Although this is a dynamic model, this study only considers steady-state calibration and verification.

Calibration

Table 1. Calibration of the model.

Component	Method of Calibration
CBOD	- First order decay coefficients determined for each reach using concentrations in each computational element. Decay coefficient for the first reach was assumed to be equal to others and the balance of the loss was assumed to be due to settling.
NBOD	- ammonia, nitrite decay determined by first order fit to concentrations along stream. - oxygen use of nitrite-N was adjusted to account for biotic assimilation.
SOD	- 0th order reaction dependent on surface area, measured in situ.
Algae	- daily averaged productivity and respiration were measured using light dark bottles. They were equal and so algae were not included in the model.
Reaeration	- calculated using methods of USEPA(1985) minor adjustments were made to achieve a better fit during model calibration. - reaeration from dams ware also calculated from existing methods.

Inputs from point source and tributaries	- measured inputs of DO, CBOD, ammonia-N, nitrite-N, flow.

The model was calibrated using data from 1985 and verified using 1980. The amount of oxygen utilized as the nitrite-nitrogen decayed was not strictly stoichiometric. It was assumed that ammonia-N → nitrite-N → nitrate-N the values of the last two will be predicted higher because the sinks such as uptake by organisms are not taken into account. DO will be correct however of the adjustment.

Dynamic algal populations were not considered and it was found that respiration = productivity and thus algae did to have an important affect on DO in the steady state model. However there was significant diurnal variability in DO as well as other parameters. In order to characterize variability in sources a 24 hour study was conducted on sources. It was found that tributaries had little ammonia, nitrite, nitrate, CBOD variability over a 24 hour period. The upper boundary stations showed variability in CBOD and nitrite. Also, there was a large amount of variability in DO at all points probably due to algal photosynthesis. There was also significant variation in all components in the effluent of one of the point sources.

Verification

This is not discussed in much depth but it appears as though parameters are adjusted according to the new temperature and flow regimes as well as the different inputs from the point sources. Model results are compared to the measured results for DO, CBOD, ammonia, and nitrite. Both the calibrated and verification model runs give a very accurate approximation of average DO, CBOD, ammonia, and nitrite from visual inspection. There is a large amount of variability in the verification data but there is no attempt at a statistical measure of the success of the model for describing concentrations of state variables.

Simulation experiments

Several simulations were run to determine which approaches should be taken to raise dissolved oxygen concentrations to acceptable levels. It was determined that although lowering inputs from the sewage treatment plants would contribute, a majority of oxygen was consumed by the SOD. To increase oxygen levels the amount of particulate matter being released from the sewage treatment plants would have to be reduced as well as the organic matter already accumulated in the impoundment areas.

Remarks

Although this model does not contain details of the biological aspects influencing dissolved oxygen, the black box approach (first order decay of NBOD, BOD) is very successful at predicting the mean dissolved oxygen level in the river. Also, using a steady-state deterministic model when inputs are both stochastic and vary diurnally does not hamper the models ability to predict mean dissolved oxygen concentrations accurately. In water quality models, both the average and distribution of concentrations of state variables are important and this paper would benefit by some analysis of the range of variability. This would require more data to determine the range of variability and distribution of concentrations within the river. The deterministic variability due to diurnal variation of the inputs is discussed in a subsequent paper.

Transport Case Study 2

G. N. Van Orden and C. G. Uchrin. 1993. Dissolved oxygen dynamics in the Whipany River New Jersey: deterministic/stochastic time varying model . Ecological Modelling 70:19-34

The first case study on this system used a steady-state deterministic model to describe CBOD, NBOD, and DO for the river. This model accurately described mean concentrations in the river. It was noted that there was significant daily fluctuations in point source inputs. There was no net oxygen consumption or production by algae when averaged over a 24 hr period but there was over smaller time periods. The steady state model cannot account for these daily fluctuations. They reanalyze the data using a model that can include deterministic fluctuations as well as stochastic variability in inputs and rates.

To analyze the daily fluctuations of NBOD, CBOD, and DO Fourier analysis was used. Each parameter can be described by the following time series:

$$f(t) = \bar{f} + \sum_{j=1}^{n} R_i \cos(w_i t + \theta_i) + f_r(t)$$

$f(t)$ - parameter value at time t

$\bar{f}$ - mean value for the time series

R_i - amplitude of the ith harmonic

w_i - angular frequency of the ith harmonic

θ_i - phase angle of the ith harmonic

$f_r(t)$- parameter residual at time t

Variability in inputs can be converted to variability at a station down the river at a later point in time by using a frequency transfer function which depends on the steady-state model used to describe important stream variables and the velocity of the stream. In this study parameters were converted to DO deficits at a station downstream of the inputs. The input parameters that were thought to be important in influencing DO variability downstream were: DO deficit in the river at the input point (later found to be unimportant due to oxygenation at other points), NBOD, CBOD and variability at the downstream station due to daily fluctuation in photosynthesis. All other parameter values were taken from the steady-state calibration used in the first study.

Results

This model showed that a large amount of both cyclic and stochastic variability at a station downstream from a point source could be explained by daily fluctuations in photosynthesis and by variability in the concentrations of CBOD and NBOD in the inputs. This has implications for other water-quality modelling efforts as it shows that deviation from steady-state equilibria can be dependent at different points in the river (with the appropriate time lags). This may make some of the statistical analysis used in water-quality studies questionable. This study shows how analysis and prediction of variability in water quality variables can be accomplished without abandoning the steady-state models which are consistently used to study water quality.

Transport Case Study 3

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

The Pigeon River Allocation Model (PRAM) was developed using the QUAL2E-UNCAS shell. The model for the mass transport of each constituent includes the effects of advection, dispersion , dilution, constituent reaction and interactions as well as sources and sinks. The models assumes that the hydraulic regime is in steady state.

$$\frac{\partial M}{\partial t} = \left[\frac{d\left(A_x D_l^{(dc/dx)}\right)}{dx}\right] dx - \frac{d\left(A_x uC\right)}{dx} + \frac{dC}{dt} A_x dx + s$$

M-mass
C- concentration
Ax- cross-sectional area
Dl- dispersion coefficient
u - mean velocity
s- external sources or sinks

The primary state variables DO, UCBOD, and chloride, organic nitrogen, ammonia, nitrate, nitrite, organic phosphorus, dissolved phosphorus, and chlorophyll-a. The important biological and chemical mechanisms included in the model were microbial/chemical degradation and transformation, respiration, primary productivity, and chemical oxygen demand. While the physical mechanisms were advection, reaeration, deaeration, and mixing. This mode also takes into account lowered decay of BOD and decay of nitrogenous compounds when there are low oxygen levels.

The measurements taken from point sources and tributaries as well as measured along the river in order to calibrate the model were: stream flow, dissolved oxygen, temperature, biological oxygen demand (BOD), sediment oxygen demand (SOD), atmospheric exchange, light attenuation, % shading, chlorophyll a, total kjeldahl N, ammonia, nitrate, nitrite, phosphorus ortho-phosphorus, chloride.

Calibration
The model was calibrated using visual correspondence between model and field observations to approximate the best 'fit'. Further calibration was done by systematically varying each parameter 10-15% to get a matrix or parameter values which yield the smallest total sum of squares error between field and modelled data. In general the model was within 95% confidence interval of the verification data.

Observed and predicted concentrations of chloride were similar so it was concluded that flow regimes were represented accurately. The major process affecting UCBOD, and phosphorus is dilution. Chlorophyll-a had very low values in both the model and the stream and it was concluded that there would be very little effect on dissolved oxygen. The major process affecting dissolved oxygen is the oxidation of ammonia and nitrite. Due to low algal biomass there was little uptake of nitrate.

Table 2. Calibration of the model.

Constituent	modelled processes	method of calibration
Hydraulic discharge	discharge coefficients	determined from available data concerning stream velocity, cross sectional area and depth all of which were either measured or calculated from measurements. Assumption of steady state.
Carbonaceos BOD	amount of CBOD	determined from lab analysis
	degradation rate	laboratory analysis
	settling	mass balance for CBOD
Nitrogen (organic nitrogen, ammonia nitrate, nitrite)	hydrolysis from organic nitrogen to ammonia	?
	settling	?
	algal excretion and uptake	?
	benthic regeneration	?
	oxidation or nitrogenous compounds	?
Dissolved oxygen	surface reaeration	calculated from physical characteristics
	artificial infusion	measured
	deaeration after infusion	experimental measurement of deaeration in pans and correcting for other losses of oxygen from respiration measurements
	photosynthesis	light and dark bottles
	SOD	measured in situ
	chemical oxygen demand	?
Phosphorus (organic, dissolved and total)	transformation cycle from organic phosphorus to dissolved phosphorus	?
	algal uptake and excretion	?
	decay	?
	settling	?
	benthic regeneration	?
Chloride	dilution	from hydrological data
all constituents	inputs from tributaries and point souses	measured during field study

Verification

Verification was done on the day following the intensive field survey to collect calibration data. Only UCBOD and DO were validated for the next day. The data for the next day were taken from different areas but flow temperature, effluents would be the same. There was successful model fit to the data. The model was also validated using data collected under a much higher flow regime and different UCBOD in effluents. In this verification only chlorides, dissolved oxygen, and nitrate were used. The model predictions were also accurate for this verification. Success for verification was when model and recorded values were regressed and there was an intercept 0 and 1 was within the 95% confidence interval of the slope.

Simulation experiments

The model was modified to predict the effects of management decisions. The first alternative was to remove the two water treatment plants discharges. This had no effect on DO or BOD concentration in the river and resulted in only a minor reduction in nitrate. Flow reduction at the pulp mill effluents would decrease BOD and ammonia directly downstream of the mill though levels would be approximately the same further down the river. Flow reduction at the mill would actually lower DO levels due to the reduction in artificial oxygenation ant the point of discharge but these also increase to nominal levels further down the river. If the oxygenators were removed, this would strongly decrease DO in the region of the oxygenators but does not affect oxygen levels further down the river.

Remarks

It is interesting that the sidestream oxygenation units do not contribute to the consumption of CBOD and the majority is transferred downstream into the lake. The role of these oxygenators is mostly to maintain oxygen levels within the river. There are many biological processes which are independently incorporated into the model but it is unclear where estimates of these processes come from. There may be too much detail for the amount of data available to calibrate this model. It does not seem justifiable to include these components if they do not change the shape of the modeled constituent profiles. If the model parameters are to be adjusted to get a good fit then including for example algal uptake and excretion, benthic regeneration, and settling separately when they are all presumably constant rate processes seems to imply a greater understanding of the system than is possible from available data.

One shortcoming of the analysis is that during model verification the null hypothesis is that the model does fit the data. There is no discussion of the power of the analysis to detect a poor fit.

Transport Case Study 4

K. Schaarup-Jensen and T. Hvitved-Jacobsen.1994. Causal stochastic simulation of dissolved oxygen depletion in rivers receiving combined sewer overflows. Water Science and Technology 29:191-198.

The model is MOUSE-SAMBA which is used to model urban runoff and includes extreme events when runoff is large. MOUSE-SAMBA is used to calculate the amount of organic matter discharged to the stream. The other part of the model MOUSE-DOSMO is used to model water quality. In combination, these models are used to describe dissolved oxygen depletion in rivers and streams receiving combined sewer overflows. This study includes variability in some parameters which are known to vary either from event to event at one location or from one location to another.

Instead of one model calibration the model is run several times with a variety of parameter values for highly variable parameters. This model is used to simulate the unsteady stream flow caused by combined sewer outflows and a transport component to simulate the daily stream DO variations in time and space.

Calibration

Table 3. Calibration of the model.

Component	Representation in model	Calibration
flow	undamped kinematic wave is used to calculate stream depths and flow in time and space.	calculated by SAMBA
soluble organic matter	first order degradation by bacteria	earlier field studies
	first order absorption by biofilm	earlier field studies
particulate organic	first order adsorption and sedimentation due to flow characteristics	earlier field studies
	first order degradation at the bottom	earlier field studies
chemical oxygen demand	first order decay	earlier field studies
dissolved oxygen	background level mean concentrations and diurnal variation	measured in the stream that was studied
	reaeration	

The major focus of this study is to look at the sources of variation, their magnitude and the effects of this stochasticity on dissolved oxygen. Data on rates of processes was assumed to be accurate and no validation was performed. The means and variances of rates were utilized. Variability in the COD of runoff was determined to be independent of rain event size and length of the preceding dry weather period and had a log-normal distribution. The model was used to describe the distribution of dissolved oxygen levels in the stream for all rainfall events on record for the stream. Three data sets were derived. One in which rate constants were chosen randomly from their distributions but COD was held constant, one in which only COD value were stochastic and one in which rate constants and COD were chosen randomly from their distributions.

Results

These simulations showed that although the reference simulation was well above water quality standards, a significant proportion of rainfall events could lower dissolved oxygen levels well below water quality criterion when the natural variability in rates and concentrations of COD is considered. This effect is strongest for rare events with a large amount of rainfall where water quality standards are lower but the natural variability produces and even larger percentage of occurrences of DO falling below water quality standards.

Transport Case Study 5
A. Taskinen, O. Varis, H. Sirviö, J. Mutanen, and P Vakkilainen. 1994. Probabilistic uncertainty assessment of phosphorus balance calculations in watershed. Ecological Modelling 74:125-135.

This study uses a simple mass balance model to describe phosphorus in a river connecting two lakes. The model describes the rate of phosphorus input into the stream from the upper lake, inputs from point sources and output into the lower lake. All biological processes, non-point inputs, resuspension and errors are contained in the residual term.

$$c_u Q_u + P_{wtp} + P_{ffp_1} + P_{ffp_2} + Y = c_l Q_l$$

c - concentration
Q - river flow
P - phosphorus load
u - upper lake
l - lower lake
wtp - water treatment plant
ffpi - tributary inputs
Y - residual term

From input and output data collected over 10 years the mass balance and residuals were calculated for March, May, August, and October. The distribution of the inputs was taken to be either truncated normal or truncated lognormal. Using weighted least squares, the expected value of the residual was obtained for each month. This estimate is weighted by the inverse of the variance in which means with the lowest variance get the greatest weight. For normal data this is the minimum variance unbiased estimator and with non-Gaussian data the estimate is the best linear unbiased estimate of the mean.

From information about the variability in inputs, probabilistic simulations were done using the Latin Hypercube method. This method divides the probability distribution into equal sections and randomly samples from each section. This is in contrast to Monte-Carlo methods which use random samples without the initial division of the probability distribution. Two different analyses were done to study uncertainty. In the first, only one parameter was varied at a time to determine the role of each parameter in influencing variability and the relative sensitivity of the model to variability in each parameter. In the second analysis all parameters were randomly chosen from their distributions to simulate actual conditions in the system.

It was determined from both analyses that uncertainty in the phosphorus flux from the upper lake and into the lower lake had the greatest effect on the variance of the residual term and thus the phosphorus balance of the system. The uncertainty in inputs can cause large uncertainty in the phosphorus entering the lower lake. So much so that the use of more detailed mechanistic models may not change the ability to predict phosphorous outputs of the system. The authors state that this analysis would be strongly impaired if only the mean behavior of the system were studied. They also point out the dangers in using complex deterministic models without a study of uncertainty.

Transport Case Study 6

B. Cazzelles, K. Fontvieille and N.P. Chau. 1991. Self-purification in a lotic ecosystem: a model of dissolved organic carbon and benthic microorganisms dynamics. Ecological Modelling 58:91-117.

Many models of water quality emphasize the importance of transport while biological and chemical processes are oversimplified into first order rates. This model includes both transport and a realistic biodegradation sub-model based on biofilm kinetics. This model is capable of modelling diffusion and heterogeneous rates throughout the depth of the biofilm but may also be integrated through the depth of the biofilm. The global model describes the evolution of five main carbon compartments:

dissolved organic carbon (C)
suspended particulate organic carbon of diameter class i (C_{spi})
benthic particulate organic carbon of diameter class i (C_{bpi})
microorganism biomass (Bi)
macroinvertebrate biomass (Ba)

This model incorporates transport, movement between physical compartments and biological processes. The main processes and compartments are shown in the following generalized model.

$$\frac{\partial C}{\partial t} = \text{Transport - Consumption by Bi + Inputs}$$

$$\frac{\partial C_{spi}}{\partial t} = \text{Transport - Sedimentation + Scouring + Inputs}$$

$$\frac{\partial C_{bpi}}{\partial t} = \text{Sedimentation - Scouring - Consumption by Bi and Ba + Mortality of Bi and Ba}$$

$$\frac{\partial Bi}{\partial t} = \text{Assimilation of C and } C_{bpi} - \text{Respiration - Mortality - Predation by Bi}$$

$$\frac{\partial Ba}{\partial t} = \text{Assimilation of } C_{bpi} \text{ and Bi} - \text{Respiration - Mortality - Predation by Bi} \pm \text{Drift - Emergence}$$

However this application of the model considers only dissolved organic carbon.

Hydrodynamical sub-model:

The river is assumed to have a trapezoid shape cross. Lateral input discharge is proportional to the flow and two channels of different slopes can be used together with a supply of water from a small tributary.

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = qd$$

A- cross sectional area of flow (L^2)
Q -discharge (L^2/T)
qd - lateral non point source in put discharge ($L^3/L/T$)

Transport sub model:

Because the flow is mainly longitudinal, a one dimensional flow model can be derived in which only longitudinal variation is considered:

$$\frac{\partial A \cdot C}{\partial t} + \frac{\partial Q \cdot C}{\partial x} = \frac{\partial}{\partial x}\left(A \cdot D_L \cdot \frac{\partial}{\partial x} C\right)$$

c - local mean concentration of dissolved substrate (M/L^3)
C - organic substrate concentration (COT or COD) (M/L^3)
K_{xj} - coefficients for local turbulent mass transfer in the j directions (L^2/T)
D_L - longitudinal dispersion coefficient (L^2/T)

Biological sub-model:

Modelling benthic bacterial decomposition processes must include transfer processes of organic material from water to sediment and mechanisms of organic matter incorporation into microorganisms biomass. To simulate dissolved organic carbon dynamics in the river a biofilm model was used. This model incorporates organic substrates transfer through the water-sediment interface, diffusion throughout the biofilm, bacterial incorporation, bacterial growth on DOC, endogenic metabolism, lethality, biofilm shearing, and use compounds produced for bacterial autolysis. Organic matter decomposition in the free flowing water is neglected (because bacterial respiration was below the sensitivity threshold for the method used). It is assumed that biodegradation reactions are limited only by organic carbon (oxygen is not limiting) and exchange length between biofilm and water is approximated by the wet perimeter of the flow (Pm).

$$\frac{dC}{dt} = -\frac{K_t P_m}{A}(C - C_f$$

$$\frac{dX_s}{dt} = \frac{K_{arr}}{H} X_f H_f$$

$$\frac{dC}{dt} = \frac{K_t P_m}{A}(C - C_f) - \left(\frac{\mu_{max}}{Y_1} \frac{C_f}{C_f + K_s} - \frac{k_2}{Y_2} - K_e \right) X_f$$

$$\frac{dX_f}{dt} = \left(\mu_{max} \cdot \frac{C_f}{C_f + K_s} - k_2 - K_{arr} \right) X_f$$

C - organic substrate concentration (C.O.T. or C.O.D.) (M/L^3)
K_t- transfer velocity at the water biofilm interface (L/T)
P_m - wet perimeter (L)
C_f - organic substrate concentration in biofilm (M/L^3)
K_{arr} - biofilm shearing rate (1/T)
X_f - biofilm cellular density(bacterial or microorganism biomass) (M/L^3)
H - flow depth(L)
H_f - biofilm thickness (L)
K_s - half saturation coefficient for organic substrate (M/L^3)
μ_{max} - maximum growth rate (1/T)
k_2- bacterial decay rate (T)
Y_1- yield coefficient expressed in g of biomass (DNA) formed per g of substrate used
Y_2 - fraction of degenerate cells that can be used by biofilm biomass.

X_S - suspended bacterial biomass (M/L^3)
K_e - endogenous metabolism rate (1/T)

Integrated Model:

$$\frac{\partial A\cdot C}{\partial t}+\frac{\partial Q\ C}{\partial x}=\frac{\partial}{\partial x}\left(A\cdot D_L\cdot\frac{\partial C}{\partial x}\right)$$

$$\frac{\partial A\cdot C}{\partial t}+\frac{\partial Q\cdot C}{\partial x}=\frac{\partial}{\partial x}\left(A\cdot D_L\cdot\frac{\partial C}{\partial x}\right)+C_q qd-K_t P_m\left(C-C_f\right.$$

$$\frac{\partial A_f\cdot C_f}{\partial t}=K_t P_m\left(C-C_f\right)-\left(\frac{\mu_{\max}}{Y_1}\frac{C_f}{C_f+K_s}-\frac{k_2}{Y_2}-K_e\right)B_f P_m$$

$$\frac{\partial P_m\cdot B_f}{\partial t}=K_t P_m\left(C-C_f\right)-\left(\mu_{\max}\frac{C_f}{C_f+K_s}-k_2-K_{arr}\right)B_f P_m$$

$$\frac{\partial A_f\cdot C_{resp}}{\partial t}=K_{resp}\left(\mu_{\max}\frac{C_f}{C_f+K_s}-k_2-K_e\right)B_f P_m$$

B_f - biofilm bacterial or microbial biomass (M/L^3)

Because the biological components of the model depend on the physical processes but not vice versa the physical model can be calibrated independently of the biological submodel.

Calibration

Table 4. Calibration of the model.

Component	Method of calibration
physical sub-model parameters	dye tracer experiments
total biomass of microorganism	estimated by a measure of DNA
Biological parameters	obtained from experimental literature, especially from values of biofilm models and form values of bacterial growth kinetics directly measured in small streams
respiration	measured in stream

A generalized sensitivity analysis was performed. The most sensitive parameters, growth rate (μ_{max}), transfer velocity at the water biofilm interface (K_t), yield of biomass per input carbon (Y_1), temperature(θ) and bacterial decay rate(k_2) have been adjusted by a simple trials-errors method (this method was not explained in this paper). The value of K_{resp} was adjusted with the experimental values of C-CO2 production measured in situ under the assumption that the production is owed to microorganism metabolic activity, the macroinvertebrate respiration being insignificant.

Validation

Validation of the model was carried out using the same values for parameters but using data from different periods. The information used in the verification was the discharge, temperature and concentration of the allochtonous diffuse organic carbon inputs. The model predictions match very well with verification data.

Monte-Carlo simulations were run in order to analyze uncertainties associated with model inputs, disturbance variables, parameters, and to some extent, into the structure of the model. To do this each input variable and parameters value was drawn from a uniform distribution with boundaries extended 15% beyond their nominal values. The graphs of average values and confidence intervals show that stochasticity in inputs is damped down the stream (probably due to the effects of the biological component) and thus stochasticity in inputs does not create much variability in values downstream.

Model Simulations

The model simulations were used to quantify the importance of benthic biofilm in the removal of DOC and the amount of DOC present in the stream is significantly lower than would be expected if the biofilm were not present. This difference in amount of organic load removal of the biofilm versus purely physical factors increases with distance down the stream. The carbon balances produced by the model are used to quantify the main biological processes which participate in the biofilm DOC degradation and to make different assumptions about biofilm species succession owing to longitudinal trophic gradients induced by the organic load (discussed in another paper, Cazelles and Fontvieille, 1989)

Reference: Cazelles, B. and D. Fontvieille. 1989. Modelisation d'un ecosysteme lotique pollue par une charge organique: prise en compte de l'hydrodynamique et des mecanismes de transport. Revue de Sciences de Eau 2: 511-541.

Transport Case Study 7

C. Y. Chew, L. W. Moore and R. H. Smith. 1991. Hydrological simulation of Tennessee's North Reelfoot Creek watershed. Research Journal W.P.C.F. 63:10-16

This study uses HSPF (hydrological simulation program-FORTRAN), which is a comprehensive nonpoint source water quality model, to study sediment deposition in a watershed. The modelling effort was restricted to hydrology, sediment washoff from pervious land segments, stream hydraulics, and sediment transport. Data pertaining to meteorological conditions, topography, soil characteristics, land use, stream flow, and pollutant sources were obtained from various sources including government agencies, personal contacts, field investigations, and recent reports of the study area. These data were used to physically characterize the watershed so that the division of land area and main channel system could be performed. Average annual rainfall measurements were available and it was known that they were accurate from plots of several stream hydrographs.

Preliminary division of the watershed was on the basis of weather and soil characteristics which are exposed to meteorological conditions designated by one set of meteorological time series in modeling efforts. In addition to this information, land use information was used to divide the watershed into four pervious land segments (PLS), representing land uses of soybeans, corn, gullies, and others (grassland and forest) for which gross erosion rates were known.

Instream processes

Segmentation and characterization of the main steam channel was determined based on channel hydrogeometry. The land area and proportion of each land cover type which drains into the reach were determined for each reach. From information of land use and area each land segment was modelled to generate runoff and sediment loads per unit area to the stream channel. Computations of runoff and sediment loads along with hydraulic and sediment processes, results in simulation of the complete watershed. In addition, best management practices have been implemented within the time period used for model calibration. Land-use changes and changes in tilling method were incorporated into the model to increase the success of calibration and to determine the effect of these best management practices.

Calibration

The calibration uses data from April 1984-1988. All important rates and processes are derived from the watershed.

Table 5. Calibration of the model.

process	important influencing features	method of calibration
Initial parameter development	parameters that can be determined from site-specific topographical, hydrological, edaphic, and other conditions. These parameters need not be altered during the calibration.	determined from known watershed characteristics
Hydrologic		achieved by comparing observed and simulated runoff volumes (annual and monthly) and individual storm hydrographs.
Runoff from pervious land segments	three components: surface runoff interflow groundwater flow.	Stream flow records are not divided into these components so the relative contributions of each source were determined by examining the shape of hydrographs and timing of many events during the continuous simulation period.
Sediment	- Sediment washoff (sediment transport was not considered important because there is negligible bed load and degradation of the channel bottom is insignificant)	These values were determined from the information about the watershed such as land use and meteorology. Only settling velocity in still water was adjusted to make the calibration more accurate.

Verification

All verification was implemented using a separate data set which was collected from 1987-1988. Comparisons of measured and simulated values was performed using correlation. The R value for monthly observed and simulated sediment loads throughout the study period was 0.6.

Results

Preliminary simulation results indicated that sediment loads at highway 22 were reduced by approximately 20% since the implementation of Best Management Practices in 1984. Several alternative scenarios have been formulated to represent watershed conditions so that the model can be applied to evaluate the effectiveness of these Best Management Practices.

Transport Case Study 8

J. T. Kuo, J. H. Wu, and W. S. Chu. Water quality simulation of Te-Chi reservoir using two-dimensional models. Water Science and Technology 30: 61-72.

The purpose of this modelling effort was to determine the controlling factors for eutrophication in the reservoir and provide guidelines for data sampling and water quality management. In order to understand eutrophication in this system it is first necessary to understand the hydraulics of the reservoir and the model described most thoroughly in this paper is the hydraulics model. The information generated in this model is then used as input for the eutrophication model which is WASP3.

Hydrodynamics Model

The hydrodynamics model is two dimensional and is averaged over the width of the reservoir. It models both movement and temperature of water using information on wind speed, tributary inflow, and the physical structure of the reservoir. Information from this model is used to divide the reservoir into segments and to calculate movement among segments in the water quality model.

Calibration

Input data for reservoir topography, stream flow and meteorological data were all available. The only parameter that was adjusted during calibration was Chezy C, which is a coefficient which is dependent on the roughness of the bottom of the reservoir.
The model was very successful and was able to predict thermal stratification and mixing.

Eutrophication model

From the hydrodynamics model segments for the Eutrophication model were determined. There were fewer segments for the Eutrophication model. The model for each constituent in each segment is as follows:

$$\frac{\partial}{\partial t}\left(V_j C\right) = -\sum_i Q_{ij} C_{ij} + \sum R_{ij}\left(C_i - C_j\right) + \sum_B B_j S_{kj} + \sum_K B_j S_{kj} + W_j$$

C_i - concentration in a constituent

V_i - volume of the segment
Q_{ij} - net flow between segments i and j
C_{ij} - interfacial concentration between segments i and j
R_{ij} - dispersive flow between segments i and j
S_{bj} - dispersive flow between segments i and j
S_{ki} - kinetic transformation rate for the constituent in segment i
W_i - point diffusive loads in segment j

Chlorophyll-a, organic nitrogen, ammonia nitrogen, nitrate nitrogen, organic phosphorus, inorganic phosphorus, and dissolved oxygen were modelled.

Calibration and Verification

A total of 49 parameters are needed to run the model. The values for the least sensitive parameters were taken from the literature, empirical formulas and additional field data. The 15 most sensitive parameters were derived through calibration of the model.

The model was verified using a separate data set for a different year but all parameters were held constant. Model output and data seemed to match very well.

Results

The eutrophication model was used to determine whether nitrogen or phosphorus was limiting in the reservoir. It was determined that phosphorus was limiting and so it should be the focus of management decisions.

This paper could benefit from some measurement of the success of the model. As well the information on temperature and mixing seemed much more extensive than the data on constituent concentrations and thus model calibration and verification are limited somewhat due to lack of data.

Food Chain Case Study 1

R. V. Thomann, J. P. Connolly, and T. F. Parkerton. An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interaction. 1992. Environmental toxicology and Chemistry 11:615-629.

The model equations are written in terms of chemical concentration in aquatic organisms on a lipid basis and for abiotic particles on an organic carbon basis (i.e. concentration in organism = μg contaminant in organism / kg lipid in organism).

compartments of the model:

water column particulate
water column water
sediment particulate
sediment water
1 - phytoplankton, detritus
2 - zooplanton
3 - forage fish
4 - piscivorous
5 - benthic invertebrates

the model describing the uptake of each chemical is as follows:

$$\frac{dv_5}{dt} = k_{u5}\left(b_{5s}c_s + b_{5w}c_w\right) + \left(p_{5s}\alpha_{5s}I_{oc,5}\right)r_s + \left(p_{51}\alpha_{51}I_{l,5}\right)v_1 - \left(K_5 + G_5\right)v_5$$

$$\frac{dv_1}{dt} = k_{u1}c_w - \left(K_5 + G_5\right)v_1$$

$$\frac{dv_2}{dt} = k_{u2}c_w + \alpha_{2,1}I_{L,1}v_1 - \left(K_2 + G_2\right)v_2$$

$$\frac{dv_3}{dt} = k_{u5}c_w + \left(p_{32}\alpha_{32}I_{L,3}\right)v_3 + \left(p_{35}\alpha_{35}I_{l,3}\right)v_5 - \left(K_3 + G_3\right)v_3$$

$$\frac{dv_4}{dt} = k_{u4}c_w + \alpha_{43}I_{L,4}v_3 - \left(K_4 + G_4\right)v_4$$

v_i - chemical conc. in the ith compartment (lipid basis) (µg / kg lipid)
c_w, c_s - freely dissolved chemical concentration water column or sediment (µg / L)
r_w,r_s - chemical particulate concentration on an organic carbon basis in water column and sediment (µg / kg organic C)
k_{ui} - chemical uptake rate from available dissolved pools per g lipid (L / d-g lipid)
$I_{l,i}$, $I_{oc,5}$ - specific feeding rate or organism i on lipid or carbon (g prey lipid / g pred lipid / day)
$I_{oc,5}$ - specific feeding rate of organisms on carbon (g organic C / predator lipid / day)
a_{ij} - assimilation efficiency of ingested chemicals (g chemical assimilated / g chemical ingested)
K_i - excretion rate (1 / day)
G_i - growth rate (1 / day)
p_{ij} - proportion of compartment i's diet composed of compartment j

b_{is}, b_{iw} - component of ingested water from sediment or water column compartment

The total amount of contaminant in a compartment can be divided into parts in order to identify the importance of different sources of contaminant. Some terms that describe these components are as follows:

biotic sediment factor (BSF)-
organisms chemical concentration on a lipid basis : sediment chemical concentration on a carbon basis. $S_i = v_i / r_s$

bioaccumulation factor (BAF)-
organism chemical concentration : free dissolved concentration in the water ($N_i = v_i / c_w$)

bioconcentration factor (BCF)-
concentration due to water exposure only : concentration in water column ($N_{iw} = v_{wi} / c_w$)

sediment partition coefficient-
concentration in sediment organic particulate matter : concentration in sediment pore water ($\pi_s = r_s / c_s \cong K_{OW}$)

sediment water partition coefficient-
concentration in sediment particulate matter : concentration in water column ($\pi_{ws} = r_s / c_w$)

water column partition coefficient-
concentration in suspended sediment: concentration in water column ($\pi_w = r_w / c_w$)

food chain multiplier -
concentration ingested through consumption : concentration lost through excretion and growth.

Calibration

Table 6. Calibration of the model.

process	important factors influencing this rate	Calibration
chemical uptake rate	respiration rate of organism, efficiency of transfer across membranes (a function of K_{OW} of the chemical)	from other independent studies
excretion rate	K_{OW} of the chemical, fecal loss, metabolism	from other independent studies
assimilation efficiency	K_{OW}	from other independent studies
ingestion rate	respiration rate, growth rate, caloric content	from other independent studies

growth rate		allometric relationship
respiration		allometric relationship
feeding preferences		fit during calibration
sediment exposure		fit during calibration
sediment water column partition coefficient	deposition, resuspension, fraction of chemical in particulate and dissolved form, diffusion, sediment decay, concentration in organic carbon	from other independent studies

Partitioning of chemicals between water and sediment did not match well with steady state predictions, and from this it was expected that sediment interactions would be very important in determining the concentration in organisms further up the food chain.

There was significant nonlinearity in concentration as a function of K_{OW} so they used a non constant assimilation efficiency. For amphipods, comparisons were made between the assumption that they consumed all sediment or all phytoplankton. The predictions for chemical concentration were very different. The assumption that food consisted of sediment only tended to overestimate amphipod concentration while the assumption that food consisted of phytoplankton only, drastically underestimated measured concentrations. After manipulating the proportion of pore and water column water as well as the proportion of sediment and phytoplankton a best fit curve was achieved. Amphipod BAF then closely approximated the model BAF for amphipods. Again, incorporation of biomagnification gives much higher predictions than considering only uptake and elimination through water. Also, uptake from sediment is more important than from phytoplankton even though sediment comprises only 20% of the diet. For Sculpin a similar sensitivity analysis was used. Again food was very important in determining contaminant concentrations in body tissue.

Verification

There is no verification of this model, the paper is mostly an illustration to show how important trophic interactions are in determining the concentration of chemicals in the biotic components (something that the original paper that published the data did (Oliver and Niimi, 1988)) and also how different factors become important when K_{OW} was at the extremes of it's range.

Remarks

This model could have benefited from an independent source of feeding preferences and water and proportion of water uptake from water column and pore water. This model is very similar to the one used by Gobas (1993) but they are difficult to compare because Gobas used comparisons between predicted and actual concentrations while this study use comparisons between observed and predicted ratios to water or sediment concentrations.

Reference: Oliver, B.G. and A.J. Niimi. 1988. Trophodynamic analysis of polychlorinated biphenyl congeners and other chlorinated hydrocarbons in the Lake Ontario ecosystem. Environmental Science and Technology 22: 388-397.

Food Chain Case Study 2

D. Mackay and J.M. Southwood. Modelling the fate of organochlorine chemicals in pulp mill effluents. 1992. Water Pollution Research Journal of Canada 3:509-537.

Rather than using concentration of a pollutant this model uses fugacity of the pollution which is related to the concentration through the relationship C = Zf where C is the concentration, f is the fugacity and Z is a proportionality constant which is a function of the nature of the chemical and properties of the phase in which it was present. In one compartment of the stream it is assumed that chemical equilibrium is established very quickly, that is, the fugacity of the components of that compartment are in chemical equilibrium. For example, the sediment layer is divided between the particulate matter and the pore water. Both the pore water and the particulate matter will have the same fugacities but the concentrations in each component will be different and depend on the chemical characteristics of that component which are lumped into the Z parameter. The use of fugacity allows for some simplification of rates of diffusion between compartments, as diffusion is easily described in terms of fugacity but may be difficult to describe in terms of concentration when the diffusion is between two different materials. The model assumes that each reach is homogeneously mixed so there is no dispersion component. Usually the steady state solution is utilized to provide a mass balance concentration and rates for each component.

$$V_w Z_{wt} \frac{df_w}{dt} = E_w + f_s(D_3 + D_4) + f_a D_s + \sum f_{wi} D_i - f_w(D_4 + D_5 + D_6 + D_7 + D_0)$$

$$V_s Z_s \frac{df_s}{dt} = f_w(D_4 + D_5) + f_s(D_1 + D_2 + D_3 + D_4)$$

parameters are given in Table 7.

Food chain model

A complex food chain is then incorporated into the model. If the chemical is not appreciably metabolized, the concentration can be deduced as ZF where Z is of the organism and is calculated as $Z_w L K_{ow}$ where Aw is for water L is the lipid content and Kow is the octanol-water partition coefficient which is assumed to equal the lipid-water partition coefficient. The fugacity of an organism is assumed to be equal to the fugacity of the compartment in which it lives. The food chain includes 6 organism classes. There are plankton, benthos, benthivores, forage fish, small piscivores, and large piscivores. Energy and contaminants move from one level to another with typical food preferences.

For the four fish classes, a mass balance equation was written and includes uptake from water and food and loss by gill water, egestion, metabolism, and growth.

Applications

This model was used on two systems, an evaluative system and for a trichlorophenol and trichloroguaiacol in a real system in Northern Ontario. The evaluative system was used to give an idea of how different chemicals are partitioned within the system and what rates are most important to their concentrations in the different components.

Calibration

Table 7. Calibration of the model.

process	method of calibration for Kam river
sediment burial (D_1 f_s)	anecdotal observation during studies
sediment transformation(D_2 f_s)	estimated rates from similar compounds
sediment resuspension(D_3 f_s)	anecdotal observation during studies
sediment to water diffusion(D_4 f_s)	?
water to sediment diffusion(D_4 f_w)	?
sediment deposition(D_5 f_w)	anecdotal observation during studies
water transformation(D_6 f_w)	estimated rates from similar compounds
volatilization(D_7 f_w)	?
air to water absorption(D_7 f_a)	?
water outflow	measured
water particle outflow(D_0 f_w)	measured
rain dissolution	?
wet particle deposition(D_8 f_a)	?
dry particle deposition	?
water inflow(D_i f_I)	?
water particle inflow	measured
direct emissions(E_w)	measured

The model was used to study the Kam river. The river was divided into three homogeneously mixed segments. The method of calibration is not covered extensively. Rates such as volatilization and diffusion are probably estimated from chemical characteristics. Since organisms are assumed to be in chemical equilibrium with the compartment in which they live, partitioning between the organism and the component is simple and basically assumes that the organism is a blob of fat and there is no regulation of chemicals entering or leaving the body.

Verification

It appears as though all rates are derived independently and model verification but are varied to get a better model fit. Goodness of fit was then tested by comparing the modeled and observed concentrations and fugacity. The model produces a steady-state mass balance diagram with concentrations in each compartment and flow rates between them. The model predictions are compared to measured concentrations of both TCP and TCG in the water, sediment and benthos.

Results

Because there is no true verification and parameters had to be modified a lot the model results may be questionable. For example, the reported modelled concentrations were for benthic organisms with a 60% lipid content where this lipid content is above that normally found. It was also found that the ratios of concentration in sediment and biota were much larger than would be expected from other studies of bioconcentration. In general, the model predictions and measured values did not agree which means that the structure of the model is probably not accurate. Many of the measured values would produce highly unrealistic rates of transport or degradation. It is possible that the river water is not well-mixed and samples have been taken from a more dilute region, or another rapid removal mechanism may be in operation. They conclude that a more thorough examination of the local hydrodynamics are in order.

While concentrations in sediment and water are lower than predicted, concentrations in the benthos are much higher. It is possible that some rates are not accounted for or that bioaccumulation is actually important in this component.

Recommendations that were made because of the lack of success of this model:
1) more data for these and other chemicals in effluents, water, sediments, and a variety of organism are needed.
2) improved estimates of partitioning and reaction properties of these chemicals.
3) assembly of mass balance models which provide a successful reconciliation between model and reality.

The model is thought to be successful in some sense because it illustrates at least qualitatively which components will have high concentrations and which will be below detection limits. This type of information will help in future sampling programs.

Food Chain Case Study 3
V. A. McFarland, J. Feldhaus, L. N. Ace and J. M. Brannon. 1994. Measuring the sediment/organism accumulation factor of PCB-52 using a kinetic model. Bulletin of Environmental Contamination and Toxicology 52:699-705.

There are several ways of measuring the bioaccumulation factor of neutral organic chemicals. Kinetic modelling uses short exposure provides an alternative to long-term exposures to achieve steady-state. Kinetic modelling has the advantage that short-term exposures offer the possibility of avoiding many conflicting rate-influencing variables. There have been many kinetic studies of bioconcentration. Some of the criticisms are: uptake and elimination rates are more complex than can be accounted for by simple first-order models; elimination rates can depend on whether exposure is constant, variable or discontinued; and when comparisons have been made, kinetic projections of steady-state bioconcentration of chemicals in fish have generally underestimated long-term laboratory or field exposures. However there are also disadvantages of long-term studies: failure to achieve near equilibrium conditions in the exposures is an obvious potential shortcoming of non-kinetic short-term exposures; in both laboratory and field experiments use of organisms that aren't in continuous contact with sediments can fail the equilibrium criterion; if desorption of the chemical from sediments is very slow, an exposed organism may never reach equilibrium bioaccumualtion; sediments may be depleted of the bioavailable fraction of a chemical thereby reducing exposure; or sublethal toxicity may occur causing loss of lipids.

In this experiment fish were exposed to water, suspended sediment, and contaminant but were not fed during the course of the experiment. Exposure was maintained for durations ranging from 1 to 120 hrs. Concentration in sediment fish and water as well as estimates of total organic carbon and lipid content were measured. These measurements were used to calibrate the following model:

$$\frac{dX_w}{dt} = k_{sw}X_s + k_{fw}X_f - k_{ws}X_w - k_{wf}X_w$$
$$\frac{dX_s}{dt} = k_{ws}X_w + k_{sw}X_s$$
$$\frac{dX_f}{dt} = k_{wf}X_w + k_{fw}X_f$$

X_w, X_s, X_f - mass of PCB in in water sediment and fish respectively
k_{ij} – rate from compartment i to compartment j
sediment/water partition coefficient - $K_s = k_{ws}/k_{sw}$
fish/water partition coefficient - $K_f = k_{wf}/k_{fw}$
accumulation factor - $AF = \dfrac{K_f/f_{lipid}}{K_s/f_{oc}}$
where f_{lipid} and f_{oc} are the fractions of lipid and organic carbon in exposed organisms and in sediment respectively.

The resulting predicted equilibrium concentrations agree with bioaccumulation factors found in a variety of equilibrium studies.

Food Chain Case Study 4

F. A. P C. Gobas. 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: Application to Lake Ontario. Ecological Modelling 69:1-17.

In this paper uses a steady state model with independent calibration to predict the concentration of many different hydrophobic chemicals in different trophic levels of a Lake Ontario food-web.

In general only chemicals in true solution can be taken up by organisms and the relationship between dissolved and sorbed concentrations is as follows:

Bioavailable solute fraction or bioavailability (BSF) -
truly dissolved chemical concentration in the water (C_{wd}(µg/L)):
total chemical concentration in the water (C_{wt}(µg/L))

mass balance of the chemical in the water shows that:

$$V_{WT}C_{Wt} = V_W C_{WD} + M_{OM}C_{OM}$$

V_{wt} - volume of total water (water and organic matter)
V_w - volume of water only
M_{om} - mass of particulate organic matter in suspension
C_{om} - chemical concentration in the organic matter

because $V_{wt} \approx V_w$ $C_{om}=K_{om}C_{wd}$ ($K_{om} \approx K_{ow}$)

so:

$$BSF = 1/\left(1+\left(K_{ow}[OM]/d_{om}\right)\right)$$

OM - concentration of organic matter in the water (kg/l)

The model describing the uptake of bioavailable chemicals is as follows:

Aquatic Macrophytes and phytoplankton:

$$\frac{dC_A}{dt} = k_1 C_{WD} - (k_2 + k_G)C_A$$

C_A- chemical concentration in the organism
C_{WD}- bioavailable concentration in the water
k_1- rate of chemical uptake from the water
k_2- rate of chemical elimination to the water
k_G- first order rate constant for growth

This gives the bioconcentration factor ($C_A \backslash C_{WD}$(=$L_A K_{OW}$, if growth is not included. $L_A$is the proportion of organism that is lipid on a weight basis)). There is no biomagnification in this compartment nor the zooplankton compartment. This equation also describes zooplankton, however the lipid content of zooplankton is usually different than that of phytoplankton.

Benthic invertebrates:

For this compartment interaction with the bioavaible concentration in the water is thought to be the most important factor influencing concentration. Equilibrium partitioning between lipids of the organism, organic carbon fraction of the sediment, and the pore water describes the concentration in benthic invertebrates:

$$C_B d_L / L_B = C_S d_{OC} / OC = K_{LW} C_P$$

C_B-concentration in the benthic invertebrate
C_S- concentration in the sediment
C_P- truly dissolved concentration in the pore water
L_B- lipid fraction of the bethos
D_L- density of lipid in the bethos
d_{OC}- density of organic carbon fraction of the sediment
K_{LW}- lipid water partition coefficient
OC- organic carbon fraction of the sediments (kg organic carbon / kg organism)

Fish:

$$\frac{dC_F}{dt} = k_1 C_{WD} + k_D C_D - (k_2 + k_E + k_M + k_G) C_F$$

C_{WD}- dissolved concentration in the water (µg/L)
C_D- concentration in the food (µg/kg)
C_F- concentration in the fish(µg/kg fish)
V_F- weight of the fish (kg)
k_1- uptake form the water vial the gills (L/kg/day)
k_2- elimination via the gills (1?/day)
k_D- uptake from food (kg food / kg fish/day)
k_E- elimination by faecal egestion (1/day)
k_M- metabolic transformation of the chemical (1/day)

Calibration

The choice for model application was made for three reasons:
1) the information for chemical concentration of PCBs and other organochlorides was extensive and thus there was a good database for verification
2) studies suggest that concentrations are near steady-state (i.e. no significant change in concentrations in fish species over time)
3) data collection was on a whole-lake basis which accounts for spatial differences.

Monte-Carlo simulations were run with a sample size of 10 000 to estimate the variability introduced in the model calculations by the variability in observed water and sediment concentrations and fish weights. These were varied because they were the parameters that were available. The mean and standard error of these parameters are taken from the literature and the distributions of parameters were found to be normal.

Table 8. Calibration of the model.

rate	important influencing component	relationship	method of calibration
gill uptake rate	-gill ventilation rate (G_V) -gill uptake efficiency ($E_W k_1$) (depends on K_{ow}) -weight of the fish (V_f) - transport rates in water or lipid (Q_W or Q_L)	$1/k_1 = (V_F/Q_w) + (V_F/Q_L)/K$ $Q_w = 88.3 \cdot V_F^{0.6 \pm 0.2}$ $Q_L = small$	other independent studies
gill elimination rate	- gill uptake rate - K_{ow} - k_1/k_2 is the chemicals partition coefficient between the fish and the water	$k_1/k_2 = L_F K_{ow}$	relationship to get uptake rate
metabolic transformation rate	- many factors	small	determined by experiment, can often be assumed =0
dietary uptake rate	- food ingestion rate(F_D) - uptake efficiency(E_D) - faecal egestion rate(F_E) - temperature (T)	$k_D = E_D \cdot F_D / V_F$ $/ E_D = A \cdot K_{ow} + B$ (A and B from experimental data) $F_D = 0.022 \cdot V_F \exp(0.06T)$	- taken to be 0.25 (k_d) from other studies (this is the most important factor influencing biomagnification
faecal egestion	- related to dietary uptake rate. - dependent on the concentration gradient in the GI tract	$k_E = 0.25 \cdot k_D$	

growth	temperature, mass	$k_G = a \cdot V_F^{-0.2}$ a depends on the temperature	- allometric relationship
feeding preferences			taken from Flint (1986)
chemical partitioning and amount of organic matter in the water			typical values

Verification

For each organism group the observed and predicted concentrations of may organic substances were compared. For PCBs in fish and benthic invertebrates it was found that there were no significant differences between observed and predicted concentrations of contaminants. However there were significant differences for phytoplankton and zooplankton, this was attributed to poor estimates of actual concentrations.

A sensitivity analysis of the water and sediment concentrations showed that concentrations in all fish species are more sensitive to changes in sediment concentration than to changes in the water concentration. Chemical uptake through the benthic food chain is very important.

In general it was thought that the model was successful and predictions are believed to be accurate within a factor of 2 to 3 (believed to reflect the variability in food chain concentration).

They suggest combining the model with models of contaminant loading and partitioning in the physical environment to achieve a greater understanding of contaminant dynamics.

Food Chain Case Study 5

L.S. McCarty, G.W. Ozburn, A.D. Smith, and D.G. Dixon L.S. McCarty, G.W. Ozburn, A.D. Smith, and D.G. Dixon. 1992. Toxicokinetic modeling of mixtures of organic chemicals. Environmental Toxicology and Chemistry 11: 1037-1047. 1992.

Toxic unit (TU) - the concentration of a particular toxic chemical in a mixture divided by the incipient or threshold exposure concentration for the biological response end-point in question.

Threshold exposure concentration - the point where the LC50 estimate becomes independent of exposure time; that is, when the asymptote is reached.

TUs are dimensionless rations so the toxicity of a mixture can be expressed as the sum of the TU contributed by each component. If TU is ≈1 the mixture is expected to produce the toxic response. From a variety of studies it has been confirmed that many toxicants have an additive effect on organisms. However, if net uptake proceeds at different rates for each chemical, then the contribution of each to the total critical body residue (CBR) will vary with time and each will achieve its respective steady-state body residue (if reached) at different times.

This paper uses a first-order, one compartment kinetic model to look at the time courses and ultimate body residues at lethality for several mixtures or organic chemicals based on data from single-chemical toxicity tests. The success of the modelling exercise was determined by qualitatively comparing the model output to toxicity data previously obtained in actual mixture toxicity test.

Model

$$Cf(t) = Cw \cdot \left(\frac{k_1}{k_2}\right) \cdot \left(1 - e^{-k_2 t}\right.$$

Cf(t) - molar toxicant concentration in the fish at time t
Cw - molar toxicant concentration in the water
k_1 - uptake rate
k_2 - elimination rate

for two chemicals:

$$Cf_A(t) + Cf_B(t) = BCF_A Cw \cdot \left(1 - e^{-k_{2A} t}\right) + BCF_B Cw \cdot \left(1 - e^{-k_{2B} t}\right.$$

Calibration and Verification

Table 9. Calibration of the model.

Parameter	Method of calibration
Threshold LC50	from literature
Uptake rate constant	from calibration (The model was fitted to LC50 estimates for various exposure times)
Elimination rate constants	literature
Bioconcentration factor	established relationship between log Kow and BCF
Critical body residual associated with 50% mortality.	from relationship with BCF

The single toxicant model was calibrated from the literature describing LC50s for various times. This model was used to predict critical body residues for the different chemicals. These predictions were verified using independent data. The verified model was used to predict the contribution of each component of a mixture to the critical body residue as well as the asymptotic LC50 for the mixture. Again, the model was very successful at predicting LC50s for mixtures as well as the critical body residue.

Results

In general the model was thought to be successful because all experimental data fell within the 95% confidence interval of the model. There are several reasons given for the success of the model including that the toxicants do behave similarly and the original LC50s of mixtures were an additive function of the individual LC50s. However, this model may not have been as successful as reported. The model has a very large 95% confidence interval implying that there was a lot of individual variation in the original calibration data. This will make it hard to predict LC50s with very much accuracy.

APPENDIX C. MODELLING APPROACHES FOR INSTREAM FLOW NEED ASSESSMENTS (Prepared by Gordon L. Walder, Sirius Aquatic Sciences)

1.0 INTRODUCTION

An important aspect of management of water resources is the allocation of water among various uses, including both instream and out-of-stream uses. As used here, instream uses refers to all uses of water in the stream channel that do not involve withdrawal, diversion or impoundment of water. Such uses include those related to environmental protection issues (management of fish resources and maintenance of ecosystem health/integrity) as well as more direct human uses (recreation, navigation, waste transport and assimilation, and aesthetic considerations).

River impoundments and diversions can have dramatic effects on the physical, chemical, and biological characteristics of downstream reaches of the river. Recognition of these effects, concern about the implications for fish populations, and interest in broader environmental protection issues have led to attempts to describe what is needed, in terms of stream flow regime, in order to achieve a desired level of environmental protection. In this context, instream flow needs (IFN) may be defined as stream flow regime characteristics, quantities of water, and water quality conditions needed to protect both the aquatic and riparian components of riverine ecosystems.

The need for addressing instream flow needs in the Northern River Basins Study (NRBS) arises primarily from issues related to flow regulation on the Peace River. Flow regulation may have adverse effects on important or critical fish habitats in the river and has clearly affected riparian habitats along the Peace River mainstem and in the Peace-Athabasca Delta.

Most instream flow need studies have dealt primarily with issues related to protection of fish and fish habitat. Two aspects of fish habitat are generally considered; physical conditions (depth, velocity, substrate, cover) needed to provide suitable habitat, and water quality conditions (e.g., temperature and dissolved oxygen) needed to sustain healthy populations. Suitability of both physical conditions and water quality conditions may be significantly affected by changes in flow regime due to river impoundment, withdrawal of water for human uses, or discharge of effluents.

A variety of different riverine habitats is used by different species and life stages of fish. In considering habitat protection needs, it is therefore necessary to consider a number of different habitat types and how each type may be affected by changes in stream discharge. Several different types of fish habitat are typically recognized, including pools, riffles, runs, and backwaters. In most large rivers there are also side channel, snye, and slough habitats.

Areas of large rivers that are particularly important, in terms of utilization by fish, include side channels, pools, snyes, and backwaters. In addition, shoals and any other shallow, low velocity areas are particularly important as habitat for rearing juveniles of many species. The amount and quality of these habitat types varies over the short term with changes in discharge. Side channels, snyes, and shallow stream margin areas are the first to be affected by a reduction in stream flow. Over the longer term the availability and quality of these habitat features may also be affected by changes in river channel morphology induced by changes in flow regime.

While it is generally recognized that maintenance of the entire aquatic community is necessary in order to maintain fish populations, components of the aquatic community other than fish have received little attention in most studies of instream flow needs. It has generally been assumed that provision of physical habitat and water quality conditions suitable for the fish species of interest will also protect other components of the aquatic community and maintain production of food organisms for the major fish species.

A few studies have, however, addressed instream flow requirements of benthic invertebrate communities (Gore, 1978; Gore and Judy, 1981; Gore, 1987). The depth, velocity, and substrate characteristics at locations used by various benthic invertebrate species are very diverse because different species are adapted to very different types of physical conditions. While conditions suitable for a single species can be described, it is difficult to describe depth and velocity conditions that would be needed to maintain any given benthic invertebrate community. Any change in flow regime that alters the availability of any of a broad range of habitat types can be expected to alter the benthic community structure to a greater or lesser degree. Changes in community structure are also related to alterations in temperature regime and availability of organic detritus (Rader and Ward, 1988). Both of these factors, and their relationship to stream discharge, are therefore important aspects of instream flow needs for aquatic ecosystems.

The two water quality variables that most influence presence or distribution of fish within a river system are water temperature and dissolved oxygen. Both of these may be significantly affected by alterations to flow regime. Changes in the temperature regime may affect species composition of the aquatic community as well as distribution, growth, spawning and reproductive success of some fish species. Maintenance of specific water temperatures and dissolved oxygen levels is therefore an important consideration in determining the instream flow needs of aquatic ecosystems.

The potential effect of changes in stream flow on fish movement is another factor that should be considered in assessments of instream flow needs. A number of natural barriers to fish movement may be present in a river system. These include rapids, waterfalls, beaver dams, and log jams. While some barriers are impassable at all flows (e.g., waterfalls) many are passable to fish at some flows but not at others. In addition, some features may represent only a partial barrier, preventing movements of some species or sizes of fish but not others. When the existence or severity of a passage barrier is flow dependent, alterations to the flow regime may significantly affect fish populations.

Several factors are involved in limiting or preventing fish movements. The first is depth of a river section at low flow, which may be too shallow to allow passage of some fish. The second is high velocity and length of the high velocity section. The effectiveness of a high velocity area at limiting fish movement may depend on how far a fish must travel without shelter from the current. The third factor is associated with rapids, low dams, or other hydraulic jumps. A fish may be able to leap the barrier at some flows but not others.

2.0 APPROACHES FOR ASSESSING INSTREAM FLOW NEEDS

Methods developed for assessing instream flow needs have been focussed primarily on the needs for protection of aquatic habitats. Approaches for determining instream flows needed to provide habitat suitable for various fish species have received the most attention. Relatively little work has been done on approaches for assessing instream flow needs for riparian vegetation. Virtually all riparian vegetation instream flow needs studies have been undertaken in areas of dry climate, and have focussed primarily on drought stress or conditions required for seedling establishment. Criteria for describing instream flow needs for riparian vegetation (e.g., Mahoney and Rood, 1993; Wagner, 1993) have not generally been based on modelling approaches.

Instream flow methods for fisheries and aquatic habitats have been reviewed by several authors (Stalnaker and Arnette, 1976; Wesche and Rechard, 1980; Morhardt, 1986; Courtney, 1995). A large number of different methods have been used for various different purposes. However, most methods can be grouped into three general types of approaches; discharge methods, rating curve methods, and methods based on habitat suitability modelling.

Discharge methods are often referred to as "office methods" because they rely solely on historical stream flow records; field studies are not required. Using these approaches, instream flow needs are expressed as single minimum or preferred flows. These minimum or preferred flows may be determined as percentages of mean or median annual flow, mean or median monthly flows, or on the basis of flow duration analysis.

The Tennant method (also known as the Montana method), or one of several modifications, is the most widely used of the discharge methods. This method was derived from studies on 11 streams in three states and has been applied and tested on many more streams in 21 states (Tennant, 1976). When originally developed, the method was based on expert opinion as to the quality of fish habitat at different discharges. However, experience with the method over many years has indicated that it can be successfully applied to protect fish habitat. The Tennant method includes a rating system for instream flow needs which specifies different percentages of natural mean annual flow to achieve different levels of habitat protection.

The major limitation of the Tennant method and other discharge-based approaches is that they do not allow development of habitat-discharge relationships. They therefore have no quantitative impact prediction capability and provide no basis for evaluating different flow regime scenarios. These discharge-based methods are not considered modelling approaches and will not be discussed further.

Rating curve methods are approaches based on single or multiple transect data to develop hydraulic rating or habitat-discharge curves that describe the relationships between one or more physical habitat variables and stream discharge at specific locations in a stream. These approaches result in what can be considered empirical models representing how some habitat characteristic (e.g., wetted width, maximum depth) varies with changes in discharge.

IFN methods based on habitat suitability modelling involve simulation of micro-habitat characteristics (depth, velocity, substrate) over a range of discharges. Habitat availability at different discharges is then compared to micro-habitat preference criteria for species of interest. By far the most widely used method based on this approach is the Instream Flow Incremental Methodology (IFIM).

3.0 SIMPLE EMPIRICAL MODELS

A variety of rating curve methods have been used to develop empirical models (hydraulic rating or habitat-discharge curves) describe the relationships between one or more physical habitat characteristics and stream discharge. These relationships are developed by simply measuring the habitat variables of interest on a stream transect at several different discharges. Habitat variables that may be measured include water surface width, wetted perimeter, cross-sectional area, mean or maximum depth, and mean velocity. Rating curve methods are generally designed to be applied at a single stream transect, but multiple transect applications may be used in some instances.

In many applications of these methods, instream flow recommendations are made on the basis of some habitat retention criteria, such as some percentage of a reference value for one habitat parameter (e.g., 50% of the bank-to-bank perimeter is wetted) or an inflection point on a rating curve. Biological criteria are sometimes used where relevant species-specific criteria are available (e.g., preferred depth or velocity for spawning).

There exists a rather large number of rating curve methods, and they have been reviewed by several authors (Stalnaker and Arnette, 1976; Wesche and Rechard, 1980; Morhardt, 1986; Courtney, 1995). The Wetted Perimeter Method and the Oregon Usable Width Method, which are described below, are typical examples of the rating curve type of approach.

The Wetted Perimeter Method is based on the relationship between discharge and the measured wetted perimeter and therefore requires data describing the cross-sectional geometry at a stream transect and knowledge of water levels at various discharges. With this method, instream flow recommendations are based on identification of an inflection point on the wetted perimeter-discharge curve. The location of an inflection point is dependant upon the shape of the stream channel and may be difficult to identify. In some cases, particularly in complex reaches, there may be several inflection points. In addition, this type of approach is of limited value for IFN assessments because there is no clear link between wetted perimeter and quality of habitat.

In contrast, the Oregon Usable Width Method employs biological criteria for developing instream flow recommendations. Transects are located in areas of known critical habitat (e.g., for fish passage or spawning). Depth and velocity are measured at a number of points across the transect at several different discharges. The usable width at each discharge is then calculated based on criteria describing the usable depth and velocity ranges for the fish species and life stage of interest
Usable width versus discharge curves can be constructed for each species and life stage and used as a basis for IFN assessments.

A limitation of all rating curve methods is that habitat is measured only at specific locations; areal extent of habitat types is not determined. These methods are therefore best suited to applications at biologically critical locations such as known spawning sites or potential barriers to movement where determination of passage flow requirements is desired.

A further limitation is that habitat assessments can be made only within the range of discharges for which habitat measurements are available. Extrapolations beyond the range of observed discharges cannot readily be made. These types of models are therefore of limited usefulness in situations where a proposed flow regime modification results in discharges outside the normal range of flows prior to the stream flow alteration.

4.0 HABITAT MAPPING MODELS

A somewhat more comprehensive empirical modelling approach is one based on meso-habitat mapping. In this approach, aquatic habitats are mapped at a meso-scale level and the amounts of different meso-habitat types (e.g., side channels, snyes, shoals, backwaters, pools, riffles) measured at several different discharges. Availability of the various habitats is quantified by measuring the areal extent of each habitat type at each discharge. The product of this type of mapping study is a series of graphs depicting relationships between amounts of each habitat type and stream discharge. These results can then be interpreted based on knowledge about use of the various meso-habitats by different species and life stages of fish or on knowledge about the importance and role of these habitat features in terms of the aquatic community in general.

A meso-habitat mapping approach was used for IFN assessment on the Susitna River, a large river in Alaska (Trihey and Associates, 1985). In that study, the mapping was based on a series of aerial photographs taken at several different river discharges. Panja et al.

(1993) have also used images collected by multi-spectral videography remote sensing instrumentation to map meso-scale features at different discharges in the Virgin River, Utah.

An IFN study undertaken as part of the NRBS was also based on meso-habitat mapping. This study was conducted as a pilot project for development and evaluation of methods for mapping aquatic habitat types on the Peace River (Courtney et al., 1995). This project was based primarily on the use of multi-spectral image data collected by airborne remote sensing equipment (CASI; Compact Airborne Spectrographic Imager), but also includes a comparative evaluation of the suitability of conventional film photography and remote sensing methods for collecting image data. This pilot project was undertaken at two location on the Peace River; an upstream segment near the Alberta-B.C. border, and a downstream segment in the vicinity of Fort Vermilion.

A significant limitation that habitat mapping models share with the simple empirical models described in Section 3.0 is that IFN assessments are limited to the range of discharges for which habitat mapping data are available. This type of approach is therefore most useful in situations where anticipated flow regime alterations do not result in discharges outside the natural range of flows.

The habitat mapping approach is, however, particularly useful on large rivers because it can be easily applied in situations where collection of the data necessary to support habitat simulation modelling is impractical or prohibitively expensive.

5.0 HABITAT SUITABILITY MODELS

IFN assessment methods based on habitat suitability modelling require knowledge of the suitability of micro-habitat characteristics (depth, velocity, substrate) for species and life stages of interest as well as the ability to relate stream discharge to the distribution of micro-habitat characteristics. The Instream Flow Incremental Methodology (IFIM) is by far the most widely used method of this type.

The IFIM was developed by the Instream Flow and Aquatic Systems Group at the National Ecology Center of the U.S. Fish and Wildlife Service (Bovee, 1982). The method is based on use of hydraulic models to simulate relationships between discharge, stage, and velocity. A study site typically includes several transects placed to represent the range of habitat conditions present. The model is calibrated to measured discharge, stage and velocity data and is then use to simulate depth and velocity conditions over a wide range of flows. Typically, calibration data are required for at least three discharges. Velocity and depth are predicted for many points on each transect, allowing computation of the areal extent of different depth and velocity conditions. Output from this modelling process is used in conjunction with information on depth and velocity preferences of fish to predict habitat availability in terms of weighted usable area (WUA) for each fish species and life stage of interest. WUA is a function of the areal extent of different depth, velocity, and substrate conditions and the relative suitability of these conditions based on fish habitat preference data.

The IFIM is currently the most comprehensive and widely accepted IFN method used in North America. Unfortunately, it is very time consuming and costly to apply, particularly on large river systems. Large rivers present significant data collection problems that increase the time and costs involved in undertaking an IFIM study. Typically, a major part of the cost of an IFIM study is in determining the micro-habitat preferences of several fish species and life stages, and this is particularly difficult in large rivers. Existing preference information may not be applicable to a broad range of different rivers. The experience in Alberta is that transferability of habitat preference curves between watersheds has been poor (Courtney, 1995).

The IFIM uses relatively simple hydraulic models that, for some applications, have been considered inadequate (Osborne et al., 1988; Ghanem and Hicks, 1992). However, it would be possible to replace the current IFIM hydraulic models with other, more realistic, models for IFN assessments using the IFIM approach. Recent developments in hydraulic modelling have resulted in a new model, based on two-dimensional finite element methods, that shows considerable promise for application to fish habitat suitability modelling (Ghanem et al., 1994).

6.0 ECOSYSTEM ORIENTED APPROACHES TO IFN ASSESSMENT

Analyses of instream flow needs for aquatic habitats have usually been based on micro-habitat requirements (i.e., depth, velocity, substrate) of one or two selected sport fish species. The most frequently used method for this type of analysis is the Instream Flow Incremental Methodology (IFIM). While an IFIM analysis can evaluate habitats for multiple species and life stages, habitat assessment for a large number of species becomes intractable due to conflicting habitat requirements and the large volume of data that must be analyzed. In addition, the role and importance of habitat diversity in maintaining community and ecosystem structure and stability has not usually been considered in previous studies.

In order to better address instream flow needs for protection of aquatic ecosystems, it is desirable to undertake types of analyses that relate to a broader range of aquatic community components than has been common in the past, and that include consideration of habitat diversity and complexity. Options for extending IFN analyses to address broader ecosystem protection issues include the following:

1. Analysis based on habitat requirements of **sensitive indicator species**. This approach assumes that protection of the most sensitive species will provide protection for the ecosystem. Different indicator species would likely be required for different situations

or parameters (e.g., fish for depth and velocity; an insect for oxygen) and the most sensitive indicators may not include the most valued sport fish species. Selection of appropriate indicator species would require knowledge of the composition of the aquatic community and the tolerances of many species.

2. Analysis based on habitat requirements of **valued species and their prey**. This approach assumes that protection of valued species and their primary prey will provide protection for the ecosystem. Knowledge of community composition and trophic relationships would be required. In addition, the number of species for which habitat suitability data would be needed is potentially large.

3. Analysis that includes consideration of habitat requirements of all **key biotic components** of the ecosystem. The primary assumption in this instance is that protection of the key biological components will provide protection of the ecosystem. This approach would require detailed knowledge of ecosystem structure and function, habitat suitability data for large numbers of species, a high level of expertise, and relatively large budget.

4. Analysis based primarily on consideration of **habitat characteristics and availability**. This approach is based on analysis of the amount, distribution, diversity, and structural complexity of aquatic habitats at different stream discharges. The primary assumption is that protection of habitats will protect ecosystem structure and function. Application of this type of analysis requires less detailed knowledge of ecosystem structure and function and only general habitat requirements information for key biotic components.

Recently, some strictly habitat-based approaches that address instream flow needs from a community, ecosystem and biological diversity perspective have been proposed (Sekerak, 1992; Bovee, 1995). The underlying principles of these approaches are that all habitat types are potentially important to the structure and stability of the community and that habitat diversity and structural complexity are key requirements of complex ecosystems. One objective in managing regulated rivers, from an environmental protection perspective, might therefore be provision of instream flows capable of maintaining a heterogeneous mix of habitat features that is similar to unregulated conditions.

One approach to the fourth type of analysis listed above is based on mapping of aquatic habitats at a meso-scale level and describing the relationships between the amounts of different meso-habitat types (e.g., side channels, sloughs, backwaters, shoals, riffles, pools) and stream discharge. Relative to other options, this type of study can be undertaken more quickly, requires less detailed information on habitat requirements of specific species, and is less costly.

The usual product of an IFN study based on habitat mapping is a series of graphs depicting relationships between amounts of each habitat type and stream discharge. Interpretation of these results is typically based on knowledge about use of the various meso-habitats by different species and life stages of fish and information about benthic communities associated with different meso-habitats. However, other types of analysis may also be useful for interpreting results in the context of ecosystem protection. Measures of habitat diversity, richness, evenness, or other descriptions of structural complexity, might be usefully employed. Because all types of habitats are potentially important to community structure, function, and stability, the relationship between habitat diversity/complexity and stream discharge may provide additional information useful in making instream flow management decisions.

IFN studies based on micro-habitat characteristics (e.g., IFIM) and those based on meso-habitat mapping provide different types of information and involve examination of habitat characteristics at very different scales. Both types of analysis provide information useful in making management decisions and are complementary to each other. It may therefore be advantageous to employ the two approaches in combination. Such a strategy has been employed previously, on the Susitna River, Alaska (Trihey & Associates and Entrix Inc., 1985).

In addition, analysis of habitat diversity/complexity and its relation to discharge can be investigated at both the micro-habitat and meso-habitat scales. Bovee (1995) described how analyses of habitat richness, diversity, and evenness can be based on output from an IFIM modelling exercise.

7.0 WATER QUALITY MODELLING FOR IFN ASSESSMENTS

Because water quality is strongly influenced by the volume of flow, an understanding of the relationship between water quality and quantity is essential for an evaluation of instream flow needs. Also of particular importance in most streams is the relationship between water quality and the aquatic communities; how the biological components and processes affect, and are affected by, water quality. For example, dissolved oxygen is a key water quality variable that influences distribution of fish and the species composition of the aquatic community. Dissolved oxygen may also be strongly affected by macrophytes and by the various benthic biological processes.

The assimilative capacity of rivers and the related flow requirements may be a significant issue in assessing instream flow needs. Many aspects of water quality is directly related to volume of stream flow and to the quantity and characteristics of effluents discharged into the system. Some minimum flows are required to assimilate effluent loadings while maintaining water quality conditions adequate to protect the aquatic ecosystem. In streams receiving effluent discharges, the instream flow needs for maintenance of the aquatic ecosystem will, at least under some conditions (e.g., periods of low flow), be greater than it would be without effluent loadings.

Water quality issues in instream flow need investigations are typically examined using one of the several available water quality models. These models vary greatly in their degree of complexity, the variables modelled, and the data inputs required. Selection of a particular model is generally project specific and is based on the specific issues and requirements in each instance. The water quality models most commonly utilized in instream flow needs investigations include the following:

1. SRQM - Stochastic River Quality Model (HydroQual and Gore & Storrie, 1989)

2. QUAL2E - Enhanced Stream Water Quality Model (Brown and Barnwell, 1987)

3. WQRRS - Water Quality for River-Reservoir Systems (Smith, 1978)

4. WASP - Water Quality Analysis Simulation Program (Ambrose et al., 1991)

5. DSSAM III - Dynamic Stream Simulation and Assessment Model III (Caupp et al., 1991)

7.1 Stochastic River Quality Model

The Stochastic River Quality Model (SRQM) consists of three modules: DOSTOC, for simulating dissolved oxygen; NUSTOC, for simulating nitrogen and phosphorus; and UNSTOC, for simulating a user-specified toxic or conservative substance. Each module requires description of a number of input parameters. The model is steady-state and is limited to one space dimension. Hydraulic characteristics of the river are represented by Leopold-Maddock equations, which are exponential functions relating mean depth, top width, and mean velocity to river discharge. Input data requirements are relatively small, compared to many other models. The model can be run as either a deterministic simulation or a stochastic simulation. In the stochastic mode, uncertainty of model predictions can be evaluated by incorporating uncertainty in model parameters and randomness of natural processes.

The DOSTOC module simulates dissolved oxygen concentration in a river based on the solution of a set of differential equations representing the interactions between oxygen demanding substances (ultimate carbonaceous biochemical oxygen demand [BOD] and nitrogen oxygen demand [NOD]) with sources of oxygen in the river. Processes represented in the model include decay of BOD and NOD in the water column, photosynthesis, respiration, and reaeration.

The NUSTOC module models organic and inorganic nitrogen as well as dissolved and particulate phosphorus. The nitrogen cycle simulation includes decay of organic nitrogen to ammonia, nitrification of ammonia to nitrate, generation of ammonia from sediments and by respiration, and loss of organic nitrogen from the water column by settling. The phosphorus simulation was designed specifically for use in the North Saskatchewan River and other turbid prairie rivers. It includes conversion of dissolved to particulate phosphorus through adsorption, release of dissolved phosphorus from bottom sediments, and removal of particulate phosphorus from the water column by settling. Decay of organic phosphorus to inorganic phosphate is not included. Both the nitrogen and phosphorus components of the model include biological uptake by photosynthesis.

UNSTOC is a simple model that calculates the concentration of a single water quality constituent that behaves conservatively. It can also be used to predict some non-conservative substances where the important processes can be represented by simple decay rates. The available instream decay processes include volatilization, biodegradation, and sedimentation.

7.2 Enhanced Stream Water Quality Model

The Enhanced Stream Water Quality model (QUAL2E) is a comprehensive water quality model designed for simulation of dissolved oxygen, nutrients, and related constituents as well as coliforms and arbitrary conservative and non-conservative constituents in a branching stream system. The following 15 water quality constituents can be simulated: dissolved oxygen, biochemical oxygen demand, temperature, algae, organic nitrogen, ammonia, nitrite, nitrate, organic phosphorus, dissolved phosphorus, coliforms, one arbitrary non-conservative constituent, and up to three conservative constituents. The model allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow. It can also compute required dilution flows for flow augmentation to meet any specified dissolved oxygen concentration. QUAL2E can best used as either a steady-state or dynamic model, but the hydraulic regime is assumed to be steady-state.

QUAL2E is based on a finite difference solution to the one dimensional advection-dispersion mass transport equation. This equation represents the effects of advection, dispersion, dilution, constituent reactions and interactions, and sources and sinks for constituents. Hydraulic characteristics of the stream are determined by the same exponential equations used in the SRQM or by solution of Mannings equation.

The QUAL2E model includes the major interactions of the nutrient cycles, photosynthesis, algal growth, algal respiration, benthic oxygen demand, carbonaceous oxygen demand, atmospheric reaeration, and their effect on dissolved oxygen concentration. The nitrogen cycle in QUAL2E includes organic nitrogen, ammonia, nitrite, nitrate, an organic nitrogen settling term, and algal nitrogen uptake. The phosphorus cycle includes organic phosphorus, which can be generated by death of algae, conversion of organic phosphorus to dissolved inorganic phosphorus, algal uptake of phosphorus, and settling of organic phosphorus. Temperature is modelled by performing heat balance computations using a variety of data, including latitude and longitude, time of year,
evaporation coefficients, a dust attenuation coefficient, and local climatological information (time of day, air temperature, atmospheric pressure, cloud cover, wind).

Uncertainty analysis can be conducted by QUAL2E on steady-state water quality simulations to evaluate the effect of model sensitivities and uncertain input data on model predictions. Three types of uncertainty analysis are available: sensitivity analysis, first order error analysis, and Monte Carlo simulation.

7.3 Water Quality for River-Reservoir Systems

The Water Quality for River-Reservoir Systems (WQRRS) model is a comprehensive water quality simulation model for river systems including up to 10 reservoirs. The model consists of three separate modules: the reservoir module, the stream hydraulic module, and the water quality module. Modelling can be done as either steady-state or dynamic simulations.

The reservoir module represents impoundments as one-dimensional systems in which the isotherms and contours of other variables are horizontal (i.e., with dominant vertical gradients. This approximation is satisfactory for small to moderately large lakes or reservoirs with long residence times and is less useful in shallow impoundments or those with rapid flow-through times.

The stream hydraulic module can simulate steady-state hydraulics and is capable of simulating hydraulics within both the gradually varied steady and unsteady flow regimes. Peak flows from storm water runoff or hydropower releases can be represented. Six hydraulic computation options are provided: steady flow with backwater hydraulic solution, finite difference solution of the St. Venant equations, solution of kinematic wave equations, input of a stage-flow relationship, Muskingum hydrologic routing, and modified Puls hydrologic routing.

The water quality module is very comprehensive and provides for complex, nonlinear relationships to represent interactions among the various constituents. Ecological processes within a lake or reservoir environment are centred around phytoplankton. The relationships between phytoplankton and nutrients and between phytoplankton and zooplankton normally controls water quality within the reservoir. In stream modelling, the ecological processes are centred around benthic algae, and the model provides for complex interactions among water quality variables and various components of the food chain. The following chemical and biological constituents are included in the water quality module: temperature, dissolved oxygen, total inorganic carbon, dissolved phosphorus, ammonia, nitrite, nitrate, alkalinity, total dissolved solids, pH, coliform bacteria, inorganic suspended solids, inorganic sediment, detritus, organic sediment, phytoplankton, zooplankton, benthic animals, benthic algae, aquatic insects, and three types of fish. Included in the water quality module is the capability to omit one or more constituents or to hold them at constant values during the simulation.

While WQRRS includes several variables for the higher trophic levels, it appears that the capability to simulate these components has not been tested in practical applications of the model. In addition, applications of WQRRS in Alberta have encountered a number of difficulties involving simulation of nutrients and primary production. Hamilton et al. (1989) reported that their review of WQRRS model processes for nutrients, algae, and aquatic plants indicated that the model configuration is deficient in that it does not adequately account for the following: nutrient flux and uptake from sediments, tissue nutrient levels limiting concentrations and luxury storage, factors affecting macrophyte bed establishment and propagation, and factors regulating plant growth and respiration as well as nutrient cycling.

7.4 Water Quality Analysis Simulation Program

The Water Quality Analysis Program (WASP) is a dynamic compartment modelling system that provides a generalized framework for modelling the transport and transformation of both conventional and toxic pollutants. WASP can be applied in one, two, or three dimensions to simulate constituents in the water column and benthos of ponds, streams, lakes, reservoirs, estuaries, and coastal waters.

The WASP modelling system consists of two computer programs, DYNHYD and WASP, that can be run separately or in conjunction with each other. DYNHYD is a hydrodynamics program that simulates the movement of water while WASP is a water quality program that simulates movement and interactions of constituents in the water. The WASP program includes two sub-models: EUTRO, for simulation of water quality problems related to conventional pollution (dissolved oxygen, biochemical oxygen demand, nutrients, and eutrophication); and TOXI, for simulating toxic pollution (organic chemicals, heavy metals, and sediment). The EUTRO model includes a comprehensive kinetic structure to represent dissolved oxygen and eutrophication, while the TOXI model includes a kinetic structure for transformation of organic chemicals as well as sediment balance algorithms. The various water quality processes in WASP are represented in a number of kinetic subroutines that can be selected from an existing library or written by the model user. The flexibility provided by this structure, which allows the model to be tailored to specific locations and situations, is unique among water quality models.

The hydrodynamic model, DYNHYD, solves the one-dimensional equations of continuity and momentum. The equation of motion, which is based on the conservation of momentum, predicts water velocities and flows while the equation of continuity predicts water levels and volumes, based on conservation of volume. This approach is suitable for most natural flow conditions in large rivers and estuaries, but high-gradient small mountain streams and dam-break situations could not be simulated with DYNHYD.

The water quality model, WASP, can simulate a wide variety of water quality constituents and processes, depending on the model configuration as described by the user. WASP is based on the principle of conservation of mass and traces each water quality constituent from the point of input (spatial and temporal) to the final point of export, conserving mass in space and time. In order to perform the mass balance calculations, the user must supply input data describing the following: simulation and output control, model segmentation, advective and dispersive transport, boundary concentrations, point and diffuse source loads, initial concentrations, and kinetic parameters, constants and time functions.

The EUTRO sub-model of WASP has the capability to represent the various physical, chemical, and biological processes of interaction among nutrients, phytoplankton, benthos, carbonaceous material, and dissolved oxygen. This includes simulation of phytoplankton production kinetics, nutrient uptake kinetics associated with algal growth, the phosphorus cycle, the nitrogen cycle, dissolved oxygen balance, and sediment-water interactions. EUTRO can be implemented at six different levels of complexity: (1) Streeter-Phelps BOD-DO equations; (2) Modified Streeter-Phelps equations (divides BOD into carbonaceous and nitrogenous fractions); (3) Full linear DO balance (divides NBOD process into mineralization and nitrification, and adds photosynthesis and respiration); (4) Simple eutrophication kinetics (simulates growth and death of phytoplankton and interactions with nutrient cycles and DO); (5) Intermediate eutrophication kinetics (adds light limitation, phytoplankton effect on mineralization of phosphorus and nitrogen, DO limitation on nitrification, denitrification); (6) Intermediate eutrophication kinetics with benthos (includes benthic interactions with nutrients, CBOD, and dissolved oxygen).

7.5 Dynamic Stream Simulation and Assessment Model III

The Dynamic Stream Simulation and Assessment Model (DSSAM-III) was designed to simulate a system where pollutants may enter the stream from a variety of sources, including point source effluents, surface water runoff, groundwater, and leaching from bottom sediments. It provides a dynamic representation of diel variation in water quality constituent concentrations, and incorporates modelling of benthic algae. Algal biomass is a dynamic variable, determined as a function of nutrients, light and temperature. DSSAM-III can be applied to river systems with distributed surface inflows and outflows and with distributed groundwater inflows and outflows. The model is implemented as two modules: a hydraulic model to represent collection and physical transport of constituents, and a water quality model that uses kinetic equations to represent processes affecting concentrations of water quality constituents.

The hydraulic equations used in DSSAM-III are based on steady non-uniform flow conditions and allow options for distributed surface water and groundwater inflows and outflows. Channel hydraulic properties are described by relationships between average cross-sectional velocity and flow, and between hydraulic radius and cross-sectional area. These relationships are represented in DSSAM-III by the commonly used Leopold-Maddock equations. The model does a flow balance on the river system and calculates average flow, average stream velocity, and width for each modelled stream element. A solar energy submodel is included to simulate water temperatures.

The DSSAM-III model is capable of simultaneously simulating the transport and kinetic reactions of 17 water quality constituents: soluble reactive phosphate, soluble non-reactive phosphate, particulate phosphorus, ammonia, nitrite, nitrate, soluble organic nitrogen, particulate organic nitrogen, biochemical oxygen demand, dissolved oxygen, acidity, alkalinity, carbon dioxide, total dissolved solids, chloride, and two components of benthic algae. The water quality module requires input data representing the boundary conditions for water quality constituent concentrations as well as kinetic coefficients for the various water quality equations. The benthic algae algorithm of DSSAM-III simulates the dynamics of the periphyton community of a river. It includes one state variable (periphyton biomass) and three rate variables (primary production, endogenous respiration, and removal processes resulting in export of biomass from the system. Algal biomass, production, and respiration are linked to pH, dissolved oxygen, phosphorus, and nitrogen. Algal removal processes included are scouring due to current velocity, and removal by benthic invertebrate activity. The model also has the capability to separately predict biomasses and growth rates for two distinct periphyton components.

8.0 FUTURE MODEL DEVELOPMENT NEEDS

Examination of the capabilities and limitations of models potentially useful for conducting instream flow needs analyses, as described in the foregoing sections, suggests a number of future model development needs. Some of these would involve either enhancement or new development of simulation models themselves, but other needs could be met by development of strategies and/or computer software to facilitate post-processing and analysis of the output of existing models. The following are seen as some of the future model development and analysis needs:

1. Enhancement of the two-dimensional finite element hydraulic model.

As discussed in Section 5.0, the types of hydraulic models that have typically been used for modelling physical stream habitat suitability have some significant limitations, and the recently developed finite element approach described by Ghanem et al. (1994) has some definite advantages. The actual algorithms implementing the two-dimensional finite element approach have been adequately developed. Additional needs are for development of software to link this hydraulic model to computation of aquatic habitat suitability and for development of a user interface for the combined modelling system that would make this approach readily available for use by instream flow needs analysts.

2. Implementation of two-dimensional water quality modelling approaches.

Virtually all water quality modelling done to support instream flow needs analysis has involved implementation of one of the available models in a one dimensional context. Such models predict, in effect, the average concentrations of water quality constituents at specific points along the length of a river channel without regard for potential lateral (across channel) variability. These model implementations have typically been calibrated to water quality data measured at mid-channel locations. In many rivers, some water quality characteristics (particularly dissolved oxygen and temperature) may be significantly different along the river margins than in mid-channel. These differences are probably most marked in large rivers with a complexity of habitats that includes side channels, snyes, shoals, and backwaters. It is precisely these habitats, as well as any shallow, low velocity stream margins, that are particularly important fish habitat in large rivers and that are also most affected by effects of flow regulation.

The WASP model, described in Section 7.0 has the capability to be implemented in a two-dimensional manner. The water quality component of DSSAM-III could also be implemented as a two-dimensional model but this would require replacing the hydraulic model component of DSSAM-III with one that has two-dimensional simulation capabilities. With either of these approaches, the data requirements to support two-dimensional modelling are very large. Because of this, implementation of two dimensional water quality modelling may prove to be intractable, for all practical purposes, in many situations. Nevertheless, it is obvious that prediction of mid-channel (or average) dissolved oxygen and temperature is of little value, for purposes of instream flow needs analysis, if these variables are significantly different at locations of important fish habitat.

3. Development of approaches that are more ecosystem oriented.

The issue of ecosystem oriented approaches to IFN assessment has been discussed in Section 6.0. New model development is not necessarily needed; new approaches to applying existing models may suffice. As discussed in Section 6.0, potential approaches to more ecosystem oriented IFN assessments involve consideration of the instream needs of a greater number of species and/or analysis and interpretation of habitat diversity and complexity. To a large extent, such approaches could be based on the habitat mapping models described in Section 4.0 and the habitat suitability models described in Section 5.0. Development of suitable software tools for post-processing and analysis of model outputs would certainly facilitate application of IFN assessments that are more ecosystem oriented. What appears to be needed most, however, is motivation and commitment among instream flow needs analysts to take up the challenge.

4. Development of riparian vegetation response models

As mentioned briefly in Section 2.0, criteria for assessing instream flow needs for riparian vegetation have not generally been based on modelling approaches. This is due primarily to the difficulty of predicting the response of riparian vegetation communities to alterations in stream flow. At the NRBS Instream Flow Needs Workshop, it was the general consensus of the participating vegetation biologists that we are not yet very close to being able to undertake quantitative modelling of the responses of riparian communities to changes in river flow regime (Walder, 1995). This was considered to be due to an insufficient understanding of system functions as well as a lack of data on specific process coefficients. However, it was also the opinion of the majority of workshop participants that riparian vegetation response modelling at the conceptual level would be a useful undertaking.

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