Canada [+] Alberta

Northwest Territories

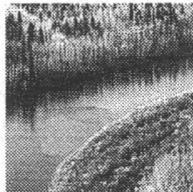### Northern River Basins Study

Prepared for the
Northern River Basins Study
under Project 2612-B7

by
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NORTHERN RIVER BASINS STUDY PROJECT REPORT NO. 18

A REVIEW OF RATE COEFFICIENTS
AND CONSTANTS
USED IN NUTRIENT AND
DISSOLVED OXYGEN MODELS
FOR THE PEACE, ATHABASCA AND
SLAVE RIVER BASINS

Published by the
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Edmonton, Alberta
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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.

This report contains referenced data obtained from sources external to the Northern River Basins Study. Individuals interested in using external data must obtain permission to do so from the donor agency.

NORTHERN RIVER BASINS STUDY
PROJECT REPORT RELEASE FORM

This publication may be cited as:

Shaw, R.D. and MacDonald, G., Environmental Management Associates, *Northern River Basins Study Project Report No. 18, A Review of Rate Coefficients and Constants Used in Nutrient and Dissolved Oxygen Models for the Peace, Athabasca and Slave River Basins*, Edmonton, Alberta, Canada, September, 1993.

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,
IT IS THEREFORE REQUESTED BY THE STUDY OFFICE THAT;
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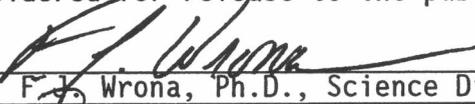
(Dr. F. J. Wrona, Ph.D., Science Director)   *26 August 1993* (Date)

Whereas it is an explicit term of reference of the Science Advisory Committee "to review, for scientific content, material for publication by the Board",
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SUPPLEMENTAL COMMENTARY HAS BEEN ADDED TO THIS PUBLICATION: [ ] Yes [✓] No

(Dr. P. A. Larkin, Ph.D., Chair)   *Sept. 8/93* (Date)

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(Bev Burns, Co-chair)   *93/09/20* (Date)

A REVIEW OF RATE COEFFICIENTS AND CONSTANTS USED IN NUTRIENT AND DISSOLVED OXYGEN MODELS FOR THE PEACE, ATHABASCA AND SLAVE RIVER BASINS

STUDY PERSPECTIVE

Modelling of river nutrient and dissolved oxygen concentrations is necessary to predict the effects of development and changes in land use within the study basins. The purpose of this project was to compile a list of rate coefficients that have been used or are appropriate for use in nutrient and dissolved oxygen models for rivers in the Peace, Athabasca and Slave river basins. Rate coefficients for nitrogen and phosphorous, algal growth and dissolved oxygen used in NRBS rivers were reviewed and compared those from other rivers in Alberta and throughout the world. The rate coefficients will be used in the water quality models for the study area.

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 stakeholders have the opportunity for input.

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1.0   INTRODUCTION

Mathematical models that simulate ecological and water quality interactions in surface water are by necessity much simplified versions of reality. These models incorporate numerous rate coefficients and constants to represent complex physical, chemical and biological processes. Values for some of these coefficients and constants are relatively well known and consistent among many different surface water systems, e.g., carbon generally comprises about 40% of algal biomass (dry weight). Values for other coefficients and constants vary greatly among different water bodies and even spatially and temporally within a single water body, e.g., in rivers, sediment oxygen demand (SOD) may vary from 0 $gO_2/m^2/d$ in pristine cold-water systems to as much as 44 $gO_2/m^2/d$ below sewage outfalls (Bowie et al. 1985).

In addition to environmental influences, the values of these coefficients and constants are dependent upon the way they are defined in the modelling formulation. For example, in some models (e.g., DOSTOC) SOD is simulated by one term that comprises all sediment-related processes that require oxygen, e.g., benthic organism respiration, degradation of organic matter, nitrification, etc.. Other models (e.g., WQRRS) separate the benthic layers into multiple components to directly simulate various oxygen demands, e.g., benthic algal and macrophyte growth routines to simulate respiration.

Given the inherent variability in many of the rate coefficients and constants used in models, their values are most often estimated as part of model calibration, subject to the constraint of a reasonable range. A first estimate of this range can be obtained from a review of comparable systems reported in the literature. The range can be further constrained if information is available from the system of interest, e.g., field and/or laboratory experiments, previous modelling work, etc.

In this report, we provide a comprehensive compilation of the values for rate coefficients and constants applicable to nutrient and dissolved oxygen models for the Peace, Athabasca and Slave River Basins. We first summarize the physical attributes of these rivers and the

ENVIRONMENTAL MANAGEMENT ASSOCIATES

modelling and field work completed to date on these systems. The major processes controlling nutrient and oxygen dynamics in these rivers is discussed along with important differences in the formulation of different models. Finally we have compiled literature, field measurements, and model calibration values for the important rate coefficients and constants required to model nutrient and dissolved oxygen dynamics in these rivers.

2.0   PHYSICAL ATTRIBUTES

An overview of physical attributes of the major rivers in the Athabasca, Peace and Slave River Basins is given in Table 1. Additional reach-specific information is available from a number of different sources. For example, Kellerhals et al. (1972) provides additional information on river geomorphology and flow characteristics. Additional flow data are available from Water Survey of Canada annual reports. Numerous Interpretive reports, cross-sections, ice-cover photos and field notes are available from Alberta Environment. Site-specific hydraulic information may also be obtained from some companies that discharge effluent to these rivers.

TABLE 1

PHYSICAL ATTRIBUTES OF THE NORTHERN RIVERS

RIVER	DRAINAGE AREA (km²)[1]	FLOW (m³/s)		WIDTH[2] (m)	MEAN DEPTH[2] (m)	MEAN CURRENT VELOCITY[2] (m/s)	BED MATERIAL[2]
		MEAN ANNUAL	7Q10				
PEACE RIVER BASIN							
Peace R. at Taylor, B.C.	97 100	1 420[3]	503[3]	524	3.35	0.82	gravel over shale
Peace R. at Peace River	186 000	1 930[3]	590[3]	469	3.47	1.10	gravel over shale
Peace R. at Peace Point	293 000	2 170[3]	761[3]	643	4.33	0.82	sand w/gravel over shale
Smoky R. at Watino	50 300	358[3]	23.0[3]	271	4.21	2.10	gravel over clay
Wapiti R. near Grande Prairie	11 300	102[1]		118	1.37	0.73	gravel over clay
ATHABASCA RIVER BASIN							
Athabasca R. at Hinton	9 780	173[1]	16.0[4]	191	2.59	1.83	gravel
Athabasca R. at Athabasca	74 600	433[1]	53.0[4]	283	1.71	0.88	gravel w/sand over clay
Athabasca R. at Ft. McMurray	133 000	667[1]	114.0[4]	448	1.37	1.07	sand w/gravel over limestone
Lesser Slave R. at Hwy 24	14 400	51[1]	11.6[4]	50.9	2.16	0.64	deepsand or silt
SLAVE RIVER BASIN							
Slave R. at Fitzgerald	606 000	3 410[1]					

1   Environment Canada (1989)
2   Kellerhals et al. (1972)
3   Shaw et al. (1990)
4   Bothe and Siemonsen (1989)

3.0   MODELLING AND FIELD STUDIES

A summary of nutrient and dissolved oxygen modelling studies within the Athabasca and Peace River Basins is given in Table 2. (No modelling work has been completed on the Slave River). Studies pertaining directly to definition or measurement of rate coefficients or constants are listed in Table 3.

In addition to the studies referred to above, a large number of oxygen, BOD and nutrient data have been collected from the northern rivers by Alberta Environment and individual pulp mills. Water quality overviews of these rivers are also available (Hamilton et al. 1985; Noton et al. 1989; Noton and Shaw 1989; Shaw et al. 1990).

TABLE 2

NUTRIENT AND DISSOLVED OXYGEN MODELLING STUDIES OF THE NORTHERN RIVERS

RIVER	REACH	SEASON	STATE VARIABLES	MODEL(S)	REFERENCE
PEACE RIVER BASIN					
Peace River	Smoky River confluence to 225 km d/s	Fall/Winter	DO, BOD, TN, TP	WASP4	Macdonald and Taylor (1990)
Wapiti and Smoky Rivers	u/s Grande Prairie STP to mouth of Smoky River	Fall/Winter	DO, BOD TN, TP	DOSTOC NUSTOC	Macdonald and Taylor (1990)
ATHABASCA RIVER BASIN					
Athabasca River	Hinton to Athabasca	Winter	DO, BOD	DOSTOC	HydroQual (1987)
	Hinton to Athabasca	Winter	DO, BOD	DOSTOC	HydroQual (1988)
	Athabasca to Embarras	Winter	DO, BOD	DOSTOC	Macdonald et al. (1989a)
	Hinton to Embarras	Fall/Winter	DO, BOD organic N, NH$_4$-N, NO$_3$-N, TN, DP, PP, TP	DOSTOC NUSTOC	Macdonald and Radermacher (1989)
	Hinton to Embarras	Winter	DO, BOD	DOSTOC	Macdonald and Hamilton (1989)
	Hinton to Athabasca	Winter	DO, BOD	DOSTOC, QUAL2E-UNCAS	Linton and Hamilton (1989)
	Hinton to Embarras	Winter	organic N, NH$_4$-N, NO$_3$-N, TN, DP, PP, TP	NUSTOC	Taylor et al. (1990)

TABLE 2 CONCLUDED

RIVER	REACH	SEASON	STATE VARIABLES	MODEL(S)	REFERENCE
	Hinton to Embarras	Winter	DO, BOD organic N, NH$_4$-N, NO$_3$-N, TN, DP, PP, TP	DOSTOC NUSTOC	Macdonald and Radermacher (1992)
SLAVE RIVER BASIN					
None					

TABLE 3

FIELD STUDIES TO DEFINE RATES AND CONSTANTS FOR NUTRIENT AND DISSOLVED OXYGEN MODELLING OF THE NORTHERN RIVERS

RIVER	REACH	PURPOSE	REFERENCE
PEACE RIVER BASIN			
Wapiti River	u/s and d/s P&G effluent	Winter SOD measurements	Casey (1990)
	u/s to mouth	Under ice time-of-travel measurements	Andres et al. (1990)
Smoky River	Bezanson and Watino	Winter SOD measurements	Casey (1990)
	Wapiti R. to mouth	Under ice time-of-travel measurements	Andres et al. (1990)
ATHABASCA RIVER BASIN			
Athabasca River	Hinton to Athabasca	Low-flow hydraulic characterization	Trevor et al. (1988)
	Hinton to Embarras	Define hydraulic parameters	Thompson and Fitch (1989)
	Hinton to Athabasca	Under ice time-of-travel measurement	Andres et al. (1989)
	Hinton to Berland River	Winter rearation measurement	Macdonald et al. (1989b)
	Hinton to Fort Assiniborne	Winter SOD measurements	Casey and Noton (1989)
	Hinton to Smith	Winter SOD measurements	Casey (1990)
	Hinton to Alpac	Winter SOD measurements	Monenco (1992)
LESSER SLAVE RIVER			
	AEC discharge to mouth	Define hydraulic parameters	Radermacher and Thompson (1989)

4.0   <u>NUTRIENTS</u>

The major processes controlling the cycling of phosphorus and nitrogen in surface water are shown in Figures 1 and 2, respectively. Most models applied to rivers do not dynamically simulate sediment nutrient processes so these were not included in our review. Thus, the major pathways for both phosphorus and nitrogen that need to be defined for models applied to the northern rivers are (1) mineralization rates, i.e., breakdown of organic nitrogen or phosphorus to inorganic (bioavailable) forms, (2) particulate settling rates, and (3) uptake and release by primary producers, which requires definition or simulation of algal and/or macrophyte growth. In addition, simulation of nitrogen requires definition of nitrification rates. Denitrification is not considered here since these rivers contain adequate oxygen levels to prevent its occurrence.

All rate coefficients (k) reported here are expressed as a first-order reaction:

$$\frac{dX}{dt} = -kX \tag{1}$$

where X is the mass of a state (simulated) variable and t is time. The solution to (1) gives:

$$X_t = X_0 e^{-kt} \tag{2}$$

where X_t and X_0 is the mass of X at time t and 0, respectively.

By convention, chemical and biological rate coefficients are generally reported at 20°C. Reaction rates at other temperatures (k_T) may, however, be considerably different and are
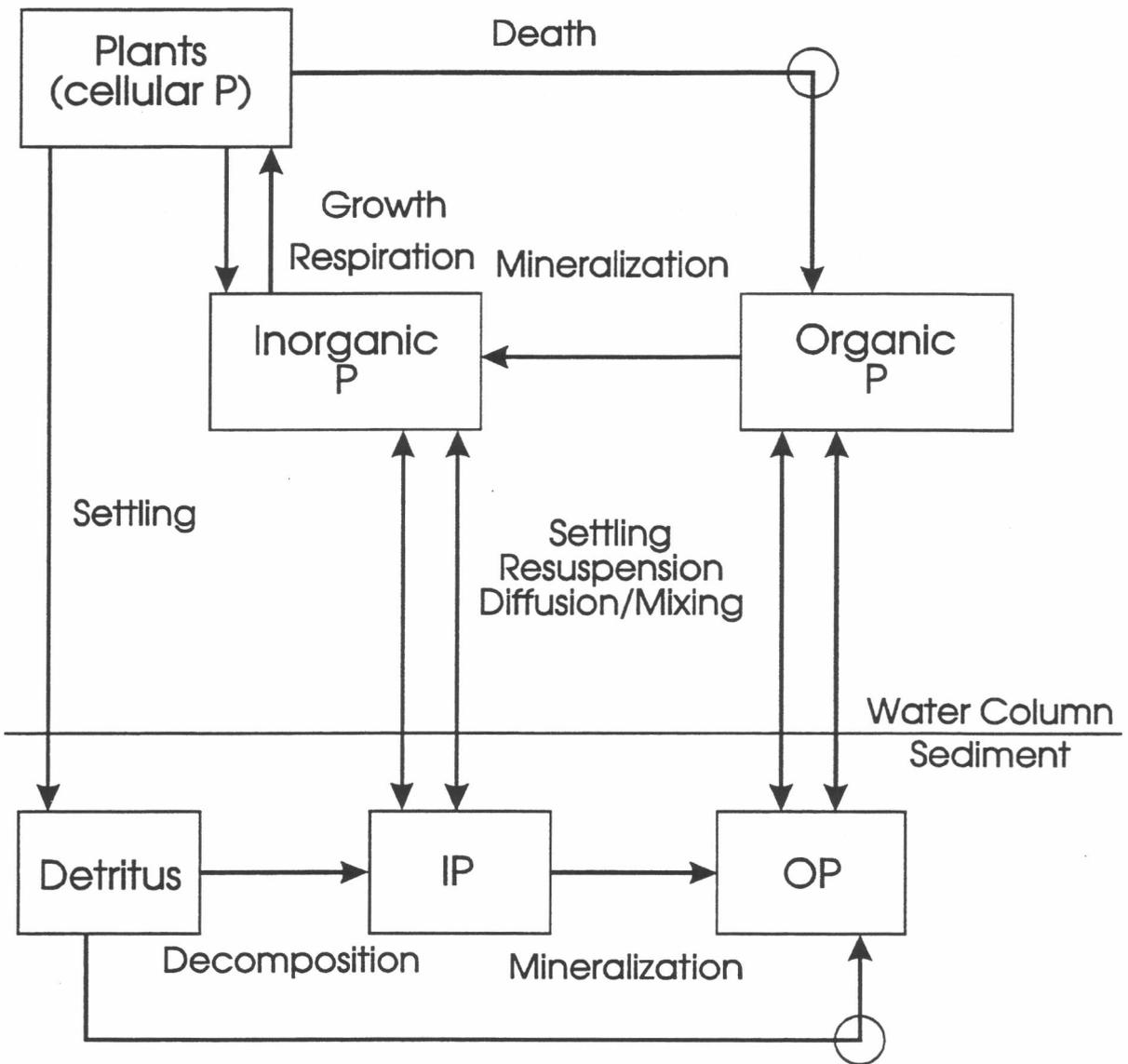
Figure 1: Generalized Phosphorus Cycle

Figure 2: Nitrogen Cycle

often computed from the following relationship (based on the van't Hoff-Arrhenius equation):

$$k_T = k_{20\,°C}\theta^{T-20°C}$$ (3)

where T is ambient temperature in degrees $°C$ and θ is the temperature coefficient.

Table 4 summarizes the coefficients and constants that may be applicable to modelling nutrients in the northern rivers. Values associated with algal and macrophyte growth are given in the following section.

TABLE 4

NUTRIENT RATE COEFFICIENTS AND CONSTANTS

| SOURCE | MINERALIZATION | | | | NITRIFICATION | | PARTICULATE SETTLING |
| | PHOSPHORUS | | NITROGEN | | | | |
	RATE (1/d)	THETA	RATE (1/d)	THETA	RATE (1/d)	THETA	RATE (1/d)
GENERAL							
Bowie et al. (1985) - Surface Water Bowie et al. (1985) - Large Rivers	0.001-0.8	1.00-1.14	0.001-0.4	1.00-1.02	0.0-9.0 0.1-0.3	1.00-1.09	
REGIONAL - MODEL CALIBRATION VALUES							
Hamilton et al. (1989) - Bow River	0.02		0.02		0.2	1.02	0
HydroQual and Gore and Storrie (1989) - North Saskatchewan River			0.03	1.08	0.5	1.08	0
Macdonald (1989) - Highwood River	0.02		0.02		0.6	1.075	0
EMA (1992) - Crawling Valley Reservoir	0.25		0.25				
EMA (1992) - Syncrude test pits	0.025	1.08	0.025	1.08	0.025	1.08	
NORTHERN RIVERS - MODEL CALIBRATION VALUES							
Macdonald and Radermacher (1989)- Athabasca River			0.03	1.08	0.19	1.08	

blanks - process not simulated or measured

5.0   DISSOLVED OXYGEN

The major processes controlling dissolved oxygen concentrations in surface water are shown in Figure 3. The major pathways of the dissolved oxygen cycle that need to be defined for most river models are (1) sediment oxygen demand, e.g., respiration of benthic organisms and decay of organic sediments, (2) nitrification rate, (3) water column BOD decay rate, (4) photosynthesis and respiration, which may require algal or macrophyte growth simulation, and (5) reaeration rate. Values for many of these parameters vary spatially and temporally within rivers.

Most models applied to rivers do not directly simulate the sediment processes that utilize oxygen. Instead, sediment oxygen demand is given as a consumptive rate, which may vary from reach to reach.

Tables 5 and 6 summarizes the coefficients and constants that may be applicable to modelling dissolved oxygen levels in the northern rivers (algal growth and respiration rates given in Table 5 are also applicable to nutrient modelling).
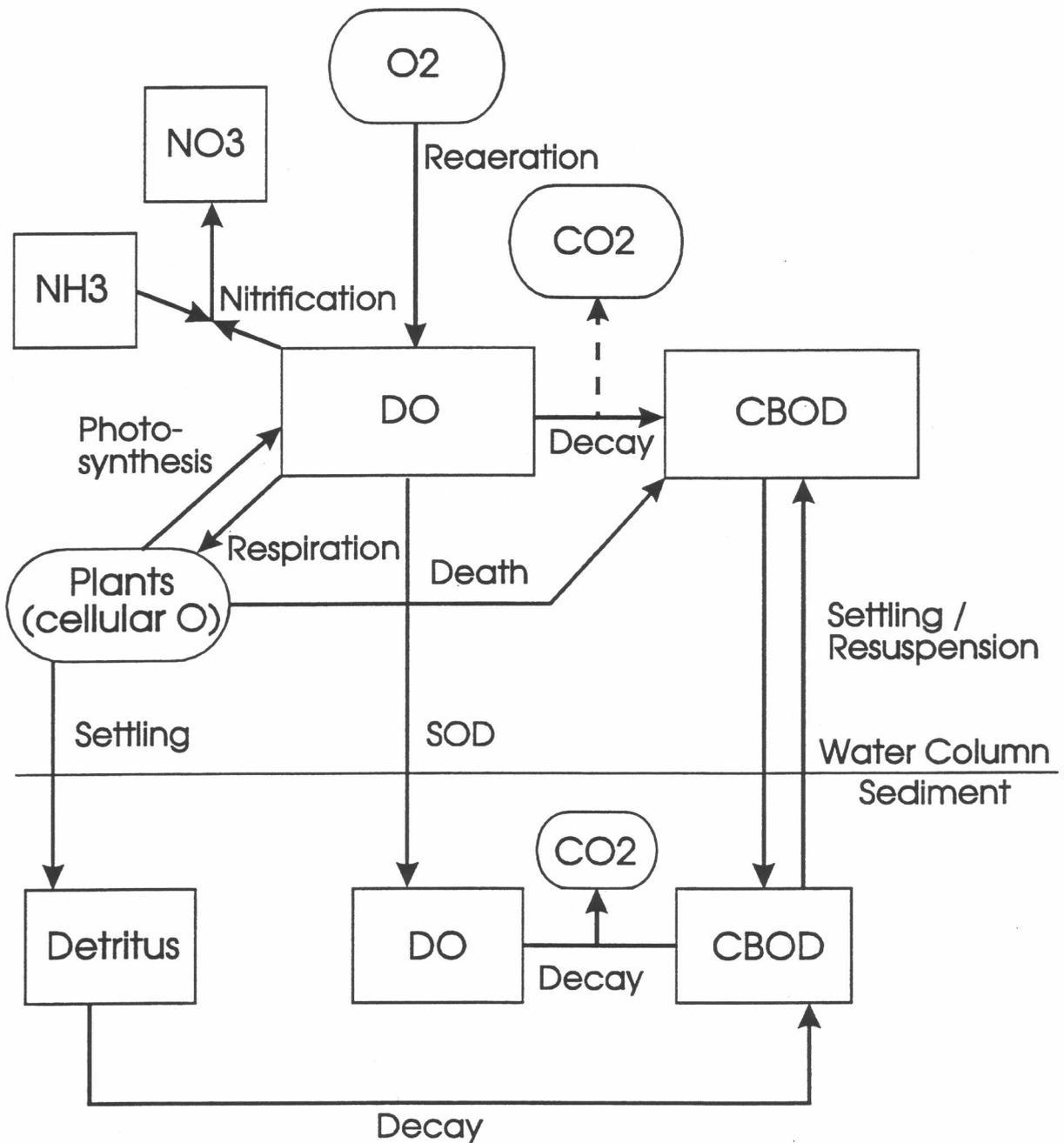
Figure 3: Dissolved Oxygen Cycle

TABLE 5

ALGAL GROWTH RATE COEFFICIENTS AND CONSTANTS

SOURCE	BENTHIC GROWTH		RESPIRATION		CELL STOICHIOMETRY			
	RATE (1/d)	THETA	RATE (1/d)	THETA	N:C	P:C	O:C	C:Dry Weight
GENERAL								
Bowie et al. (1985) - (Diatoms)	0.55-5.0	1.01-1.2	0.03-0.59	1.01-1.2	0.067-0.21	0.003-0.14	1.6-2.66	19-53
REGIONAL - MODEL CALIBRATION VALUES								
Hamilton et al. (1989) - Bow River	1.6-2.0		0.8		0.20	0.03	1.6	0.4
HydroQual and Gore and Storrie (1989) - North Saskatchewan River	0.41	1.066	0.15	1.065	0.10	0.01	1.6	
Macdonald (1989) - Highwood River	0.48		0.15		0.20	0.03		0.4
EMA (1992) - Crawling Valley Reservoir	2.5		0.08		0.010	0.018		0.49
EMA (1992) - Syncrude test pits	3.0*	1.05	0.30	1.025	0.025	0.02	2.0	
NORTHERN RIVERS - MODEL CALIBRATION VALUES								
Macdonald and Radermacher (1989)- Athabasca								
Macdonald and Taylor (1990) - Wapiti-Smoky Rivers					0.1	0.01		

blanks - process not simulated or measured

* Phytoplankton

TABLE 6

DISSOLVED OXYGEN RATE COEFFICIENTS AND CONSTANTS

SOURCE	CBODu DECAY RATE (1/d)	CBODu DECAY THETA	MAXIMUM PHOTOSYNTHESIS RATE g02/m2/d	MAXIMUM PHOTOSYNTHESIS THETA	RESPIRATION RATE g02/m2/d	RESPIRATION THETA	SOD RATE (g02/m2/d)	SOD THETA	WINTER REARATION RATE (1/d)	WINTER REARATION THETA	BODu: BOD5
GENERAL											
Bowie et al.	0.004-4.24	1.02-1.15	4-40		0-36		0.004-44	1.02-1.13			1-30
REGIONAL - MODEL CALIBRATION VALUES											
Hamilton et al. (1989) - Bow River	0.2	1.075									
HydroQual and Gore and Storrie (1989) - North Saskatchewan River	0.12-0.42	1.075	0.49-1.75	1.065	0.16-0.6	1.065	0.16-0.6	1.065	0.065	1.075	2.0
Macdonald (1989) - Highwood River	0.6	1.075									
EMA (1992) - Crawling Valley Res.	0.2						3				
EMA (1992) - Syncrude test pits	0.4	1.047					0.25	1.08			
NORTHERN RIVERS - MODEL CALIBRATION VALUES											
Macdonald and Radermacher (1989)* - Athabasca River	0.18	1.08					0.01-9.0****		0.1-1.81		2.0,5.5*
Macdonald and Taylor (1990) - Wapiti- Smoky River	0.02,0.035***	1.08					0.38		0		2-6.6**
NORTHERN RIVERS - FIELD STUDIES											
Casey (1989) - Athabasca River							0.001-0.515				
Casey (1990) - Athabasca River							0.00-0.59				
Monenco (1992) - Athabasca River							-0.002-0.38				
Casey (1990) - Wapiti River u/s P&G							-0.03- -0.01				
Casey (1990) - Wapiti River d/s P&G							0.18-0.42				
Casey (1990) - Smoky River							0.02-0.7				

* 2.0 - fast BOD; 5.5 - slow BOD

** 5.0 - mill effluent; 6.4 - headwater tributaries; 2.0 other effluents

*** 0.02 - background; 0.035 - effluents

**** site-specific for each reach

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7.0   GLOSSARY

Biochemical Oxygen Demand (BOD) - utilization of dissolved oxygen by aquatic microbes to metabolize organic matter, oxidize reduced nitrogen, and oxidize reduced mineral species such as ferrous iron.

Carbonaceous Biochemical Oxygen Demand (CBOD) - utilization of dissolved oxygen by aquatic microbes to metabolize organic matter.

Denitrification - reduction of nitrate to N_2 under anaerobic conditions.

Five-Day BOD (BOD_5) - measure of the amount of oxygen consumed in laboratory tests on a water sample over a five-day period, usually at 20°C.

Mineralization - breakdown of organic matter to inorganic forms, e.g., organic phosphorus to orthophosphate.

Nitrification - transformation of reduced forms of nitrogen (ammonia) to more oxidized forms (nitrate).

Sediment Oxygen Demand (SOD) - all processes related to bottom sediments that require oxygen, e.g., respiration by benthic organisms, degradation of organic material.

State variables - variables for which a model simulates transports and transformation reactions to project concentrations.

Theta (θ) - temperature correction coefficient for biological rates (see equation (3)).

Ultimate BOD (BOD_u) - measure of the amount of oxygen consumed in laboratory tests on a water sample over a long period of time (>120 days), usually at 20°C.

Uptake - accumulation of inorganic nutrients (C,N,P) by plants during photosynthetic growth.

APPENDIX I

TERMS OF REFERENCE

SCHEDULE A - TERMS OF REFERENCE

Project 2612-B7: Compilation of Rate Coefficients for Water Quality Models

I.   Objective

The purpose of this project is to compile a report that compiles a table of rate coefficients that have been used, or are appropriate for use, in water quality (nutrients) and dissolved oxygen models for rivers in the Peace, Athabasca and Slave river basins.

II.   Requirements

1)   Compile a table of rate coefficients that have been used, or are appropriate for use, in water quality (nutrients) and dissolved oxygen models for the Peace, Athabasca and Slave river basins. The table should include information on the source of the coefficient: values from the literature should include footnotes with complete citations. Coefficient estimated by adjustment during calibration should be so indicated. The table should include biological (e.g., primary producer known kinetics by plant type like macrophytes, blue-green algae, phytoplankton; BOD; herbivory, etc.), physical and chemical rates and constants. A glossary should be included to describe briefly the role of coefficients in the water quality models. This may be particularly important for non-standard formulations. For each rate (e.g., ammonia decay) there may be multiple entries (e.g., for each river or river reach modelled). Where appropriate, include any rate coefficients that may be useful for water quality modelling of the Peace, Athabasca and Slave basins but, to date, have not been used or incorporated into the models. A separate table would be prepared that includes descriptive information for the modelled rivers.

2)   The table and supporting text will constitute a contribution to the proceedings of a Northern River Basins Study Water Quality Workshop to be held March 22nd and 23rd, 1993 in Saskatoon, Saskatchewan.

III.   Reporting Requirements

1)   Prepare a comprehensive compilation of rate coefficients that have been used, or are appropriate for use, in water quality models for rivers in the Peace, Athabasca and Slave river basins. The report should contain compilation tables of rate coefficients such as ammonia decay, oxygen re-aeration under ice and during open water, Q_{10} BOD decay, etc., used in modelling the water quality of the rivers of the Peace, Athabasca and Slave river basins. In addition, the report should contain a table that lists a summary of attributes of the various rivers (i.e., river, latitude, longitude, length of modelled reach, minimum and maximum discharge, river width, river depth, bed type and primary sources of oxygen demand).

2)   Ten copies of the draft report are to be submitted to the Project Liaison Officer (Greg Wagner, Office of the Science Director, Northern River basins Study - phone: (403) 427-1742, fax: (4033) 422-3055) by March 19th, 1993.

3)   Three weeks after the receipt of review comments on the draft report, the contractor is to submit ten cerlox bound copies and two unbound, camera-ready originals or the final report to the Project Liaison Officer. An electronic copy of the report, in Word Perfect 5.1 format, is to be submitted to the Project Liaison Officer along with the final report. The final report is to contain a table of contents, list of figures (if appropriate) list of tables, acknowledgements, executive summary and an appendix containing the Terms of Reference for this contract.

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