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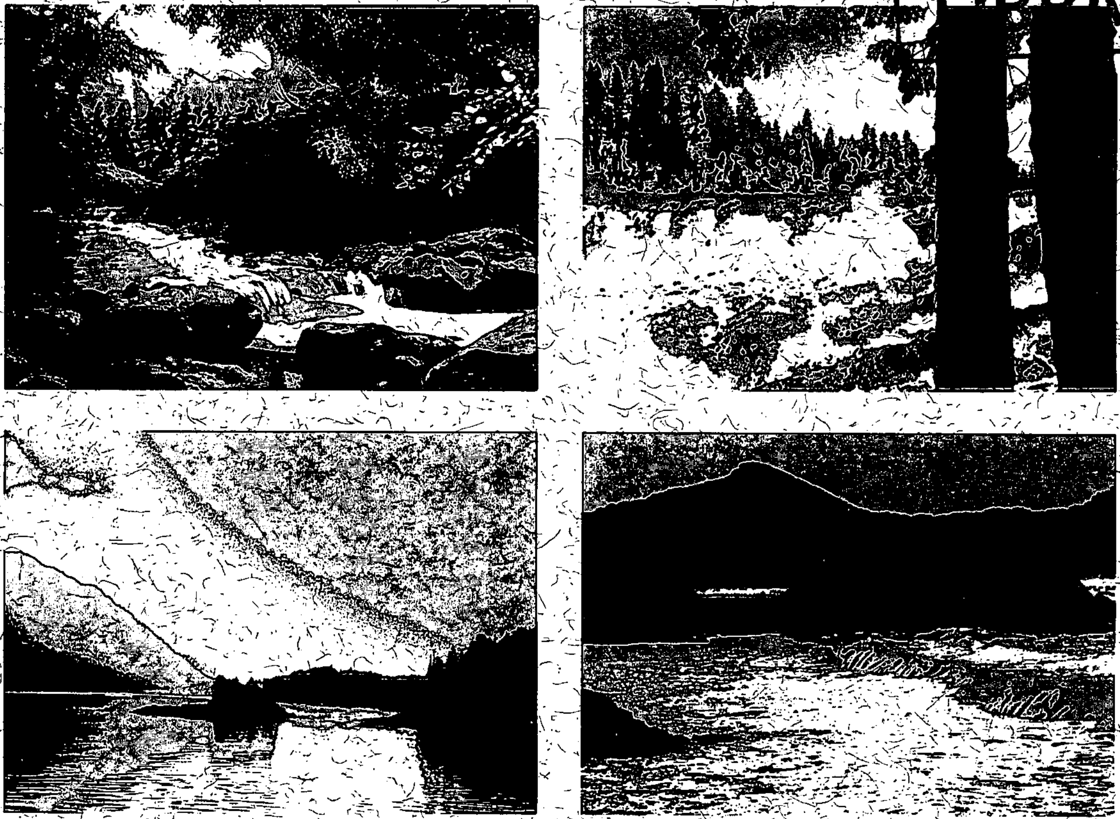
Water Quality Modelling of the Upper Saint John River: A Comparison Study

H. Cheng and D. Lockerbie



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ENVIRONMENTAL CONSERVATION SERVICE
OTTAWA, ONTARIO, 1994

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Abstract

Two computer models were used in this comparison study: the Environment Canada One-dimensional Hydrodynamic model (the One-D model) and the U.S. Environmental Protection Agency (EPA) water quality model QUAL-IIe. The two models were first calibrated and verified with the same data, which contained numerous lateral inflows and point source wastewater discharges from local municipalities and industries. The results of simulation from the two models indicated remarkably similar responses to waste loadings, as represented by the various profiles of biological oxygen demand (BOD), dissolved oxygen, total alkalinity, total suspended solids, and nutrient families. A sensitivity analysis of several parameters was also conducted for both models. It was found that either one of the two models could be used with confidence to evaluate vital water quality parameters in the Upper Saint John River at various points of interest in the future.

Résumé

Dans cette étude comparée, on s'est servi de deux modèles informatiques : le modèle hydrodynamique unidimensionnel (1-D) d'Environnement Canada et le modèle de la qualité des eaux QUAL-IIe de la U.S. Environmental Protection Agency (U.S. EPA). Les deux modèles ont d'abord fait l'objet d'étalonnage et de vérification avec les mêmes données comportant de nombreux apports latéraux et des déversements ponctuels d'eaux usées provenant de municipalités et d'industries du voisinage. Les résultats de la simulation effectuée à l'aide de chacun des deux modèles étaient semblables aux charges de résidus, ce qui se reflète par les divers profils de la DBO (demande biologique d'oxygene), de l'oxygène dissous, de l'alcalinité totale, des matières solides totales en suspension et des familles d'éléments nutritifs. On a aussi réalisé pour les deux modèles une analyse de sensibilité de plusieurs paramètres. On a trouvé que l'un ou l'autre de ces deux modèles pouvait être utilisé avec confiance pour évaluer à l'avenir les paramètres vitaux de la qualité des eaux à divers endroits dans le cours supérieur de la rivière Saint-Jean.

Water Quality Modelling of the Upper Saint John River: A Comparison Study

H. Cheng and D. Lockerbie

INTRODUCTION

The objective of this paper is to demonstrate the calibration and application of two water quality models in the Upper Saint John River water quality study and to address some of the problems and concerns of water quality modelling from a practical engineering point of view. This comparison study attempts to establish both the One-D model and QUAL-IIe model as convenient and useful tools in future modelling applications. They can be used to evaluate the environmental impact of waste load on river water quality, as well as to assist the development of water quality guidelines and objectives for rivers including boundary waters.

Since the original mass balance model was developed to determine dissolved oxygen (DO) in a river (Streeter and Phelps, 1925), numerous more sophisticated water quality models have evolved and have been widely applied in water pollution studies. In recent years, many regulatory agencies in the U.S.A. routinely use water quality models for waste load allocation and stream assimilative capacity analyses. Satisfactory application of predictive water quality models mainly depends on accurate calibration and verification. The computation of oxygen transfer at the air–water interface is the most important factor in the simulation of various key water quality constituents. The simulation of interactions involving nutrients, DO and probably other conservative and non-conservative materials in the natural stream environment is usually very complex. In the practical application of a model, several technical difficulties can arise because of the inherent limitations of the model, inadequacies in the observed data used in calibration and testing, user judgement, and the existence of unknown or unaccounted for pollution sources.

Based on the knowledge gathered from numerous previous studies on the Saint John River and other local sources, a one-dimensional water quality model would appear to be adequate for simulating the prevailing hydraulic and water quality conditions — at least of the upper stretch of the river. Both the One-dimensional Hydrodynamic model (One-D Model) and QUAL-IIe model are strictly one-dimensional with respect to space and time. Consequently, lateral and vertical directional variations in flow and water quality are not accounted for in the simulation.

RIVER BASIN

The Saint John River flows in a relatively rural area through some small municipalities and three major cities in New Brunswick: Edmundston, Fredericton and Saint John. It then discharges into the Bay of Fundy to the south-east. The river serves as the international boundary between Quebec and New Brunswick, and Maine in the U.S.A. The area of interest for this study covers approximately 100 river kilometres from St. Francis to St. Leonard, which is just 20 km upstream from the Grand Falls dam (Fig. 1). The estimated drainage area of the river at St. Leonard is approximately 21 000 km^2.

The Upper Saint John River is not influenced by the tidal effects of the Bay of Fundy, which extend about 97 km from the ocean. The land in the region is gently rolling with many lakes and swamps. The bedrock consists of altered sedimentary rocks and much of it is covered by glacial drift and recent marine sediments. The economy of the Saint John River basin depends mainly on the development of forestry resources. A variety of farming is practised in the Canadian part of the basin. Sport fishing, particularly for Atlantic salmon, is an important recreational activity.

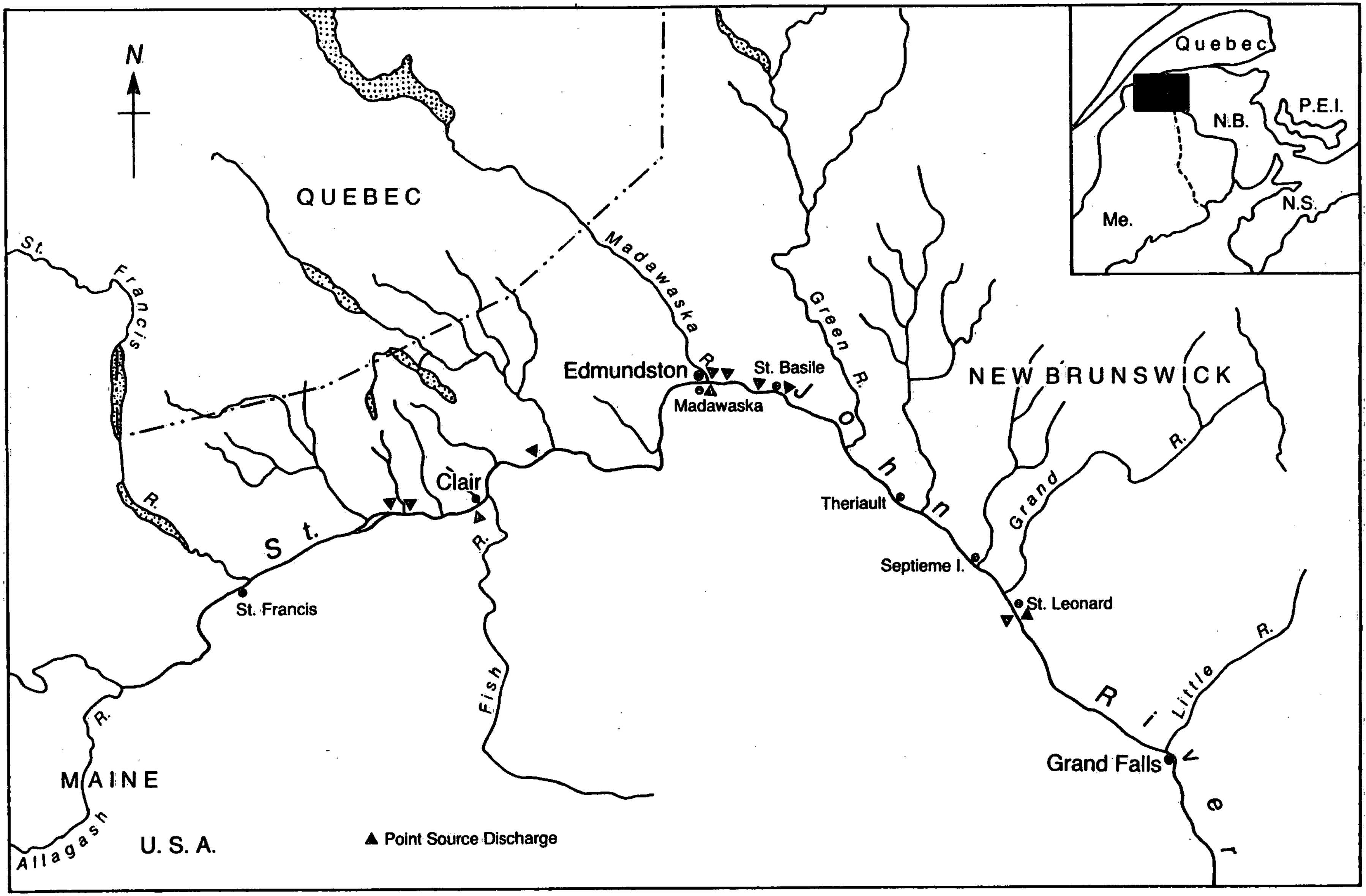

Figure 1. Upper Saint John River.

BACKGROUND ON WATER QUALITY

In the Upper Saint John River basin, water quality is good despite some high turbidity and colouring. The three major sources of pollution in the study portion of the river are municipal treatment facility discharges, industrial plant effluents, and non-point sources. The latter include agricultural land runoff, logging activities and leaching from dumps—the result of increasing urban, industrial and hydro developments. In the 1960s, the salmon population was virtually eliminated up to the Aroostook River, primarily as a result of the construction of hydro dams at Beechwood and Mactaquac.

In 1976, water quality objectives were developed by the International Technical Advisory Subcommittee on Water Quality in the Saint John River. These objectives apply to the boundary portion of the river and its tributaries. Government agencies of Canada, Quebec, New Brunswick and the State of Maine cooperate in monitoring the river to determine if the water quality objectives are met. They also gather baseline information used to assess the environmental impact of future developments and waste load allocations on the river.

Since 1972, water pollution control facilities for municipalities and various industrial plants were built with the goal of eliminating up to 90% of the BOD loading to the river. In general, water quality in the Saint John River continues to improve. Dissolved oxygen (DO) concentrations and overall environmental problems are now of less concern. Recent data show a marked reduction in the rate and degree of oxygen depletion. Biological oxygen demand loading and suspended solids have also been greatly reduced, although occasional and isolated problems with phosphate, fecal coliforms and heavy metals still occur. Nevertheless, an over 80% reduction of BOD and suspended solids from point sources in the basin during the past decade is a satisfactory achievement (International Saint John River Water Quality Committee, 1984).

MODEL DESCRIPTION

The One-D model is based on a theory developed at the Massachusetts Institute of Technology in the early 1970s (Gunaratnam and Perkins, 1970; Dailey and Harleman, 1972). The model has evolved in Canada from its initial application to the St. Lawrence River Study and later to numerous other hydraulic and water quality studies in Canada. It is capable of simulating one-dimensional unsteady flow in a network of branching and/or looping channels which may consist of over bank or embayment storage areas, various hydraulic control structures and tidal boundary conditions. The governing equations are the Saint Venant equations of conservation of mass and momentum of flow. An implicit finite-difference numerical scheme is used by applying a weighed residual method to the linearized matrix of the flow equations to obtain an unconditionally stable solution.

The water quality module is an integral part of the One-D model. Up to 13 water quality constituents can be simulated based on the mass balance of the one-dimensional advection–dispersion equation which is coupled with the hydraulic solution of the model. These constituents are salinity, temperature, BOD, dissolved oxygen, organic nitrogen, inorganic nitrogen, organic phosphate, inorganic phosphate, phytoplankton, zooplankton, fecal coliform, decaying lignins and conservative lignins. Currently, the model and its subroutines are supported by Environment Canada Water Planning and Management Branch (1988).

The river system to be simulated is divided into a network of reaches and nodes, containing computed cross-sectional areas and other details from surveyed data. Channel boundary conditions and lateral inflows are input to the network. Figure 2 shows the schematic diagram of the One-D model as used in this study. In general, the segmentation of the river into reaches is dependent upon the variabilities of the river cross sections, the river flow regime, and the minimum mesh spacing requirements of the model. If a reach is divided too finely by mesh spacing, model computation time will increase unnecessarily without any gain in modelling stability and output accuracy. Conversely, a coarse model will definitely not provide enough detail in terms of hydraulic and water quality profiles along the simulated reaches or an acceptable level of accuracy in the solution. When a computer model is generated to simulate a particular project, there are 19 dimensional variables that must be determined and input. These variables represent different types of input data groups and their sizes determine the size of the computer model. Output of the model is user-specified and can contain computed hydrographs and hydraulic profiles, with discharge, water surface elevation, flow depth, velocity and frictional coefficient tabulated.

The water quality model QUAL-IIe is an enhanced version of QUAL-II, which was developed by the National Council for Air and Stream Improvement (NCASI, 1985). In recent years, it has been widely used for waste load allocations, discharge permit determinations, and other conventional water pollution evaluations by both regulatory personnel and consultants in the United States. It is now one of several computer models maintained in updated format by the U.S. EPA Center for Water Quality Modeling in Athens, Georgia.

The QUAL-IIe can predict both the temporal and spatial quantities of the following water quality variables: temperature, BOD, algae as chlorophyll *a*, up to three conservative constituents, organic nitrogen, ammonia, nitrite, nitrate, organic phosphorus, dissolved phosphorus, dissolved oxygen, coliform, and one arbitrary non-conservative constituent. The model includes the major interactions of the nutrient cycles, algae production, benthic and carbonaceous oxygen demand, atmospheric reaëration, and their effects on the dissolved oxygen. It permits simulation of any branching, one-dimensional stream system and basically works in steady mode for boundary and input conditions such as flows, waste loads, and biochemical coefficients. The model also has a limited dynamic mode that can handle diurnal variations in meteorological data. An implicit finite-difference numerical procedure is used to solve the governing advection–dispersion mass transport equations for each water quality constituent being simulated. Hydraulic simulation is computed by mass balance of streamflow, with velocity, cross-sectional area and depth as output. As in the One-D model, dispersion in QUAL-IIe is allowed in the longitudinal direction only.

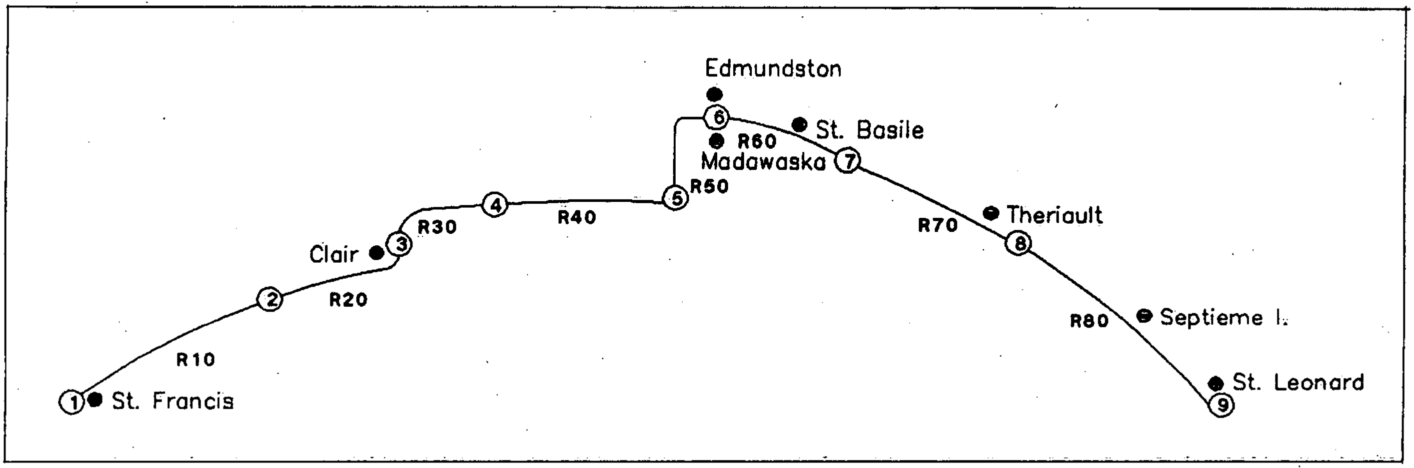

Figure 2. ONE–D model schematic diagram.

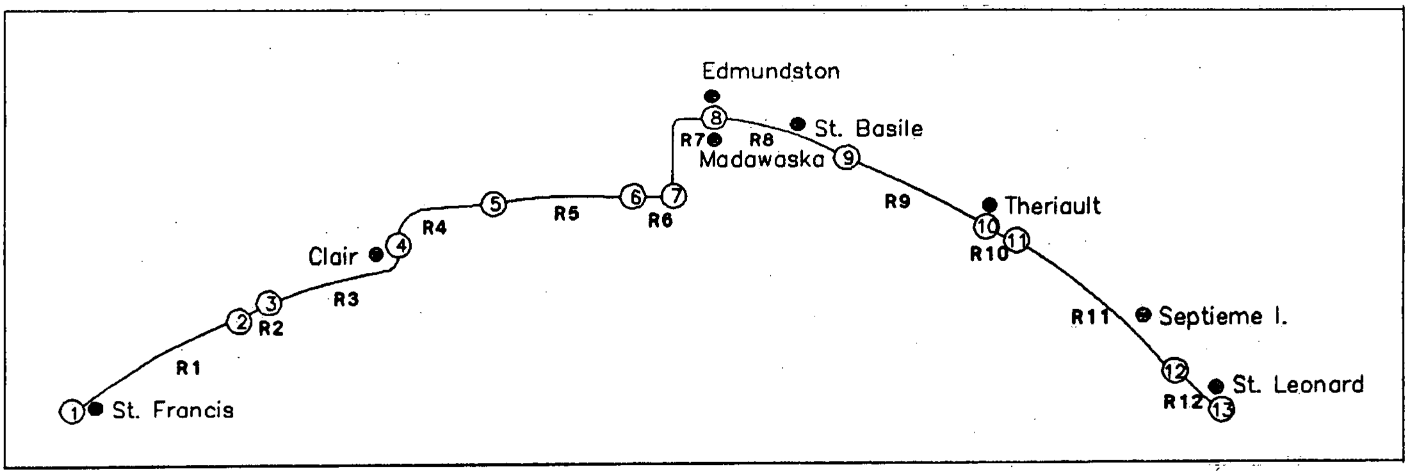

Figure 3. QUAL–IIe model schematic diagram.

Figure 3 shows the schematic diagram of the QUAL-IIe model as used in this study. The river is subdivided into reaches, which are stretches of river that have uniform hydraulic characteristics. In the model, each reach is then divided into computational elements of equal length. River reaches are the basis of most data input. The length, and hence the number of computational elements in each reach, usually determines the accuracy and degree of detail in the model solution. The number of computational elements is subject to the dimensional limitation of the program. There is also a limitation on the maximum number of reaches in a model. However, QUAL-IIe incorporates features of ANSI FORTRAN 77 that allow these and other limitations to be easily changed.

DATA COLLECTION METHODS

The Upper Saint John River usually has heavy runoff from snowmelt in April, at times combined with storm runoff. This is followed by a summer low-flow period in July and August. The average annual discharge at Fort Kent for 1987 was 219 m^3/s. Average daily discharges of the Allagash River at Dickey in Maine, which has an upstream starting point at St. Francis, are used as boundary condition flows for modelling. Other major tributaries included in the model are the St. Francis River, Fish River, Madawaska River, Green River and Grand River (Fig. 1). Average daily discharges are available from the United States Geological Survey (USGS) and Water Survey of Canada (WSC) records. Downstream boundary conditions need not be specified in QUAL-IIe. For One-D, a stage-routing boundary condition is used for the downstream end, as there is neither a stage nor discharge gauge at St. Leonard, and the discharges recorded at the Grand Falls gauge further downstream are not suitable for use because of the backwater effects of the Grand Falls dam.

Cross-sectional data of the river were provided by the Atlantic Region Water Planning and Management Branch of Environment Canada. Out of the 93 cross sections available from St. Francis to St. Leonard, 59 were selected by reviewing and comparing channel variations and were processed for use in the One-D model. Locations of these cross sections are shown in Figure 4. The QUAL-IIe model does not require exact cross-sectional areas; it has an option to use flow equations containing coefficients and exponents.

In order to obtain the relevant values of the coefficients and exponents, the One-D model was used to make simulation runs under various flow conditions to obtain velocity, depth and discharge values for each reach. These values were then used to calculate the coefficents and exponents of the flow equations for each reach which could then be used according to the model manual (Brown and Barnwell, 1985).

Water quality data used for this study were collected by the Atlantic Region Water Quality Branch of Environment Canada during two survey periods — in May 1986 representing a high-flow period and in August 1987 representing a period of low flow. In each survey,

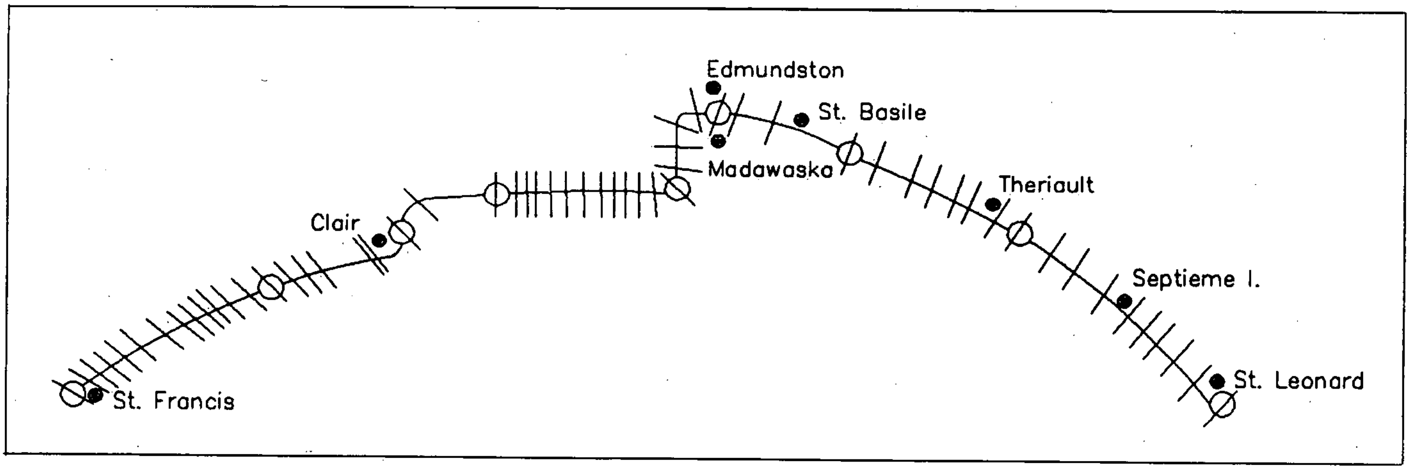

Figure 4. ONE D model cross-sections.

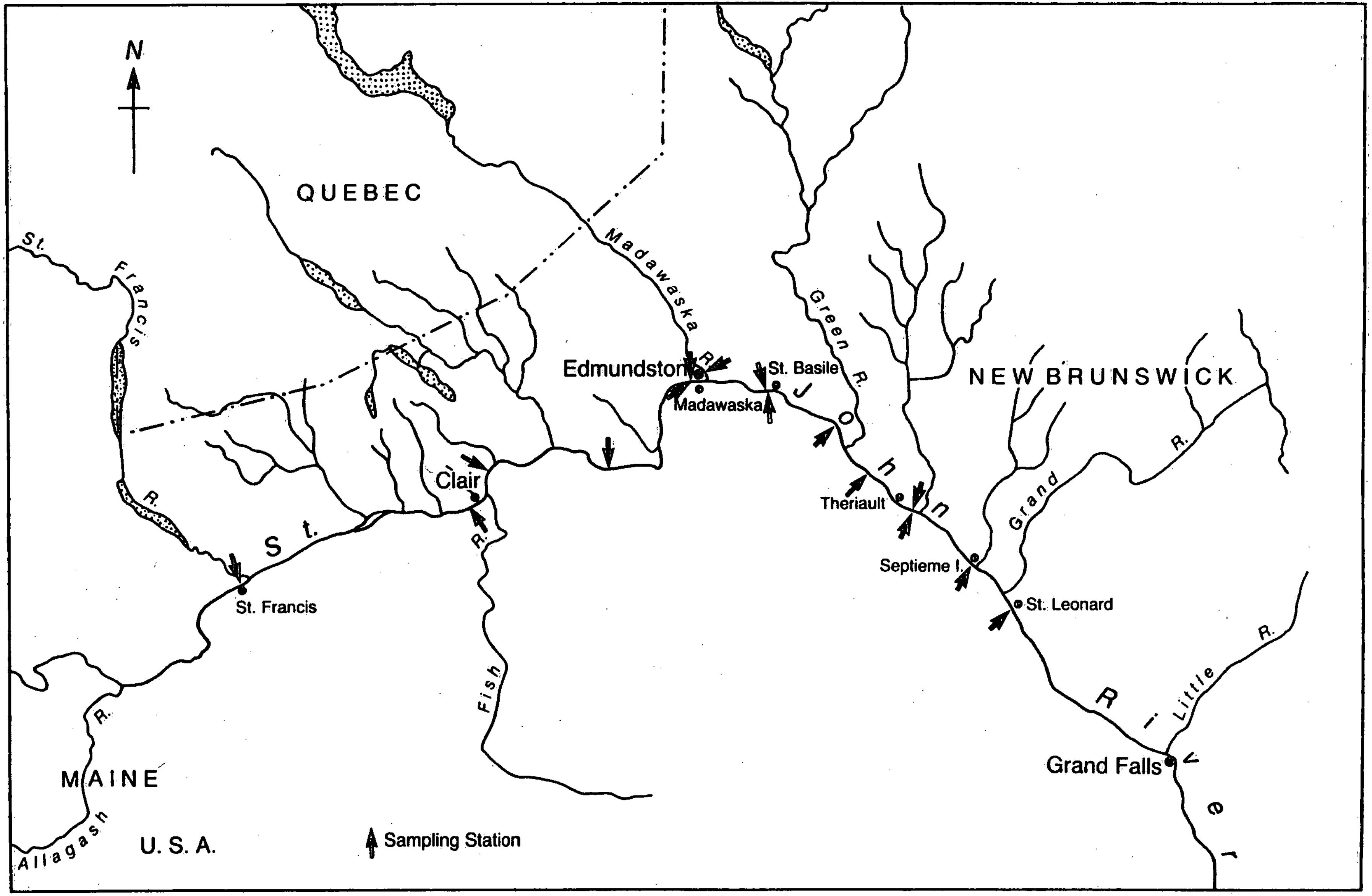

Figure 5. Sampling station locations.

four tributaries and eight point source effluents were sampled for up to 24 water quality parameters for three consecutive days. The May 1986 data were also augmented by a sampling of tributaries and point sources on the Maine side of the river. This sampling was undertaken by the Bureau of Water Quality Control, Department of Environmental Protection (DEP) of Maine during the same three-day period.

Additional data covering factors such as temperature, DO, ammonia, nitrite, nitrate, total phosphorus, phosphate, total suspended solids (TSS), total BOD and carbonaceous BOD were obtained from DEP of Maine for three-day periods in July 1987 and September 1988. These data were previously used in the Maine DEP Saint John River waste load allocation study. Locations of the sampling stations are shown in Figure 5. For the purpose of this comparison study, only the usable data of the water quality parameters that can be readily simulated by both models were selected from the previously mentioned sources. Discharges from various municipal and industrial treatment facilities included in the model were as follows:

- Nadeau poultry sewage lagoon
- St. François sewage lagoon
- Fort Kent sewage treatment plant
- Baker Brook sewage lagoon
- Madawaska sewage lagoon
- Fraser St. Basile sewage treatment plant
- Fraser Paper Madawaska sewage treatment plant
- Edmundston sewage lagoon
- St. Basile treatment plant
- Van Buren treatment plant
- St. Leonard treatment plant

Locations of the point source discharges are shown in Figure 1.

The sampling and measurement methodology adopted by the Atlantic Region Water Quality Branch basically follows the Standard Methods (APHA, AWWA, and WPCF, 1971). Dissolved oxygen and water temperature measurements were made *in situ* with a YSI Model 57 dissolved oxygen meter equipped with a Model 5739 dissolved oxygen probe and Model 5795A submersible stirrer. The Clark-type membrane-covered sensor was calibrated once a day before measurements were made by collecting duplicate samples from the river near the sensor in 300-mL BOD bottles using an Ohio River type dissolved oxygen sampler. The Azide Modification of the standard Winkler method was used to measure dissolved oxygen in the collected samples, and the results were averaged and used to calibrated the YSI probe.

Water temperature measurements were made at the same time as dissolved oxygen measurements using the built-in thermister in the probe. Water temperature was also checked once a day with a mercury-filled NBS certified thermometer to ensure that the probe thermister readings were accurate.

Grab samples were collected by hand dipping 1-L polyethylene bottles into the river from a boat at a depth of approximately 30 cm below the water surface. The bottles were previously washed in the laboratory and rinsed with water from the river. Samples were then placed in insulated picnic coolers with coldpacks for transportation to the Moncton laboratory at the end of the week. In the laboratory, samples were analyzed for a variety of analytes including major ionic constituents, nutrients and heavy metals. Table 1 lists the analytical methodology employed.

MODEL CALIBRATION

The primary purpose of constructing a valid water quality model for a river system is to enhance the basic understanding of the impact of pollution on water quality. The model can be used as a tool in the decision-making process related to river basin planning and management. In simulating a river system, evaluation of model performance normally involves testing whether observed hydraulic and water quality values can be adequately simulated using one set of system parameters under different sets of boundary conditions. By means of the calibration procedure, questions about the validity and credibility of the model should be addressed, and the predictive ability of the model can therefore be reasonably determined. However, because of the complex structure of water quality models and the interactive nature of different variables in a river system, the calibration procedure is seldom a straightforward process. Uncertainty and infeasibility are further heightened by the unavailability of observed

Table 1. Analytical Methodology Employed for Water Quality Tests

Analyte	NAQUADAT code	Units	Methodology
Specific conductivity	02041L	µS/cm	Conductivity meter with platinum (Pt) electrodes
pH	10301L	pH units	Electrometric method with glass and calomel electrodes
Colour	02011L	Hazen units	Visual comparison in a Hellige Aqua Tester
Turbidity	02073L	NTU	Photometry on a Hach Turbidimeter
Total alkalinity	10101L	mg/L as $CaCO_3$	Potentiometric titration with standard H_2SO_4 to pH = 4.5 and 4.2
Ca^{++}	20110L	mg/L	Automated Atomic Adsorption
Mg^{+}	12107L	mg/L	Automated Atomic Adsorption
Na^{+}	11103L	mg/L	Flame photometry with internal standard on an Autoanalyzer
K^{+}	19103L	mg/L	Flame photometry with internal standard on an Autoanalyzer
$SO_4^{=}$	16304L	mg/L	Autoanalyzer with barium chloride
Cl^{-}	17205L	mg/L	Specific Ion Electrode
NO_2+NO_3-N	07110L	mg/L	Colorimetry on an Autoanalyzer
Total nitrogen	07601L	mg/L	Ultraviolet digestion and colorimetry on an Autoanalyzer
Total phosphorus	15413P	mg/L	Colorimetry on an Autoanalyzer

data and the inaccuracy of monitoring methods. In the selection and adjustment of coefficients and rate constants, assumptions and judgements have to be made. All these factors make the calibration procedure more of an art than an exact science.

For the purpose of hydraulic simulation, the same sets of headwater conditions and lateral inflows were used in both the One-D and QUAL-IIe models. The boundary flows at the upstream end of the river were the sum of the flows in the Saint John River at Dickey in the U.S.A., and in its tributary, the Allagash River. Data for both flows were obtained from the U.S. Geological Survey data. Various lateral inflows included in the two models were from the St. Francis River, the Fish River, the Madawaska River at Edmundston, the Green River, the Grand River, and major wastewater treatment plants, such as the Madawaska, Edmundston and St. Basile sewage treatment plants.

Although some data sets can be applied to both models for hydraulic computation, differences must be accounted for. The QUAL-IIe model does not require any downstream boundary conditions, whereas the One-D model offers various options. The stage-routing boundary condition was chosen for this study, because the nearest Water Survey of Canada station is at Grand Falls (WSC01AF002) and was not considered to be suitable to be transferred to St. Leonard.

In the calibration process of the One-D model, Manning's coefficient is the main parameter to be calibrated. Values of 'n' for the entire study section were obtained from New Brunswick Power, based upon previous hydraulic studies of the Saint John River. Simulated results were then compared with the discharge data at Fort Kent (WSC01AD002) and the stage data at Edmundston (WSC01AD004) to check the validity of hydraulic computation. Disagreement between observed data and the data derived from the models of about 0.5 m in water level at Edmundston was found and the reason was not known, except that if a correct downstream boundary condition of either stage or discharge at St. Leonard is available for use, a different water surface profile might be produced which would result in a slightly different water level reading at Edmundston.

The QUAL-IIe model has two options to describe the hydraulic characteristics of the system. The first option uses a functional relationship, while the second option uses a geometric representation in the shape of a trapezoid (NCASI, 1985). In the absence of observed data for each reach in this study, numerous runs were made for different high- and low-flow conditions to obtain their respective flow velocity and flow depth values. These simulated values of velocity, depth and discharge for each reach were then used to develop the individual coefficients and exponents in the velocity and depth functions as specified in the first option. The hydraulic computation was based upon this set of functions, and no further calibration was performed for the QUAL-IIe model.

In order to simulate water quality, observed data from the May 1986 and September 1988 surveys were used for calibration of the two models. The water quality variables chosen to be included in this study were DO, ultimate carbonaceous BOD, total alkalinity (as calcium carbonate), total suspended solids (TSS), organic nitrogen, inorganic nitrogen, phosphorus and inorganic phosphorus. Previous studies have found that algal activity was low on the Saint John River. The chlorophyll *a* value averaged about 4 ppb and the algal photosynthesis-respiration were considered to be negligible on the oxygen balance of the river. Water temperatures varied slightly along the river stretches but were kept constant as input to the model for all runs.

The determination of input system parameters for the two models is based upon direct use of measured values from field samples, literature values and calibrated values from comparison of observed and simulated profiles. The first step normally is the calibration of the BOD decay rate (K_d). Higher rates are usually obtained in rapid and shallow rivers, while lower decay rates are obtained under slower and deeper conditions. After applying engineering judgement to the calibrated results, a range of K_d of 0.4/d to 0.05/d resulted from the upstream to downstream portion of the study section. A lower K_d range of 0.2/d to 0.05/d resulted from the calibration of the One-D model. For DO computation, QUAL-IIe provides eight options for estimating the reaeration coefficient (K_2). The option using O'Connor and Dobbins equation (1958) was selected because it generally works well on large rivers like the Saint John. The One-D model uses an equation similar to the QUAL-IIe. Both equations have a constant that can be slightly adjusted if necessary during the calibration procedure. Sediment oxygen demand (SOD) can be included in both models. From the substrate core sample measurements made in the summer of 1988 by the Maine DEP, SOD rates of 1 g/m^2-d to 3.8 g/m^2-d were found. A decision was made to assign a SOD rate of 2 g/m^2-d to both models. For the nutrient families, average values of reaction coefficients recommended by the QUAL-IIe model manual and other literature (Bowie, 1985) were used in both the QUAL-IIe and One-D runs:

- rate for hydrolysis of organic-N to ammonia	0.02/d
- rate for organic-N settling	0.00/d
- rate for biological oxidation of ammonia to nitrite	0.50/d
- benthos source rate for ammonia-N	0.00/d
- rate for biological oxidation of nitrite to nitrate	2.00/d
- rate for decay of organic-P to dissolved P	0.05/d
- rate for organic-P settling	0.00/d
- benthos source rate for dissolved-P	0.00/d

Figures 6, 7, 8 and 9 show observed values and simulated profiles of DO, total alkalinity, inorganic nitrogen and organic nitrogen from both models using the May 1986 data set. Figure 10 shows the calibration results for BOD using the September 1988 data set which covered the river section from Edmundston to St. Leonard. The high-low bars represent the observed range of field data during the three-day sampling period. The calibration for phosphorus was not done because of very low concentrations — in the range of less than 0.01 ppm, which is too low to allow for credible output from the QUAL-IIe model, the precision of which is limited to two decimal places. In general, good agreement between observed and simulated variable values was achieved by the calibration procedure with the exception of BOD values near St. Leonard. It is possible that some unrecorded local source of BOD might have contributed to slightly higher than average BOD values in the river. Profiles obtained from the two model runs resemble each other very closely.

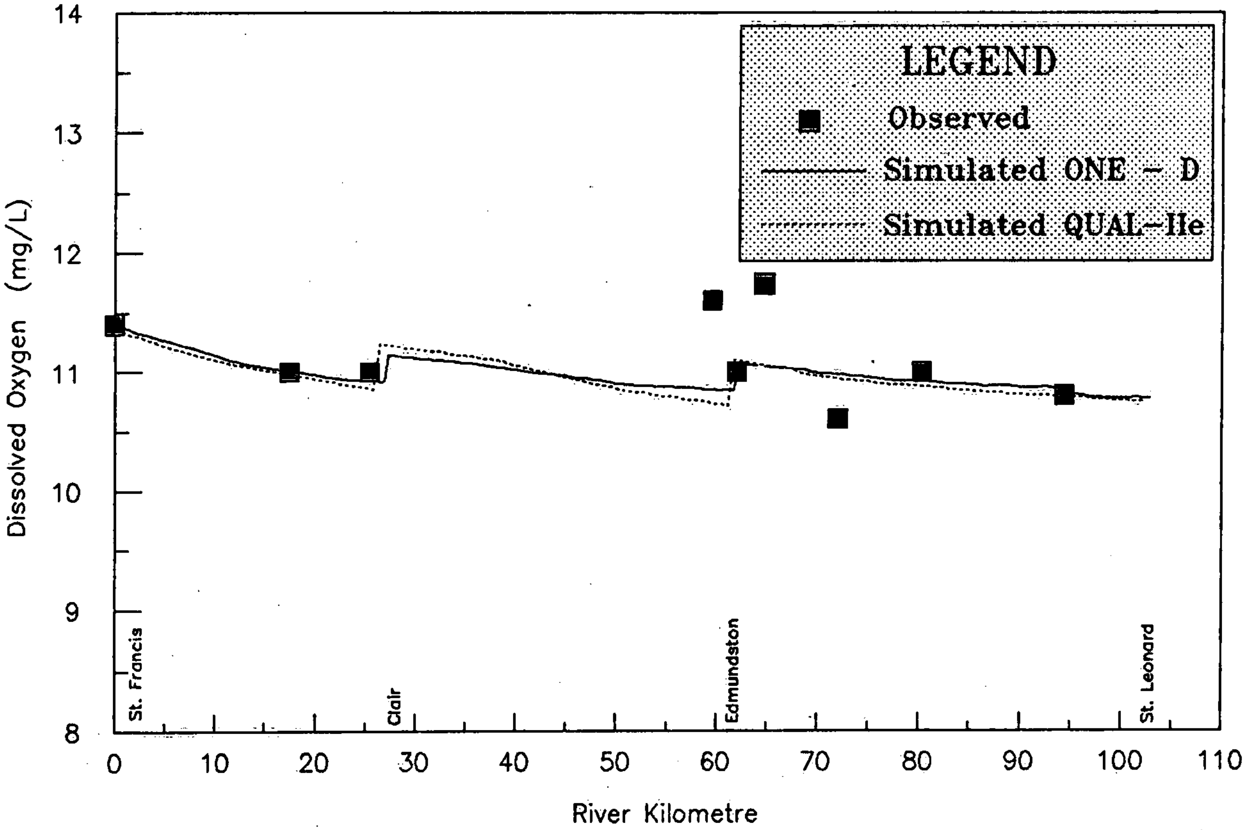

Figure 6. Model calibration - dissolved oxygen profile (May 1986).

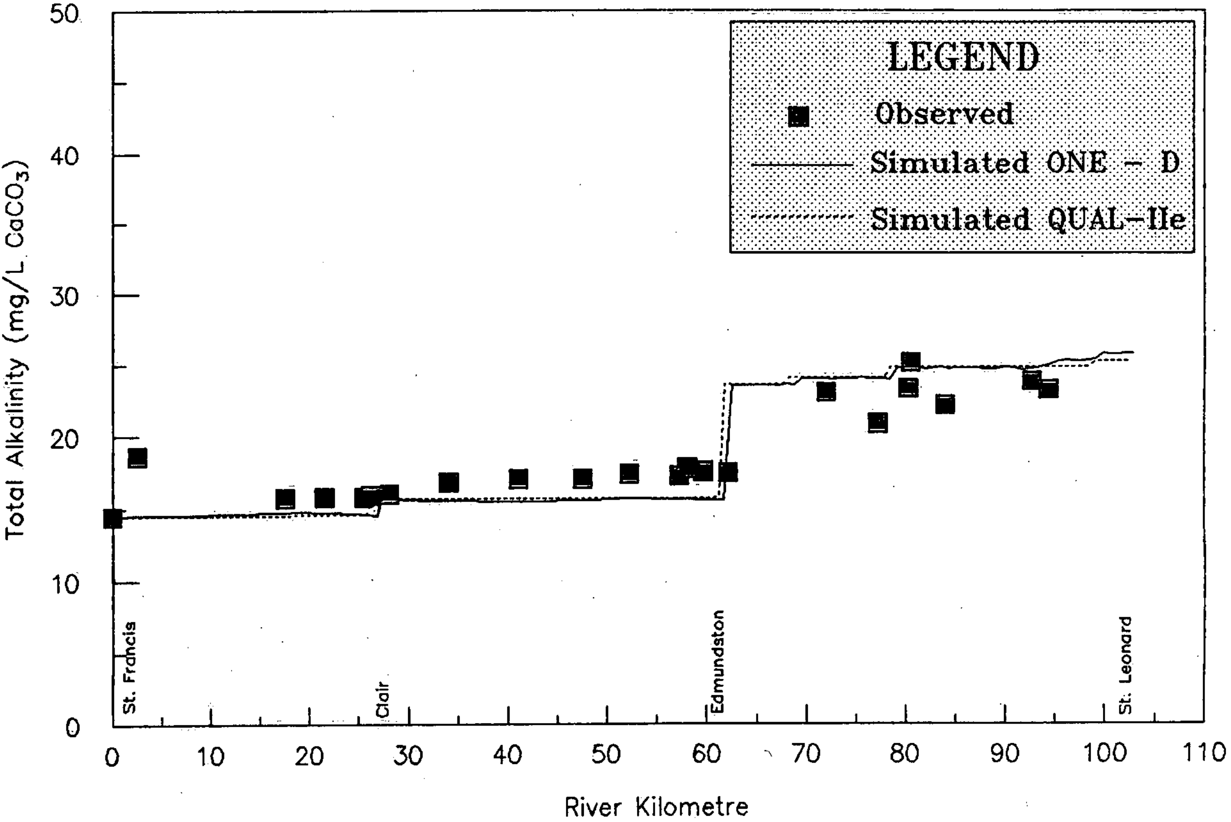

Figure 7. Model calibration - total alkalinity profile (May 1986).

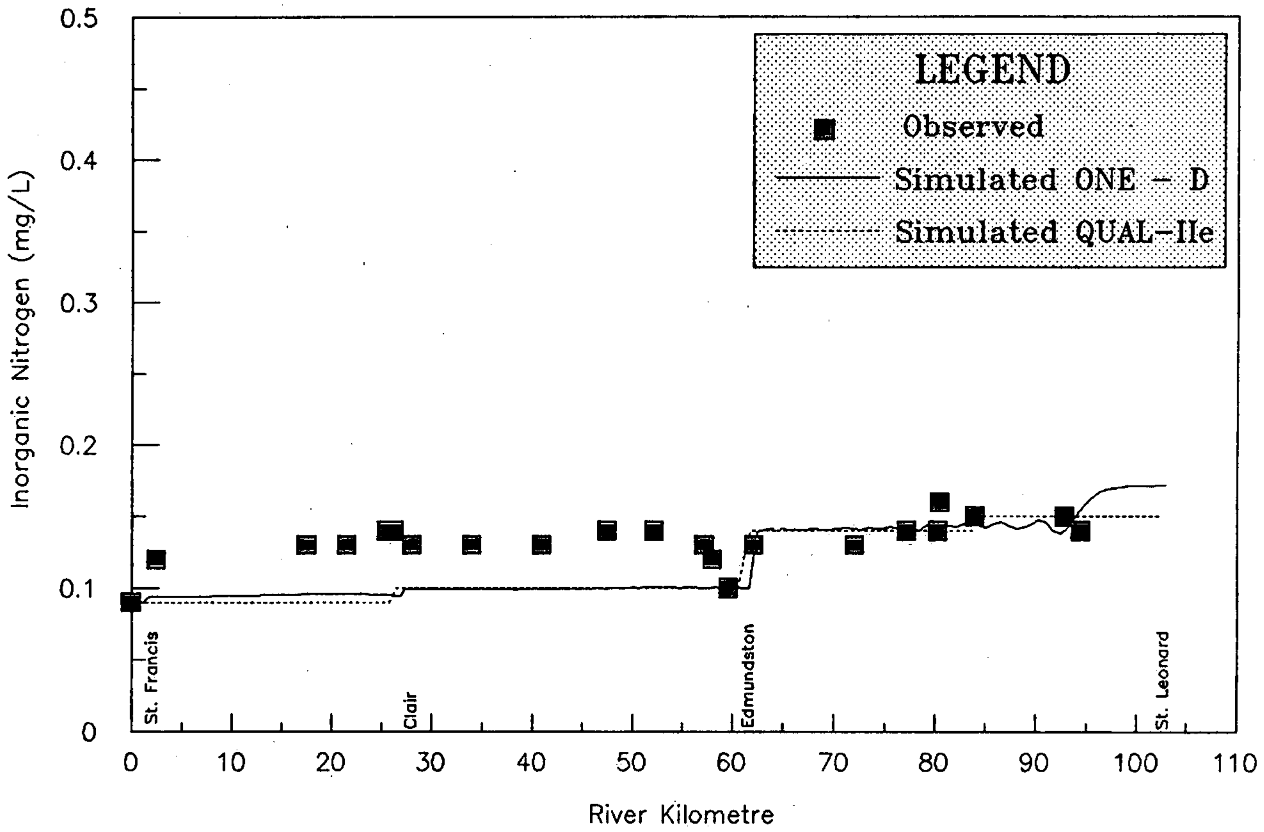

Figure 8. Model calibration - inorganic nitrogen profile (May 1986).

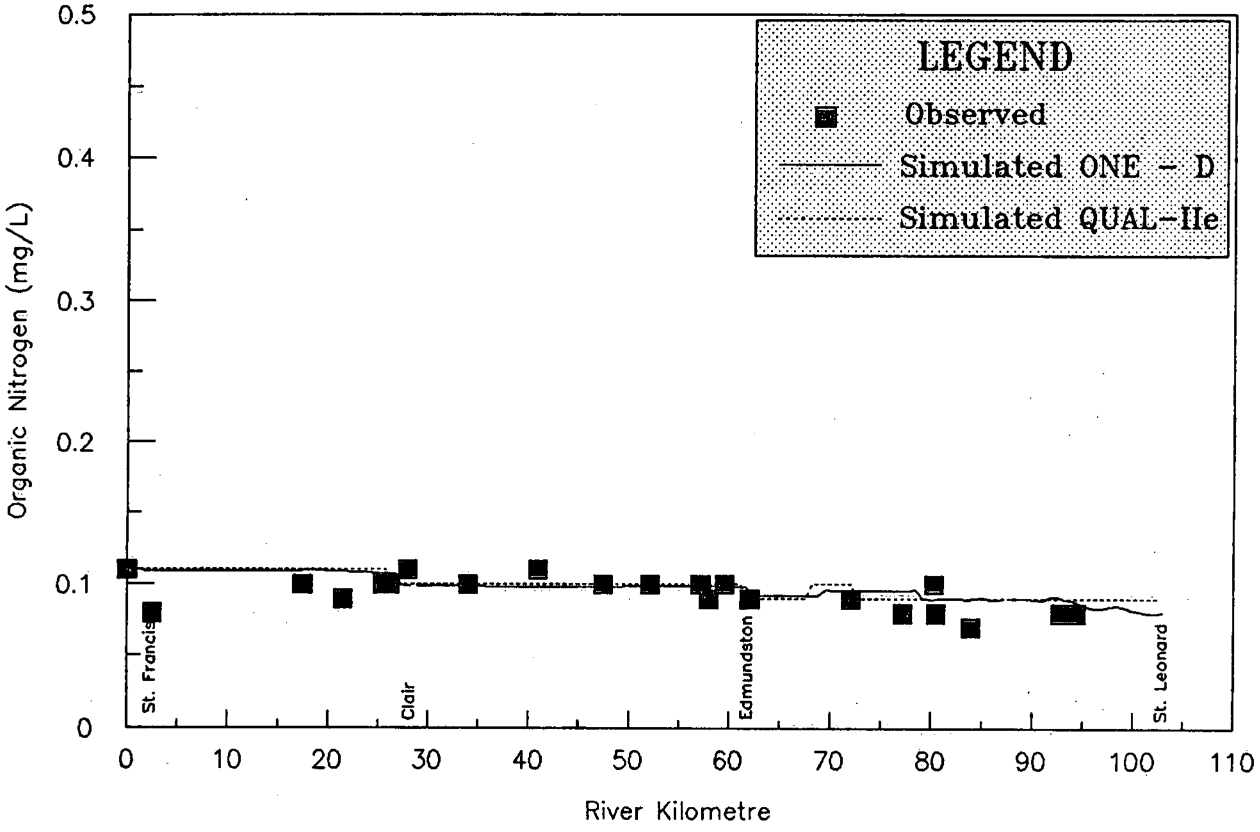

Figure 9. Model calibration - organic nitrogen profile (May 1986).

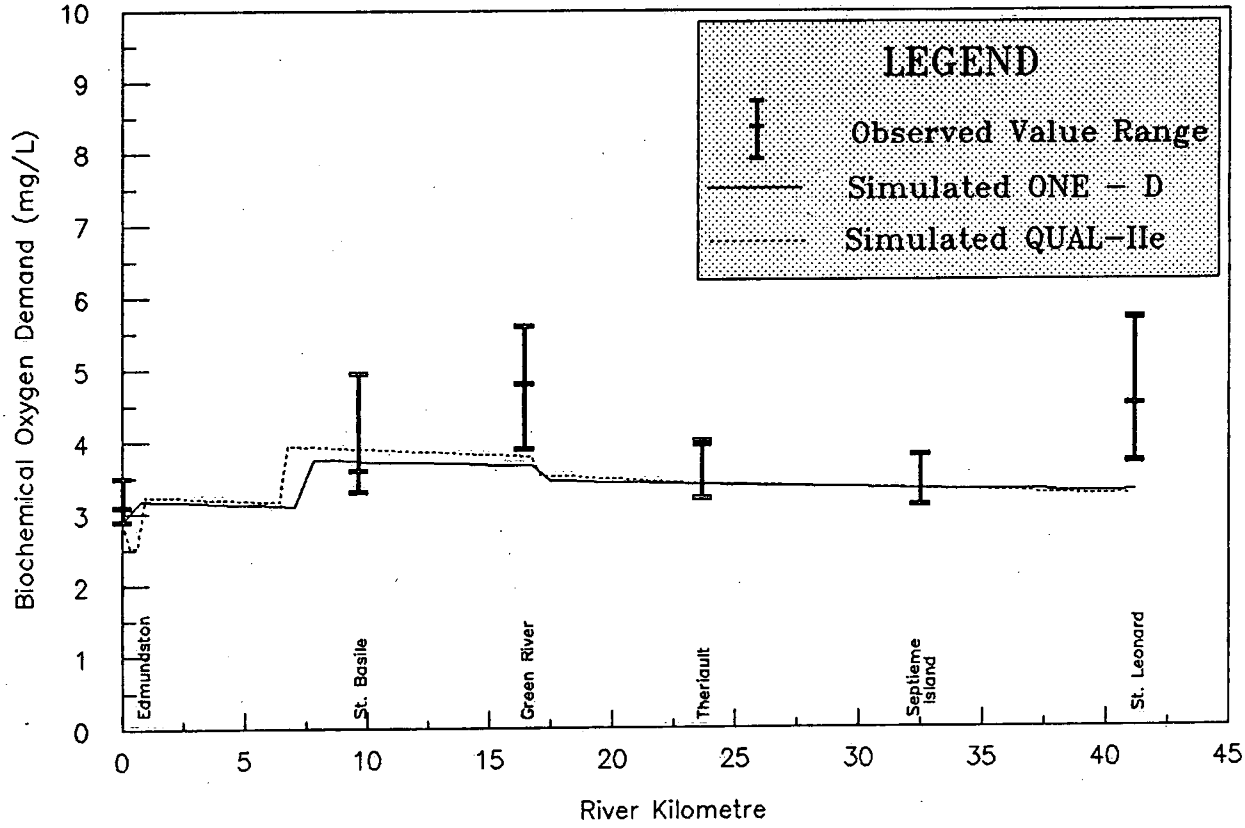

Figure 10. Model calibration - biochemical oxygen demand profile (Sept. 1988).

MODEL VERIFICATION

Model verification normally involves testing of the calibrated models to different sets of observed field data, preferably under different flow or waste load conditions. The July 1987 data set, which covered the river stretch from Edmundston to St. Leonard, and the August 1987 data set, which covered the river stretch from Clair to St. Leonard, were used for verification of the two models. The first data set was used for verification of BOD, DO and TSS. The second data set was used for verification of DO, total alkalinity, inorganic nitrogen, organic nitrogen, inorganic phosphorus and organic phosphorus. Both TSS and total alkalinity as calcium carbonate are treated as conservative materials in both models.

Figures 11 to 19 present a comparison of the simulated results from the two models plotted against the range of observed data. The verification runs serve as a test of the simulating capability of mixing processes in the river system. In most cases, the test runs resulted in a good fit of the simulated profiles from the two models and the observed data.

In the case of TSS, some high values were observed in the portion of the river below the Green River (Fig. 13). There is some potato-growing activity in this subbasin, and erosion from potato fields is a common problem in this part of the basin, particularly following sometimes intense rain showers during the summer months. These might have been the source of the high suspended solids values observed in the Saint John River downstream of the mouth of the Green River. In other words, it was possible that some unaccounted for source of pollution could have existed for just a very short period of time upstream of the sampling points.

For the verification run of the August 1987 data, the DO profiles downstream from Edmundston from both the One-D and QUAL-IIe models were higher than the observed values (Fig. 14). A possible cause for this difference in values might have been the operation of the Grand Falls power dam downstream. Although its influence on the water quality, particularly DO, was reflected in the collected data, the dam's influence was not included in the model simulations at all.

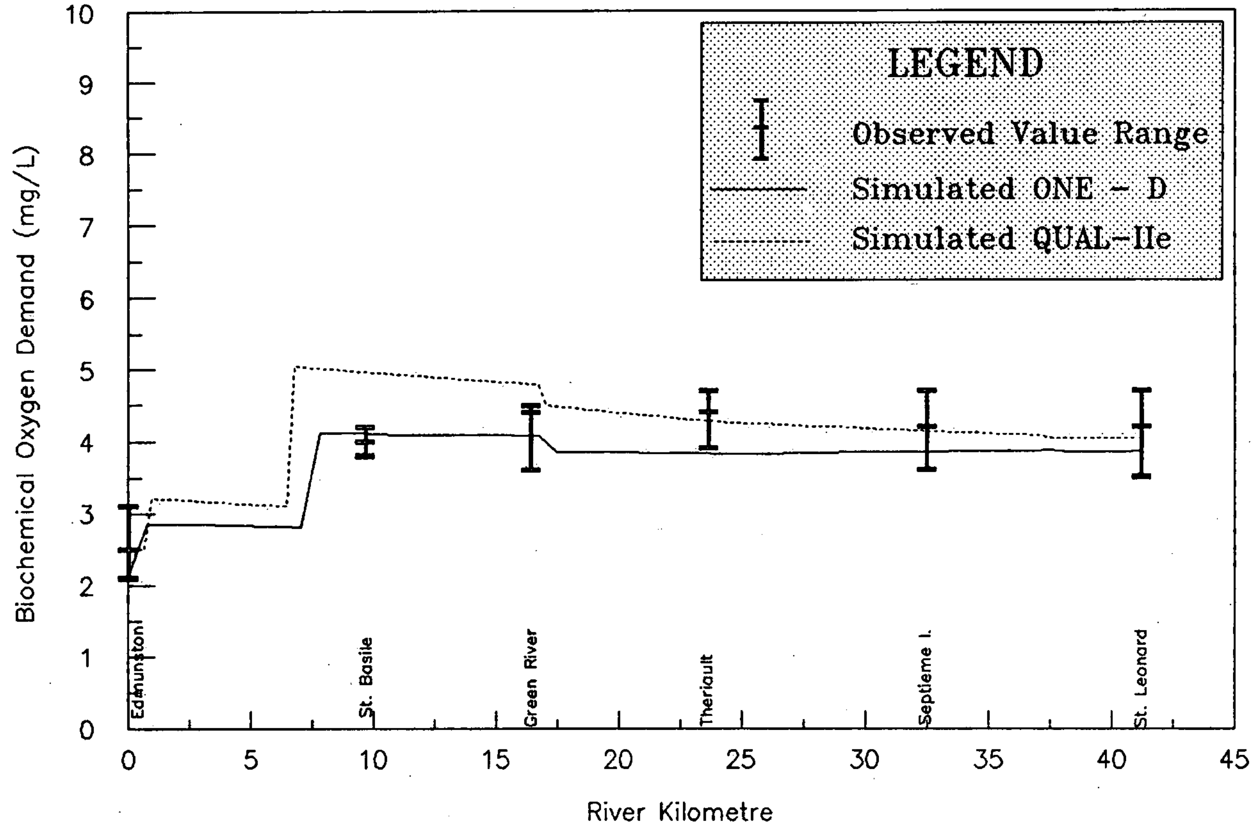

Figure 11. Model verification - biochemical oxygen demand profile (July 1987).

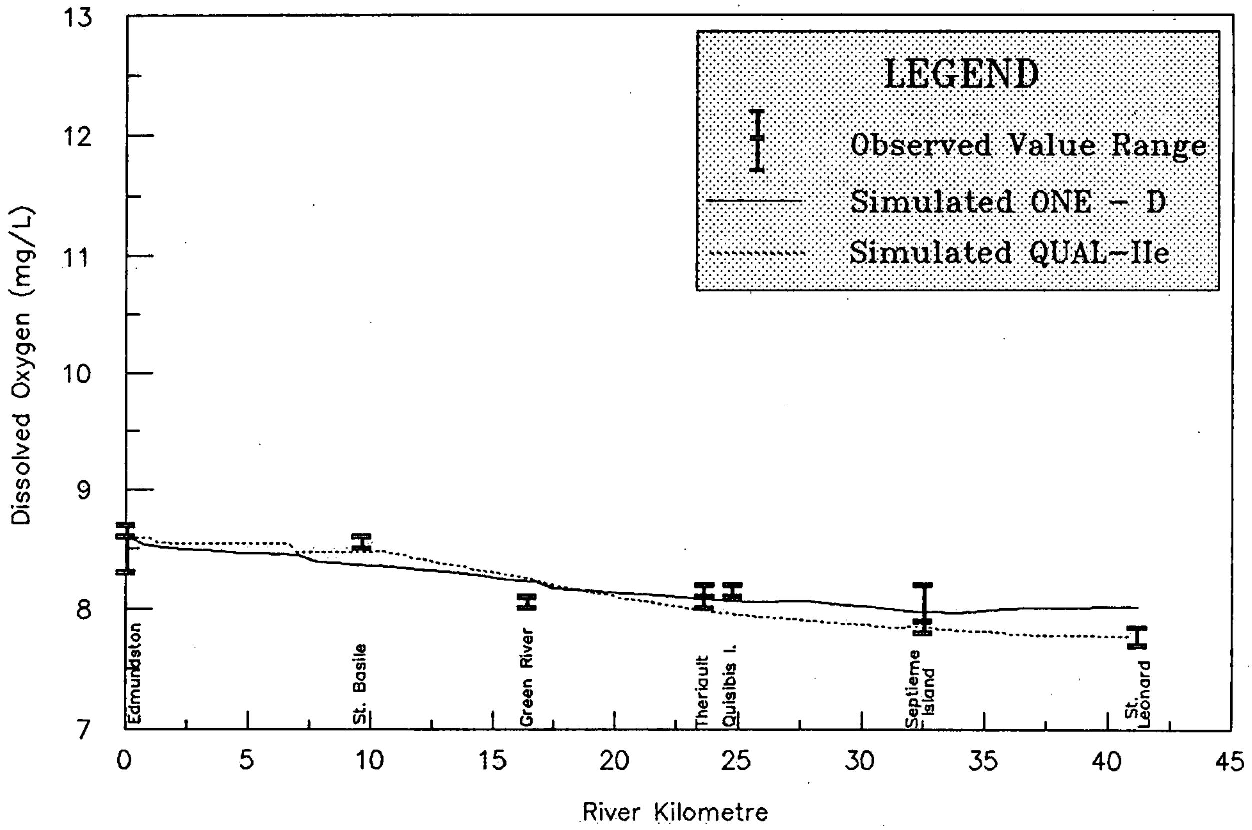

Figure 12. Model verification - dissolved oxygen profile (July 1987).

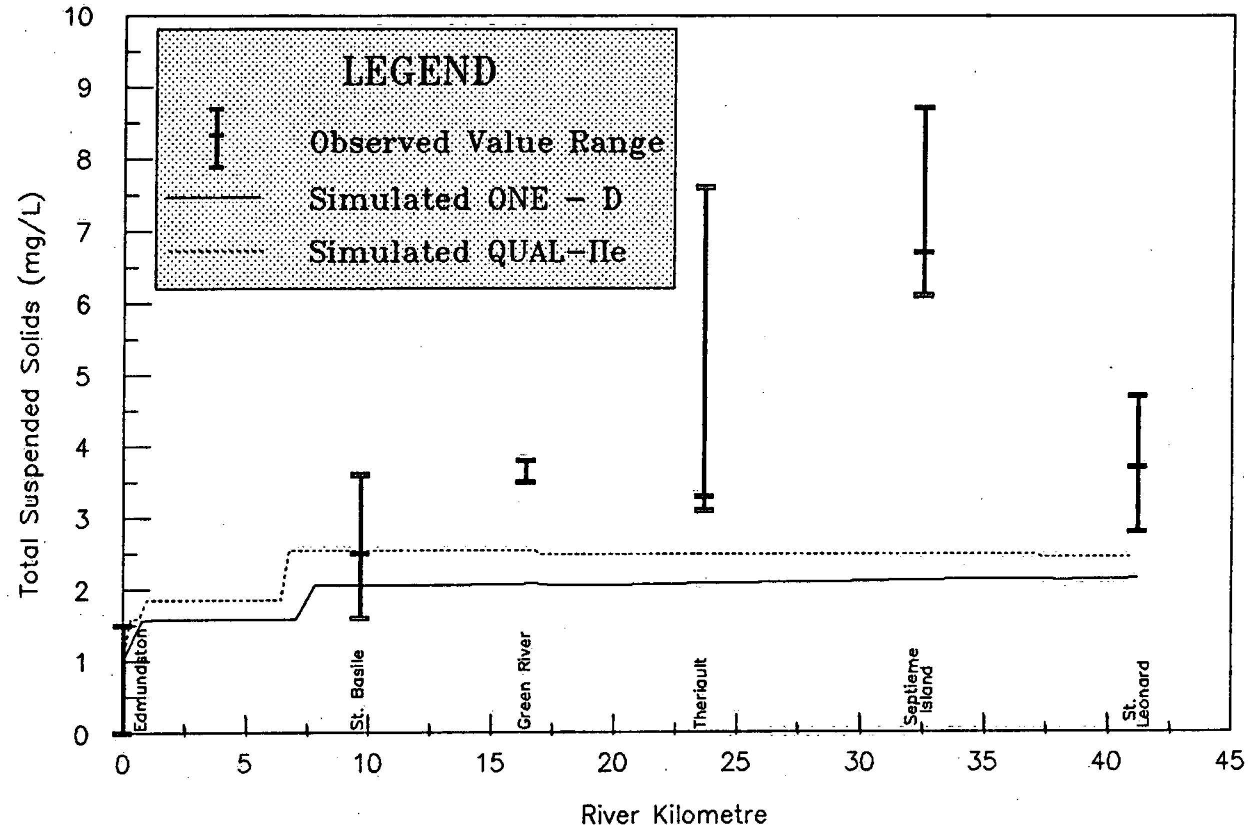

Figure 13. Model verification - total suspended solids profile (July 1987).

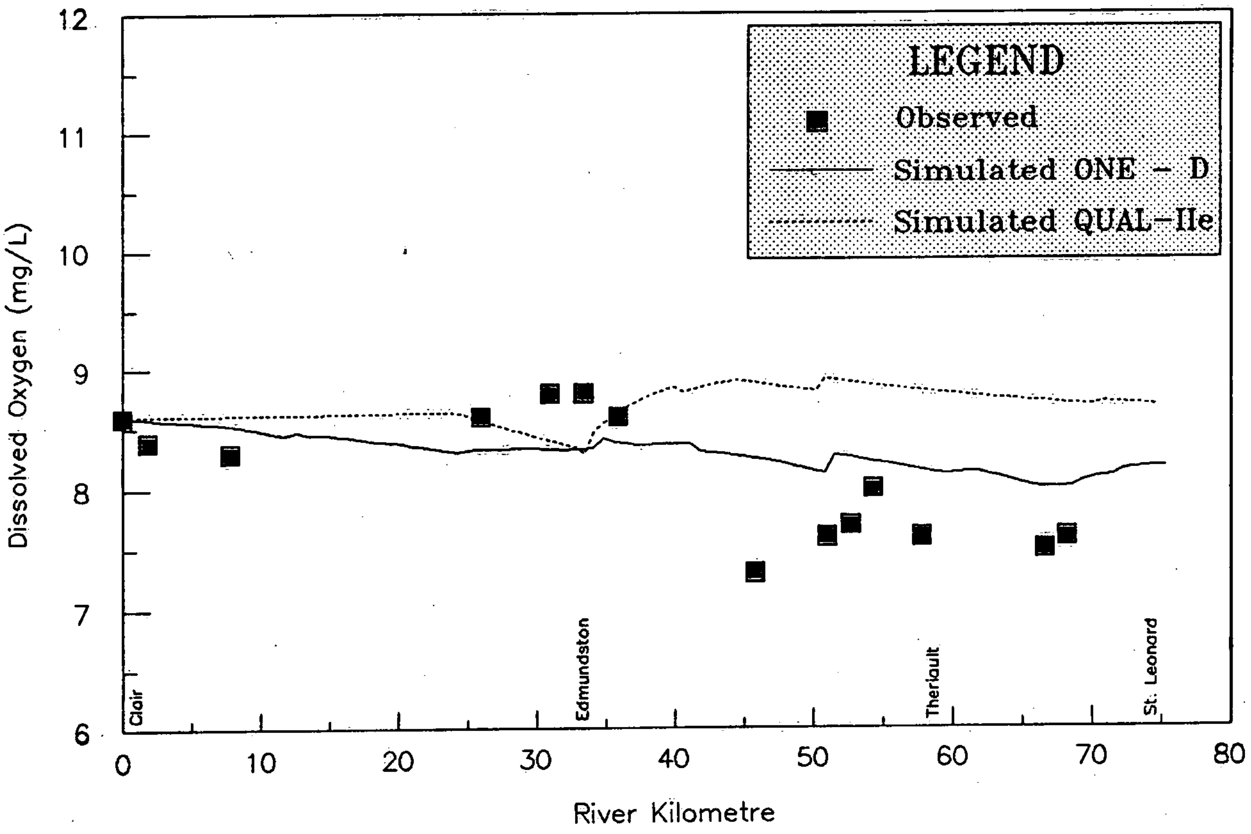

Figure 14. Model verification - dissolved oxygen profile (August 1987).

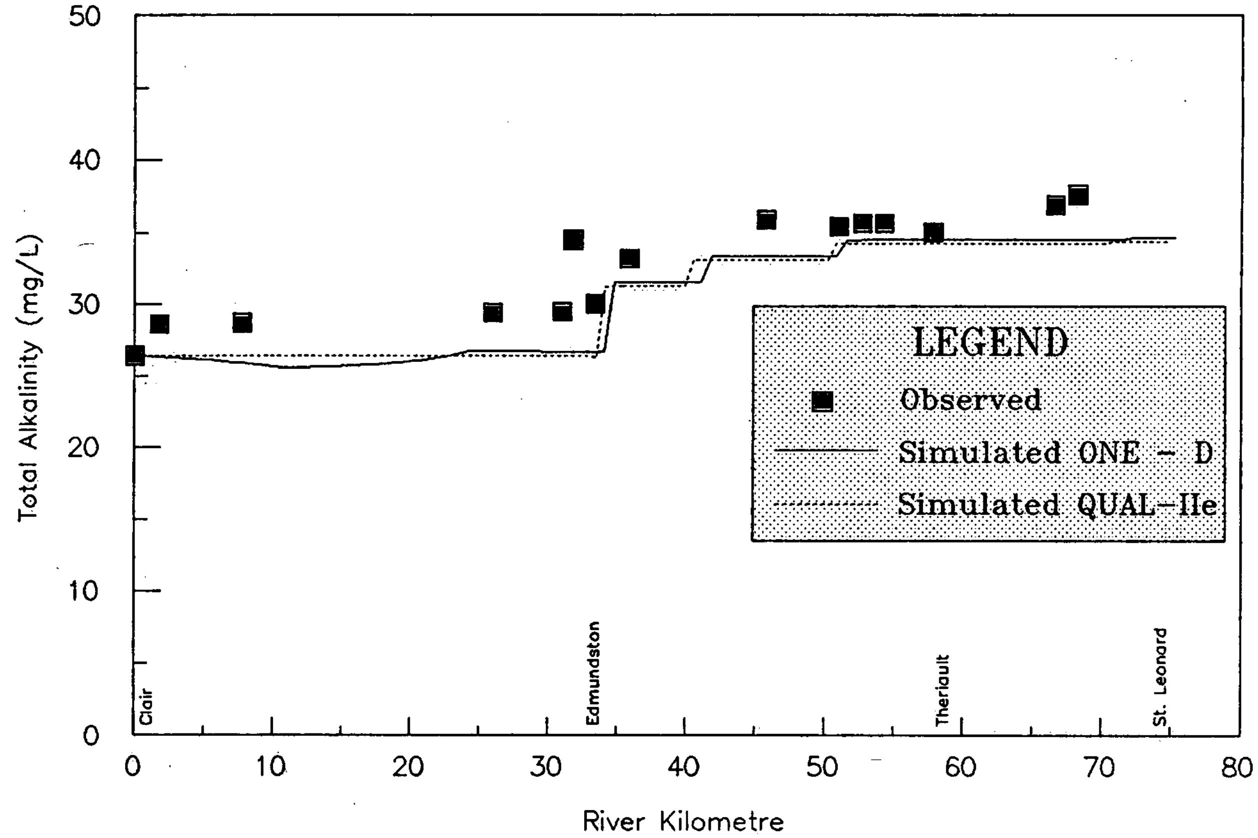

Figure 15. Model verification - total alkalinity profile (August 1987).

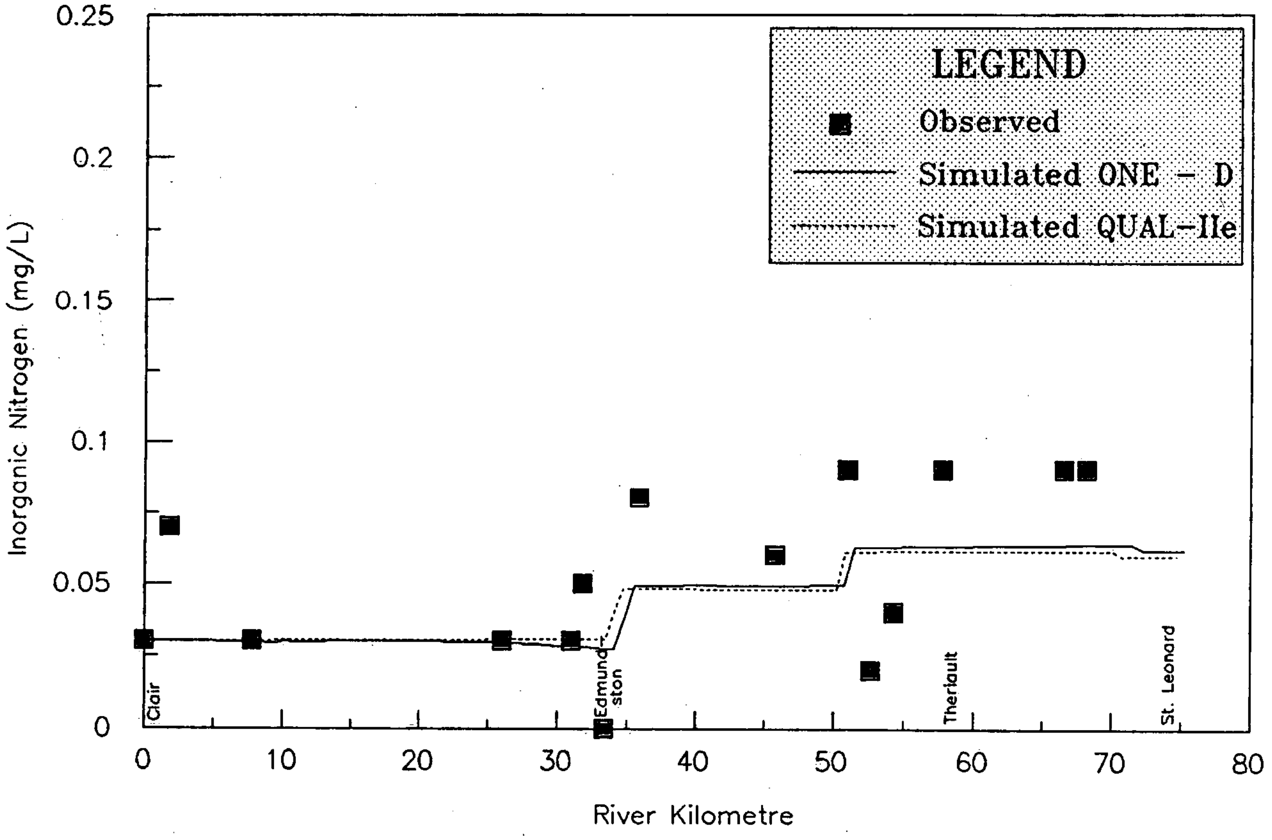

Figure 16. Model verification - inorganic nitrogen profile (August 1987).

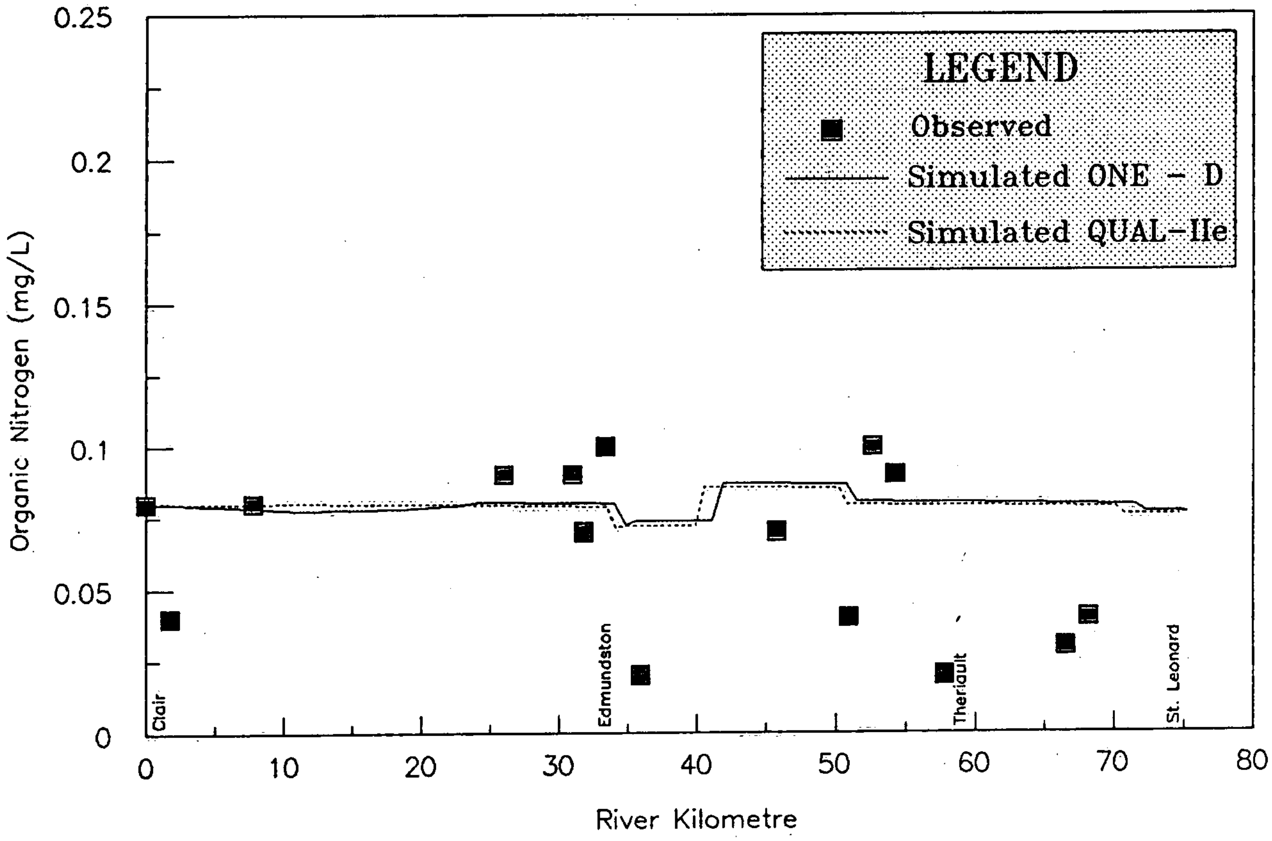

Figure 17. Model verification - organic nitrogen profile (August 1987).

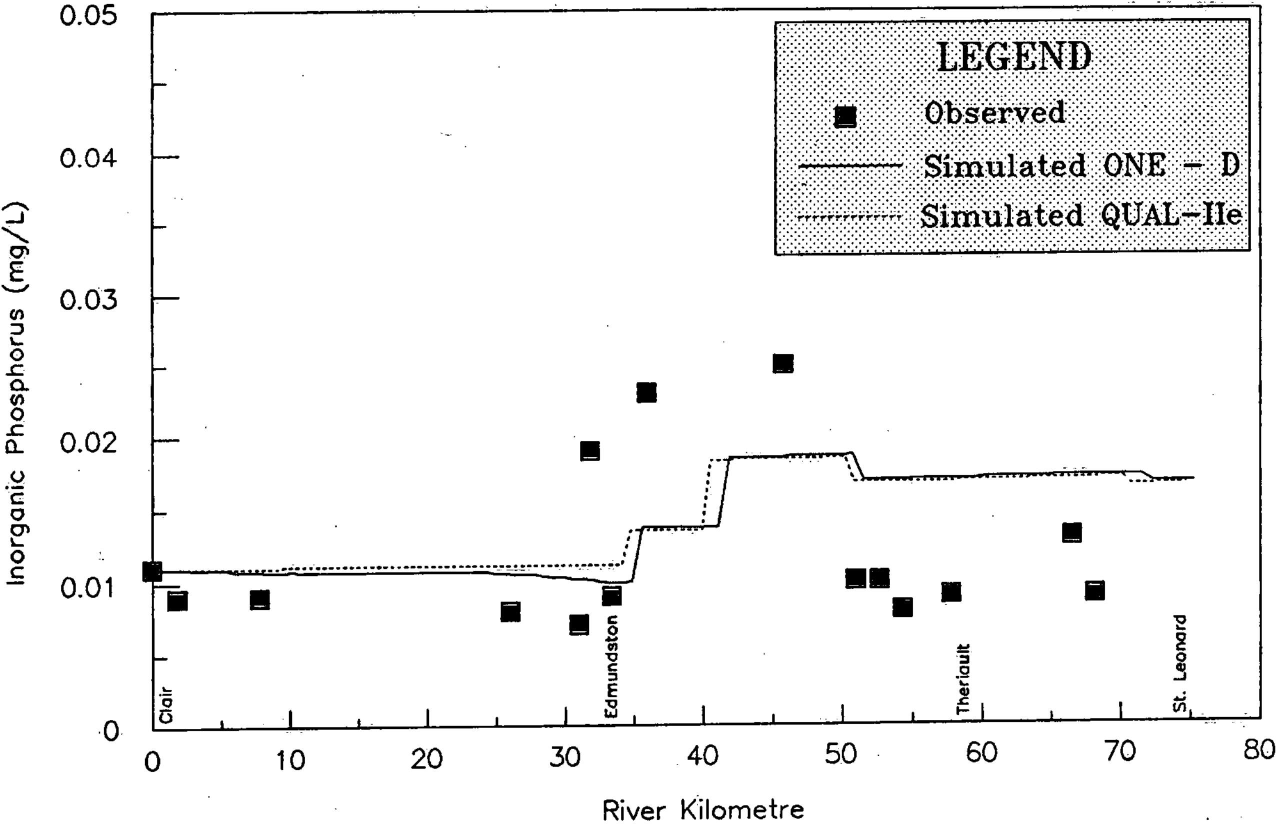

Figure 18. Model verification - inorganic phosphorus profile (August 1987).

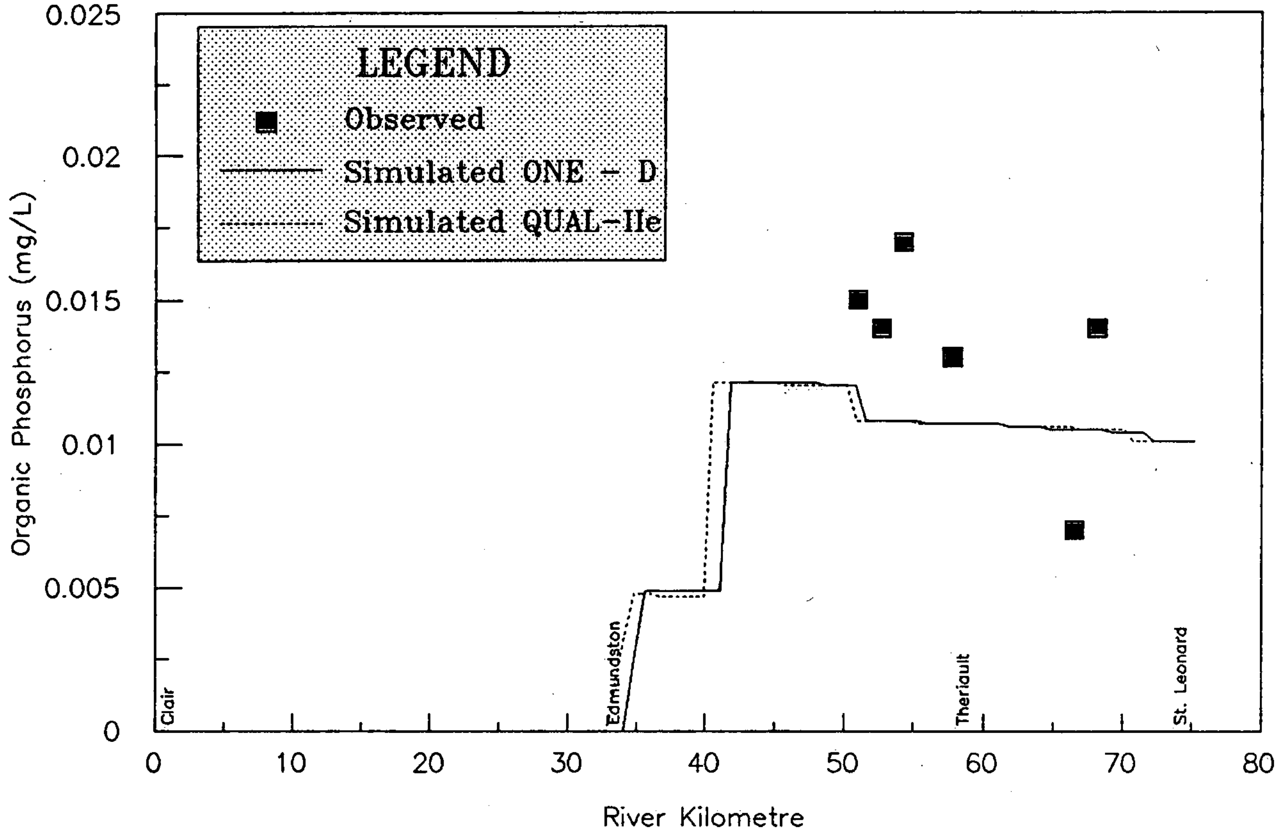

Figure 19. Model verification - organic phosphorus profile (August 1987).

SENSITIVITY ANALYSIS

The relative effects of the BOD decay rate (K_d) on the BOD profile and sediment oxygen demand (SOD) on the DO profile were examined by means of sensitivity analysis. The calibrated parameter values were varied within a reasonable range to test the responses of the two models to the particular changes. During the first stage of the procedure, two separate runs using the May 1986 data set were made with K_d doubled (+100%) and halved (-50%) for each of the two models. Sensitivity of the One-D model to K_d is very low — at least for the low-calibrated K_d condition as shown in Figure 20. Sensitivity of the QUAL-IIe model to K_d was found to be about twice the magnitude of that of the One-D model, given that the calibrated K_d value range for QUAL-IIe was also about double that of One-D (Fig. 21). The sensitivity of DO to SOD was then tested by running the models with the SOD values increased and reduced by a normal range of 50%, using the same May 1986 data set. In comparison, the QUAL-IIe model was found to be slightly less sensitive to SOD than the One-D model, as presented in Figures 22 and 23. As can be seen in both the cases of K_d and SOD, the effects of variation of the parameters on the concentrations of BOD and DO tend to increase gradually as the river proceeds downstream.

To express the model sensitivity in numerical terms, an indicator called sensitivity coefficient can be used (Table 2). It is defined as the ratio of the change in the output variable to the change in the input parameter of the model. For comparison purposes, the sensitivity coefficients are expressed in absolute values based on the simulated output at the downstream end of the river, i.e., St. Leonard.

Table 2. Sensitivity Coefficients

	One-D model	QUAL-IIe model
BOD/K_d	2.80	6.6-8.4
DO/SOD	0.256-0.257	0.183-0.197

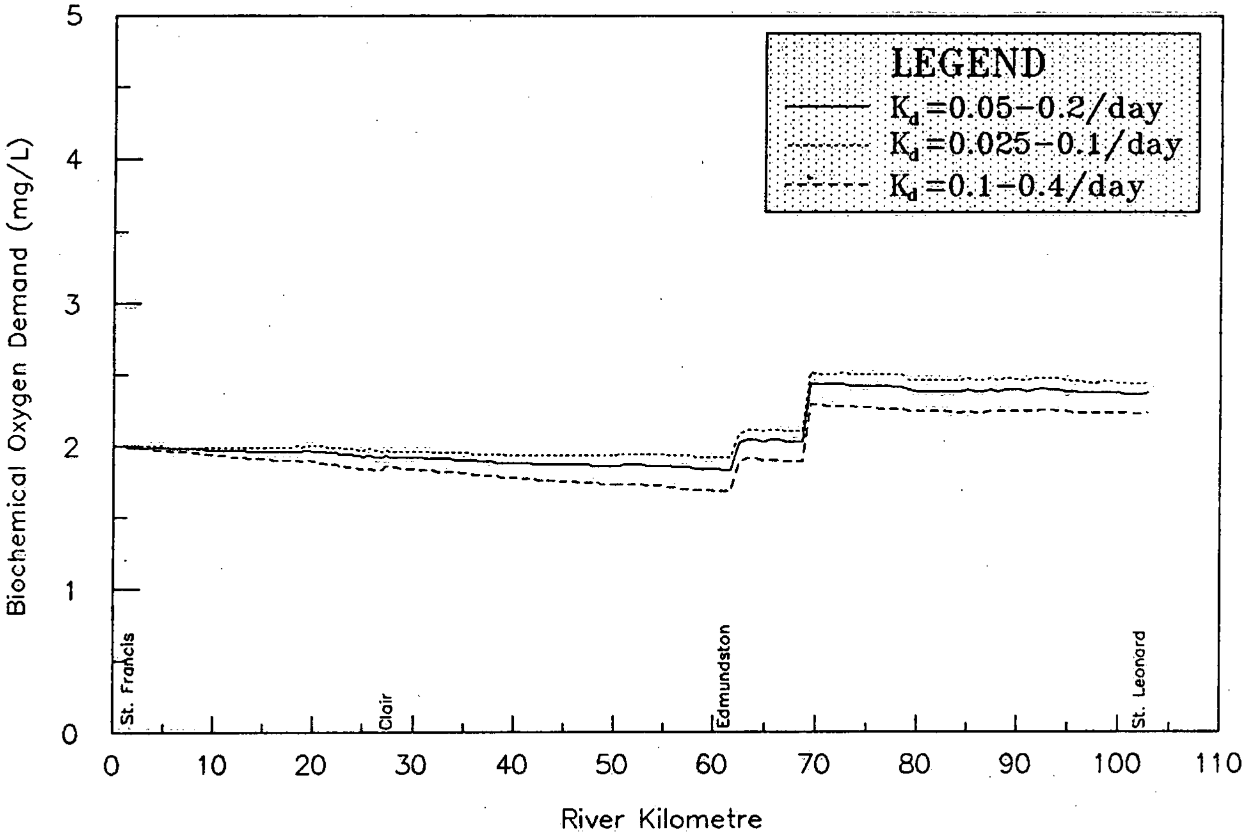

Figure 20. Sensitivity analysis of K_d-ONE–D model BOD profile (May 1986).

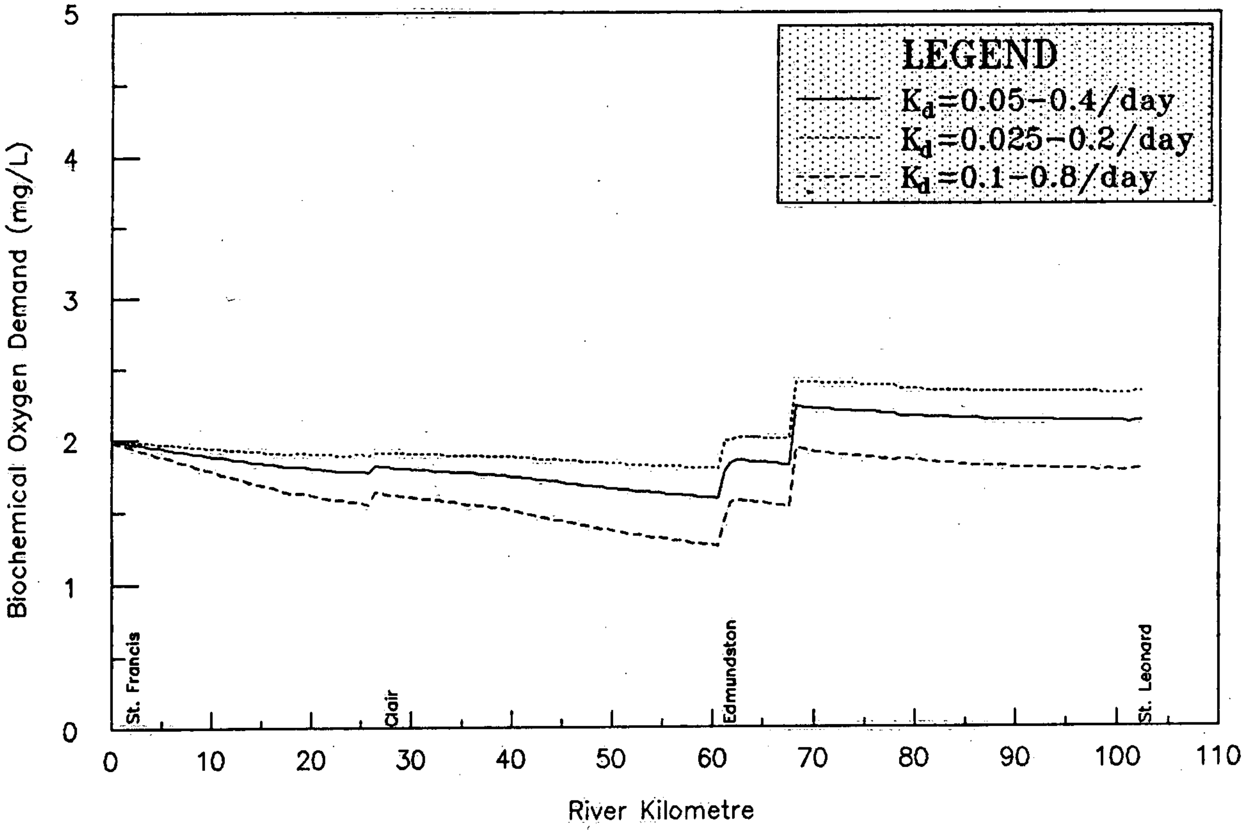

Figure 21. Sensitivity analysis of K_d-QUAL–IIe model BOD profile (May 1986).

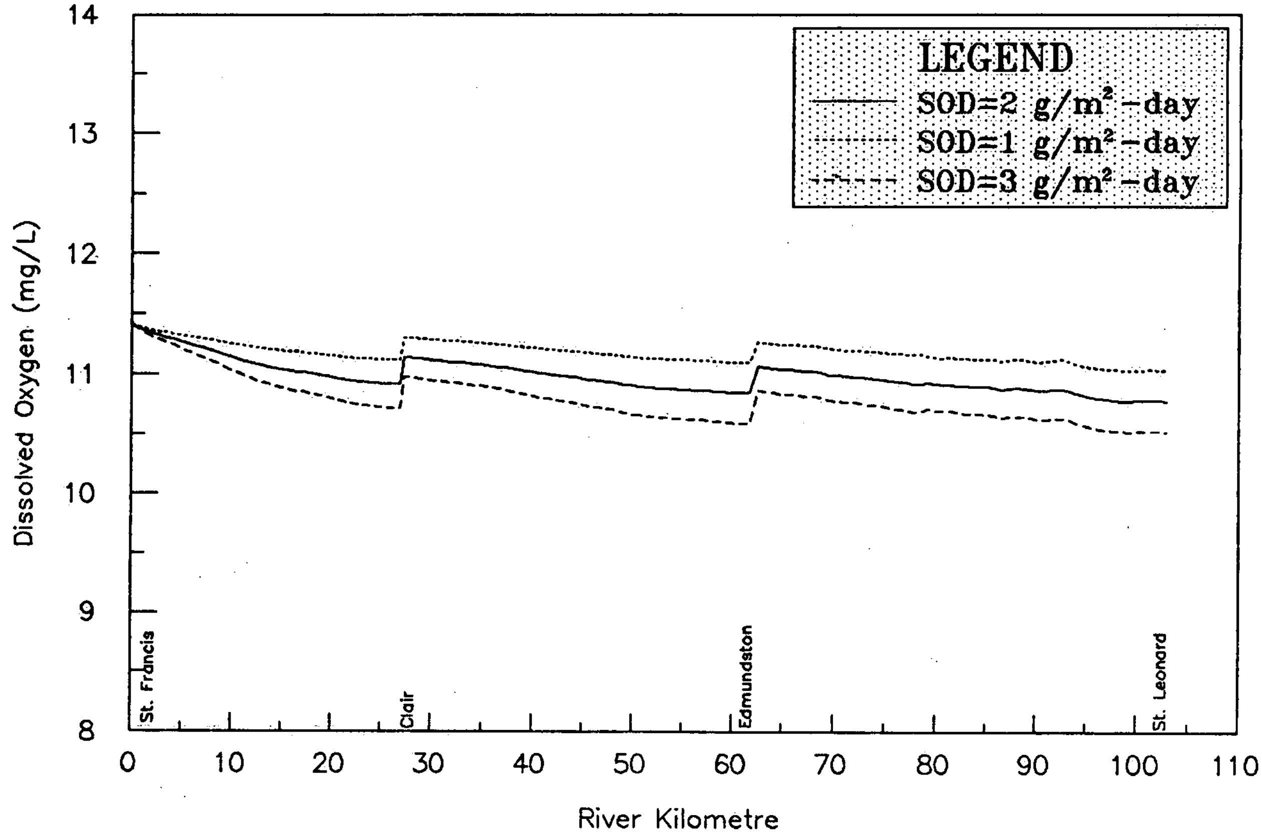

Figure 22. Sensitivity analysis of SOD (sediment oxygen demand) - ONE-D model DO profile (May 1986).

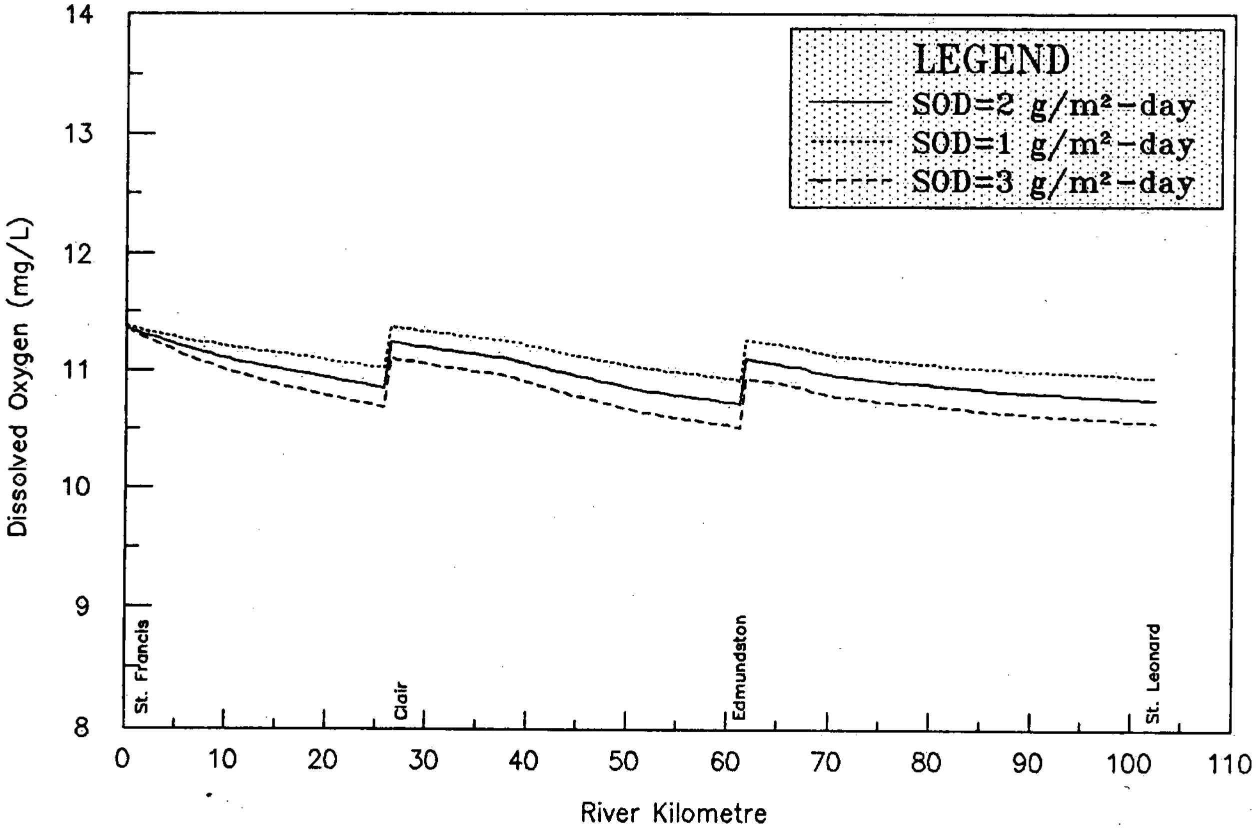

Figure 23. Sensitivity analysis of SOD (sediment oxygen demand) - QUAL-IIe model DO profile (May 1986).

It can be seen that the sensitivity of BOD to the change in K_d for the QUAL-IIe model is greater than two times that of the One-D model. In the case of the sensitivity of DO to the change in SOD, the sensitivity-coefficient values are in a much lower range; and the One-D model is more sensitive to SOD than the QUAL-IIe model.

DISCUSSIONS AND CONCLUSIONS

In the application of the One-D and QUAL-IIe models to the Upper Saint John River, results for BOD, DO, conservative materials, organic nitrogen and inorganic nitrogen profiles were generally in agreement with each other and with the observed data. This has been achieved by using parameter and coefficient values within reasonable ranges in the calibration procedure.

At St. Leonard in the downstream end, it would be expected that the observed flow and water quality data may occasionally experience temporal variability, resulting from the operation of the Grand Falls dam. This would make the fitting of the model results more difficult. However, the flow regimes during the various data collection periods were found to be quite steady, at least up to Edmundston (no discharge records were available at St. Leonard). Consequently, the dynamic model One-D was not required to simulate rapidly changing conditions in this study even though it has the capability to perform such a task. The steady-state model QUAL-IIe handled both hydraulic and water quality computation satisfactorily. A more intricate modelling study could be done if necessary long-term water quality data were available for the simulation of hydraulic and water quality dynamics over a longer period of time.

In order to run QUAL-IIe efficiently on a microcomputer, the version provided by the U.S. EPA has certain dimensional limitations. Notably, the program can only handle up to 25 reaches, which are stretches of river with uniform hydraulic characteristics, and up to 20 computational elements per reach. Each element can take only one tributary inflow. However, limitations on reach and element numbers can easily be changed in the QUAL-IIe FORTRAN 77 program code. The running time of QUAL-IIe on an IBM AT is usually below 1 minute.

The One-D model, due to its large memory requirements resulting from more detailed input data and its numerical solution scheme, was mainly run on the Cray X-MP supercomputer. The running time on the Cray X-MP was approximately 8 seconds. The estimated running time for the One-D model on an IBM AT is 20 minutes for a simulation period of 1 day. The model can take more than one lateral inflow at a given point — an advantage when modelling several inflows close to each other.

As far as observed data are concerned, measurements of nutrient families at the very low concentrations found typically in the Saint John River always tend to be less reliable. The input and output of inorganic nitrogen to the QUAL-IIe model can be presented separately as ammonia, nitrite and nitrate, while the One-D model considers the three components as one lump-sum term. It also has to be realized that results from ultimate BOD tests can be influenced by several factors such as algae, nitrification and laboratory interpretation. In terms of the quantity of observed data, model enhancement was to some extent inhibited by physical and fiscal constraints which precluded the collection of additional data under a wider variety of river flow or waste discharge conditions.

Based on experience in applying the two water quality models to a general river setting, the QUAL-IIe model is simpler to use and faster to run on a microcomputer to produce a steady-state solution. The One-D model is capable of simulating water quality coupled with complex and dynamic hydraulic conditions such as flow variation, hydropower operation and backwater conditions that are commonly found in river basins in Canada.

With respect to sensitivity to input parameter variations which may normally occur in the Upper Saint John River, the two models demonstrated different responses for both BOD and DO. It is conceivable that similar differences might be observed with other input parameters too. With the availability of more redundant input data, other elaborate uncertainty analyses on model output could also be carried out in the future. Nonetheless, this study has demonstrated that a properly developed and calibrated QUAL-IIe or One-D model would provide a good scientific basis for future water quality evaluation of the Saint John River.

RECOMMENDATIONS

From the perspective of river basin planning, water quality assessment has become an increasingly important component of environmental reviews and engineering studies. This study has illustrated that the use of a suitable computer model can greatly improve our understanding of the water quality aspects of a river.

Therefore, the predictive capability of a model and its speed as a planning tool can play an important role in the domain of water quality management.

There is an immediate need to investigate the assimilative capacity of the Upper Saint John River for the purpose of future water quality planning work. The QUAL-IIe model is highly recommended for this purpose in order to gain more in-depth knowledge of the river's responses under different flow and effluent discharge conditions, because the setup is relatively easy and the running time is short. Dissolved oxygen and BOD would be the two primary constituents to be modelled; nutrients and probably algae could be included at a later stage, depending upon the needs and resources available.

In order to carry out a credible assimilative capacity study, a field program should be developed specifically to entail cost-effective monitoring of the streamflow and effluent discharge after identifying the water quality constituent, location, frequency and duration. If more calibration and verification work is deemed necessary after the initial phase of work, several intensive sets of data should be collected preferably covering both the high- and low-flow regimes of the Upper Saint John River.

ACKNOWLEDGEMENTS

The authors would like to thank the Atlantic Region Water Planning and Management Branch and Water Quality Branch of Environment Canada for supplying the necessary hydraulic and water quality data for this study. The authors are also grateful to the Maine Department of Environmental Protection for their cooperative effort in collecting the data on the Upper Saint John River and for permission to use their other water quality data.

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APPENDIX A

Table A-1. Saint John River Water Quality Data, May 13 to 14, 1986

Station node no./ lateral inflow	Temp. (°C)	Dissolved oxygen (mg/L)	Inorganic nitrogen (mg/L)	Organic nitrogen (mg/L)	Inorganic phosphorus (mg/L)	Total alkalinity (mg/L $CaCO_3$)	BOD_u (mg/L)
2	9.6	11.4	0.09	0.11	0.006	14.5	
33	10.9	11.0	0.14	0.10	0.008	15.8	
36	10.8	11.4	0.13	0.11	0.006	16.0	
47	11.1	11.4	0.13	0.11	0.011	17.0	
59	11.1	11.2	0.13	0.10	0.005	17.2	
66	11.1	11.0	0.13	0.09	0.008	17.4	
79	10.6	11.0	0.14	0.10	0.013	23.3	
83		10.5	0.15	0.07	0.010	22.1	
Grand River	10.6	10.5	0.14	0.06	0.010	52.0	
Green River	9.4	11.0	0.20	0.01	0.004	34.3	
Fish River	7.0	12.8	0.12	0.07	0.014	20.1	
Madawaska River	7.4	12.6	0.20	0.07	0.011	52.9	
Baker Brook Lagoon			0.03	6.37	4.3	86.4	
Fort Kent STP			0.37	5.33	3.0	181.4	220.1
Edmundston STP			4.3		1.9	57.6	
Fraser Madawaska STP							70
Madawaska Lagoon			13.0		4.2	63.8	111.8
Nadeau Poultry Lagoon			0.06	1.14		240.8	
St. Basile Lagoon			0.20	1.40			143.6
St. Francois Lagoon			4.10		4.9	29.1	
Van Buren STP							133

Selected from the original data set supplied by Water Quality Branch, Atlantic Region, Environment Canada and the Department of Environmental Protection, Maine, U.S.A.

APPENDIX B

Table B-1. Saint John River Water Quality Data, July 21, 1987

Station	Temp. (°C)	Dissolved oxygen (ppm)	Inorganic nitrogen (ppm)	Organic phosphorus (ppb)	Inorganic phosphorus (ppb)	Total suspended solids (ppm)	BOD$_u$ (ppm)
Madawaska Bridge (Edmundston)	2.0	8.7	0.04	8	<1	<1	3.1
St. David (St. Basile)	20.6	8.7	0.04	13	4	3.6	4.2
Grande Isle (Green River)	20.6	8.2	0.042	7	15	3.5	4.4
La Grande I. (Theriault)	20.6	8.0	0.052	22	<1	3.1	4.7
Quisibis I.	20.6	8.2					
Septieme I.	20.8	7.8	0.059	24	4	6.1	4.2
Van Buren Bridge (St. Leonard)	21.0	7.9	0.037	18	1	3.7	4.7
Green River	18.0	8.4	0.15	4	1	1.8	1.5
Madawaska River	20.0	8.8					
Fraser Madawaska STP			0.077		11	16.7	96
Fraser St. Basile STP			0.55	500	300	70.5	232
McCain STP			0.61	1820	180	55.3	306
Madawaska STP			11.6	440	760	12.1	127
Van Buren STP			6.6	200	4000	8.1	20

Selected from the original data set supplied by the Department of Environmental Protection.

Table B-2. Saint John River Water Quality Data, July 22, 1987

Station	Temp.(°C)	Dissolved oxygen (ppm)	Inorganic nitrogen (ppm)	Organic phosphorus (ppb)	Inorganic phosphorus (ppb)	Total suspended solids (ppm)	BOD$_u$ (ppm)
Madawaska Bridge (Edmundston)	19.0	8.3	0.04	21	< 1	1.5	2.5
St. David (St. Basile)	19.4	8.6	0.03	37	< 1	2.5	3.8
Grande Isle (Green River)	19.8	8.1	0.03	39	< 1	3.8	3.6
La Grande I. (Theriault)	19.6	8.2	0.04	21	< 1	7.6	3.9
Quisibis I.	19.6	8.1					
Septieme I.	19.9	7.9	0.02	31	< 1	6.7	3.6
Van Buren Bridge (St. Leonard)	20.0	7.7	0.04	20	< 1	4.7	3.5
Green River	17.5	8.1					
Madawaska River	19.5	8.4	0.03		< 1	4.4	2.7
Fraser Madawaska STP			0.11	420	80	71.2	130
Fraser St. Basile STP			0.52	600	150	100.3	223
McCain STP							
Madawaska STP			11.5		1000	9.5	60
Van Buren STP			1.6		3750	10.2	14

Selected from the original data set supplied by the Department of Environmental Protection, Maine, U.S.A.

Table B-3. Saint John River Water Quality Data, July 23, 1987

Station	Temp. (°C)	Dissolved oxygen (ppm)	Inorganic nitrogen (ppm)	Organic phosphorus (ppb)	Inorganic phosphorus (ppb)	Total suspended solids (ppm)	BOD_5 (ppm)
Madawaska Bridge (Edmundston)	19.8	8.6	0.05	7	< 1	< 1	2.1
St. David (St. Basile)	19.8	8.6	0.02	42	1	1.6	4.0
Grande Isle (Green River)	20.0	8.1	0.03	39	1	3.8	4.5
La Grande I. (Theriault)	20.1	8.1	0.06	29	1	3.3	4.4
Quisibis I.	20.1	8.2					
Septieme I.	20.2	8.2	0.05	29	1	8.7	4.7
Van Buren Bridge (St. Leonard)	20.0	7.7	0.07	19	1	2.8	4.2
Green River							
Madawaska River	19.0	8.6	0.03	18	1	2.7	3.3
Fraser Madawaska STP			0.08	89	1	56	148
Fraser St. Basile STP			0.40	550	200	94	264
McCain STP							
Madawaska STP			11.7	750	1000	11.6	88
Van Buren STP			8.1	3750		10.5	36

Selected from the original data set supplied by the Department of Environmental Protection, Maine, U.S.A.

APPENDIX C

Table C-1. Saint John River Water Quality Data, August 11 to 12, 1987

Station node no./ lateral inflow	Temp. (°C)	Dissolved oxygen (mg/L)	Inorganic nitrogen (mg/L)	Organic nitrogen (mg/L)	Inorganic phosphorus (mg/L)	Organic phosphorus (mg/L)	Total alkalinity (mg/L $CaCO_3$)
34	20.3	8.6	0.03	0.08	0.011		26.4
36	21.0	8.4	0.07	0.04	0.009		28.6
40	21.0	8.3	0.03	0.08	0.009		28.7
56	20.6	8.6	0.03	0.09	0.008		29.4
59	21.0	8.8	0.03	0.09	0.007		29.5
60	19.0		0.05	0.07	0.019		34.5
62	19.6	8.8	<0.01	0.10	0.009		30.0
66	19.5	8.6	0.08	0.02	0.023		33.2
71	19.2	7.3	0.06	0.07	0.025		35.9
77	19.0	7.6	0.09	0.04	0.010	0.015	35.4
79	19.1	7.7	0.02	0.10	0.010	0.014	35.6
81	19.3	8.0	0.04	0.09	0.008	0.017	35.6
83	19.5	7.6	0.09	0.02	0.009	0.013	35.0
90	19.8	7.5	0.09	0.03	0.013	0.007	36.9
91	20.3	7.6	0.09	0.04	0.009	0.014	37.6
Green River	17.1	9.7	0.15	0.04	0.005	0.003	
Madawaska River	19.0	9.0	0.09	0.035	0.011	0.011	
Baker Brook Lagoon			13	10	4.1	0.7	63.2
Edmundston STP			6.9	0.9	2.2	1.3	58.3
Clair Lagoon			11	1			25.0
Fort Kent STP			9	0.5			63.5
Fraser St. Basile STP			0.03	1.2	0.4	0.6	177.4
Fraser Madawaska STP			<0.01	<0.1	0.011	0.24	11.4

Selected from the original data set supplied by Water Quality Branch, Atlantic Region, Environment Canada.

APPENDIX D

Table D-1. Saint John River Water Quality Data, September 13, 1988

Station	Temperature (°C)	Dissolved oxygen (ppm)	Inorganic nitrogen (ppm)	BOD_u (ppm)
Madawaska	12	9.2	0.07	3.5
St. David	14.8	9	0.022	4.95
Grande Isle	15	8.5	0.023	5.6
La Grande I.	14.8	8.8	0.047	4
Quisibis I.				
Septieme I.	15	8.6	0.042	3.8
Van Buren	15	8.7	0.048	4.5
Madawaska River	13	8.9	0.021	2.8
Fraser Madawaska STP			0.13	117
Fraser St. Basile STP			0.67	138
Van Buren STP				7
Madawaska STP				7

Selected from the original data set supplied by the Department of Environmental Protection, Maine, U.S.A.

Table D-2. Saint John River Water Quality Data, September 14, 1988

Station	Temperature (°C)	Dissolved oxygen (ppm)	Inorganic nitrogen (ppm)	BOD_u (ppm)	Sediment oxygen demand (mg/ft^2 per day)
Madawaska		9.2	0.032	3.1	
St. David	13.1	9.7	0.032	3.3	
Grande Isle	13.1	9.2	0.032	4.8	
La Grande I.	12	9.7	0.097	3.2	
Quisibis I.	12.8	9.4			120
Septieme I.	13.2	9.1	0.050	3.8	80
Van Buren	13.9	9.0	0.046	3.7	370
Madawaska River			0.022	1.8	
Fraser Madawaska STP			0.051	130	
Fraser St. Basile STP			0.247	114	
Van Buren STP			9.7	14	
Madawaska STP			9.2	19	

Selected from the original data set supplied by the Department of Environmental Protection, Maine, U.S.A.

Table D-3. Saint John River Water Quality Data, September 15, 1988

Station	Temperature (°C)	Dissolved oxygen (ppm)	Inorganic nitrogen (ppm)	BOD$_u$ (ppm)
Madawaska		9.2	0.043	2.9
St. David	12.3	9.9	0.043	3.6
Grande Isle	12.5	9.4	0.043	3.9
La Grande I.	12.4	9.5	0.047	3.95
Quisibis I.	12.2	9.6		
Septieme I.	12.2	9.3	0.082	3.1
Van Buren	13	8.9	0.075	5.7
Madawaska River			0.043	1.7
Fraser Madawaska STP			0.35	154
Fraser St. Basile STP			0.826	102
Van Buren STP				
Madawaska STP				

Selected from the original data set supplied by the Department of Environmental Protection, Maine, U.S.A.