

Grand River Simulation Model



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Preface

The Grand River Simulation Model (GRSM) is a water quality model of the Grand River in southwestern Ontario applied by scientists, engineers, and planning staff to understand how proposed changes to a watershed might affect the quality of water in the investigated river. GRSM is a versatile model that can be adapted to other watersheds. This flexibility rests in the fact that all the simulation parameters can be updated based on the unique characteristics of the subject watershed.

GRSM focuses on dissolved oxygen (DO) as the most important indicator of river water quality because DO levels play a large role in determining the level of stress on fish communities and diversity of the fishery in the river. Since DO levels are significantly affected by discharge of treated wastewater to the river, they are good indicators of the impact of wastewater discharges on the river environment. GRSM also models biochemical oxygen demand, nitrogenous oxygen demand, nitrate, suspended solids and total phosphorus.

History

1970	<p>The Ministry of the Environment (MOE) and the Grand River Conservation Authority (GRCA) developed GRSM in the 1970s. It built on similar work that had been done in Southwestern Ontario, in which a dynamic simulation model was used to evaluate strategies to control eutrophication in the Thames River. The Grand River Implementation Committee used GRSM in 1982 to evaluate water management options for the Grand River Basin Water Management Study.</p>
1980	<p>Aside from the initial development period, GRSM remained unused for a number of years, until the issue of increased waste water treatment plant (WWTP) discharges was raised by the MOE and several municipalities in the early 1990s. Urban development in Guelph and the Regional Municipality of Waterloo led to plans for WWTP expansion.</p>
1990	<p>In the mid 1990s, the model underwent a major upgrade to overcome limitations due to hardware and software constraints. The new version had a more streamlined input and output process. Subsequently, the equations describing plant growth and inhibition were reviewed, and in some cases revised, to improve the model's consistency with recent research and to bring calibrated oxygen minima closer to observed levels.</p>
2000	<p>As part of the Middle-Grand River Assimilative Capacity Study completed in 2010 by Stantec Consulting Ltd. (Stantec) for the Region of Waterloo, ammonia volatilization and denitrification were incorporated into GRSM to provide a more comprehensive picture of important nitrogen cycle processes occurring in the Grand River. Stantec also updated and consolidated GRSM user documentation to reflect the changes that have been made to the model over the years.</p>
2010	<p>The improvements and modifications that have been made to GRSM since its inception are a testament to its adaptability and versatility.</p>

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Region of Waterloo



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1. Introduction

This Technical Guidance Document provides the background information that explains the science behind the Grand River Simulation Model (GRSM).

1.1 The Grand River Simulation Model (GRSM)

GRSM is a dynamic (non-steady state), one-dimensional water quality model that enables users to study the impacts of alternative water management strategies on nutrients and dissolved oxygen concentrations in a river. Although GRSM is currently applied to the Grand River watershed, it is a versatile model that can be adapted to other watersheds. This flexibility rests in the fact that all the simulation parameters can be altered based on the unique characteristics of a given watershed.

As a complex mathematical computer simulation model, GRSM can simulate up to 10 water quality parameters and three aquatic plant species for a period of up to 25 years, using a finite time step of two hours. GRSM can incorporate input from up to 30 point sources, such as wastewater treatment plants, urban catchments (maximum 30), tributaries (maximum 100) and water withdrawal sites (maximum 100). GRSM can also incorporate information generated by other hydraulic models, such as loading from rural diffuse runoff and groundwater inflow.

The water quality parameters presently simulated are:

- Dissolved oxygen (DO)
- Carbonaceous biochemical oxygen demand (CBOD)
- Nitrogenous oxygen demand (NOD)
- Nitrate (NIT)
- Suspended solids (SS)
- Total phosphorus (TP)
- Un-ionized ammonia (UIA*)

*Although not directly modelled as a state variable, UIA is estimated from the simulation results based on temperature, pH and background organic nitrogen concentrations.

The three aquatic plant species modeled in GRSM are *Cladophora glomerata*, *Potamogeton pectinatus* (note: this species was renamed *Stuckenia pectinata*, however for consistency with previous documentation it will be referred to in this document simply as *Potamogeton*), and *Myriophyllum spicatum* (which replaced periphyton in 1995). These species' daily growth and processes of photosynthesis and respiration are modeled to determine the impacts of aquatic vegetation upon nutrients and DO. No other available model simulates species-specific plant/algae growth dynamics as GRSM does for these three aquatic plant species.

GRSM is composed of a linked series of sub-models that replicate the many chemical, biochemical and biological processes occurring within the river system. The river system is visualized as a series of reaches connected by node points. Each reach is a small section of the river that exhibits uniform physical, hydraulic and waste assimilative

characteristics. The model takes into account the effects of BOD and NOD decay, weir aeration and atmospheric reaeration, sediment oxygen demand and the rates of photosynthesis and respiration of aquatic plant communities. In 2010, ammonia volatilization and denitrification were incorporated in GRSM to provide a more comprehensive picture of the important nitrogen cycle processes occurring in the Grand River.

At each of the node points, flows from consecutive reaches are added or split according to the geometry of the systems. Point source inflows, local diffuse inflows and urban stormwater inflows are input and mixed at the appropriate nodes for each time step during the simulation. The water quality for each of the parameters modeled for each inflow is either calculated by individual sub-models or read in the external system data files. Mixing and decay processes are allowed to occur as the water is routed through each reach, thereby yielding the instream water quality at any river location at each simulation time step.

The simulation repeats the above process for each time step for each day of the specified portion of the year. To further account for random factors in the natural system, simulation of the specified portion of the year can be repeated on another set of conditions by utilizing the multi-year simulation option.

Figures 1 and 2 are a conceptual representation of the processes accounted for in each reach simulated by GRSM. The aquatic plant community respire continuously, utilizing oxygen from the stream and releasing soluble nutrients to the stream at night. As photosynthetically available radiation (PAR) increases during daylight hours, photosynthesis increases, resulting in the net uptake of nutrients, production of biomass and the production of oxygen. These processes are governed by stream temperature, dissolved oxygen concentration, nutrient supply, and available light at plant depth. Advective inflow and outflow of nutrients and dissolved oxygen are dependent upon the flow rate. Oxygen sink terms are included to account for BOD, nitrification (i.e. oxidation of ammonia to nitrate) and sediment oxygen demand. The import and export of oxygen across the air-water interface (i.e. atmospheric reaeration) is driven by diffusion and the deviation of instream dissolved oxygen from saturation conditions (oxygen deficit). Ammonia may be lost from the system through volatilization to the atmosphere or it may be transformed by nitrification into nitrate. In GRSM, nitrification is modeled as a single first order reaction where it is assumed that nitrite is negligible. Nitrate loss from the water column as a result of denitrification is also accounted for. The standing crop of plants can be gradually and/or drastically altered by death and washout. Since GRSM simulates processes that are affected by the degree of solar radiation, different chemical, biochemical, and biological processes will dominate, depending on the time of day. Figure 1 illustrates the processes that dominate in the daytime, whereas Figure 2 illustrates the processes that dominate in the nighttime.

Figure 1: Daytime dominant processes (temperature dependent)

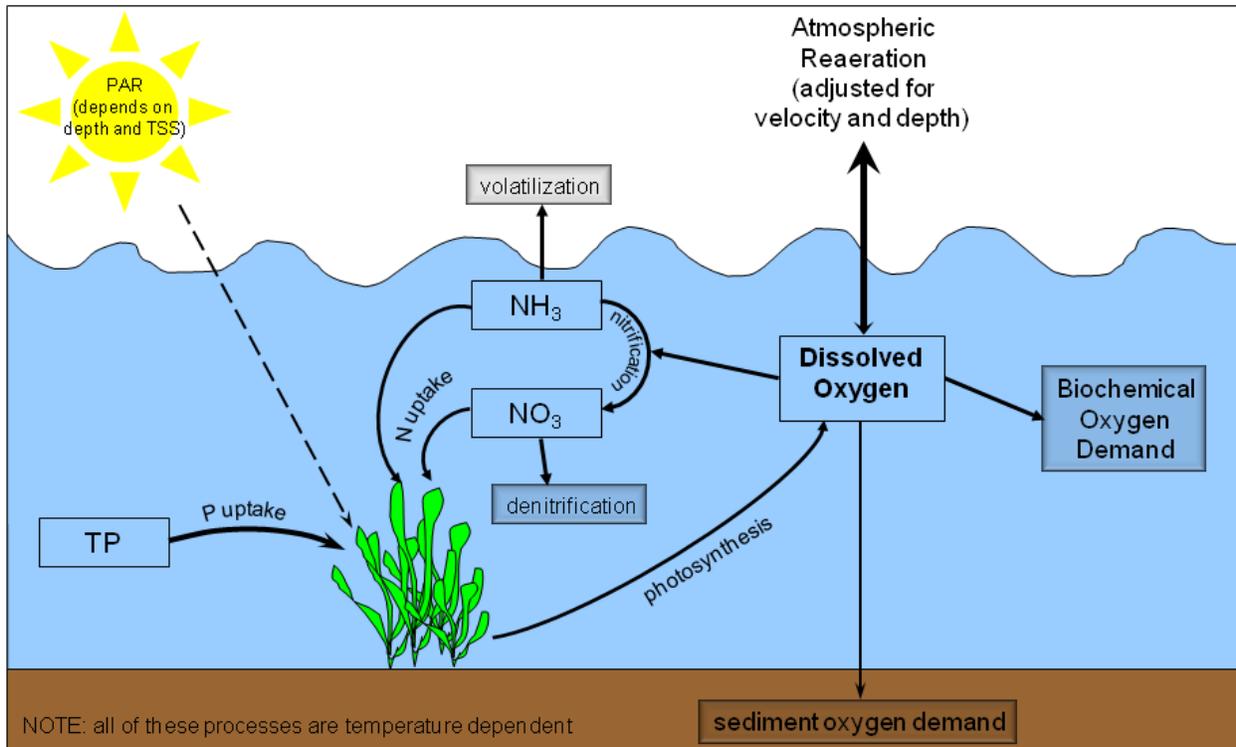
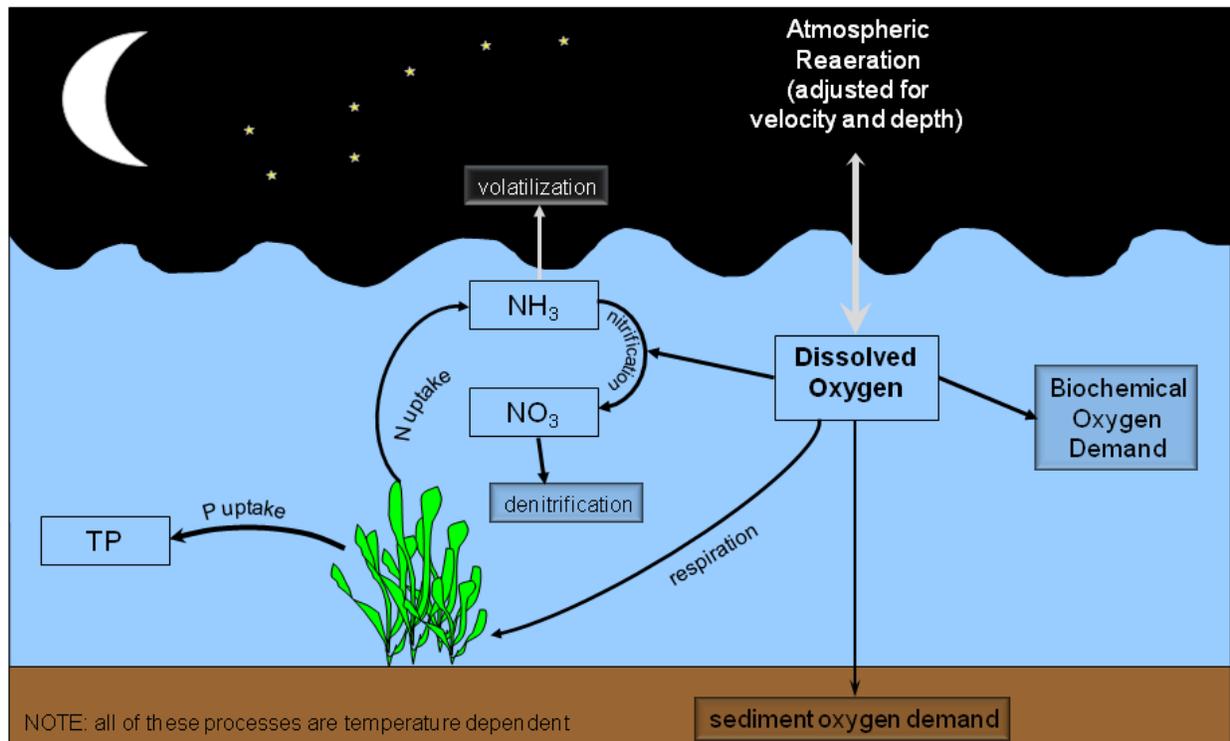


Figure 2: Nighttime dominant processes (temperature dependent)



1.2 Model Uses

GRSM is a fully mixed, one-dimensional model that can be used to evaluate water quality impacts on a watershed scale. It cannot provide all the information required for undertaking a complete receiving water impact assessment, but is to be used with other tools to provide a complete picture. For example, GRSM cannot be used to assess the extent of mixing zones, toxicity effects from un-ionized ammonia or residual chlorine, pathogen issues or other near-field issues.

GRSM has been shown to be an excellent decision support tool to evaluate the assimilative capacity of the Grand and Speed Rivers. The model can be used to evaluate a number of scenarios that describe a range of potential future conditions and provide watershed managers with an evaluation of the relative improvements associated with each management option. For example, the Regional Municipality of Waterloo used GRSM to assist in the development of a Wastewater Treatment Master Plan. Similarly, the City of Guelph applied GRSM to support planned upgrades to their wastewater treatment plant.

Future scenarios are simulated by modifying the input files to reflect anticipated increased wastewater effluent flows and/or decreased effluent nutrient concentrations. For example, several model runs can be completed to simulate future increased effluent flows with different wastewater treatment alternatives such as nitrification or sand filtration at one or several wastewater treatment plants. The model can be used to evaluate the relative benefits of different technologies; simultaneously evaluate upgrades at several wastewater treatment plants; or evaluate strategic upgrades to specific plants that are discharging into a sensitive or stressed reach of the river. The output from these model runs are compared to see what improvements in river water quality are associated with each option relative to current conditions.

The real value of most models lies in the ability of the model to predict the response of the system to changes in model inputs that can be related back to particular management strategies. GRSM should be used as a tool to evaluate management scenarios and the potential impacts that these scenarios may have on water quality. This means that the model results should not be used to determine the specific outcome of a particular set of conditions or management scenario; rather they should be used to determine the relative benefits/drawbacks between scenarios. With any modeling exercise it is imperative to have an adequate amount of good quality data to set up, calibrate and validate the model in order to have confidence in the resulting output.

1.3 Grand River Conservation Authority License Agreement

A copy of the Grand River Conservation Authority (GRCA) License Agreement (“License”) is available online, through the GRCA’s website:

<http://www.grandriver.ca/grsm>

Before using the GRSM, you will have to read and agree to the License Agreement.

1.4 Intended Users

This Technical Guidance Document was written for consultants, municipal employees, agents, and/or researchers studying the effect of effluents on river systems dominated by the types of aquatic plants simulated by GRSM (e.g., *Cladophora glomerata*, *Potamogeton pectinatus*, and *Myriophyllum spicatum*). It is assumed that the user is familiar with computer operation and with determination of the data required for running large, complex water quality simulation models.

1.5 Technical Guidance Document Scope and Purpose

This document provides background information that explains the technical aspects of the GRSM. The Technical Guidance Document is divided into several sections to facilitate its use as a reference document for the required input parameters. Detailed descriptions of the subroutines are also included.

1.6 User Manual

For additional information regarding the installation, execution, and troubleshooting of the GRSM, please refer to the GRSM User Manual, available under separate cover.

2. Glossary

2.1 Common Terms

Block: Refers to a specific section of an input file for GRSM. The User Manual describes the structure and content of each input file and identifies the blocks that make up each file.

Boundary Flow: Major tributary entering the model domain. Where possible, model input for each boundary flow is based on daily average measured flow at the nearest flow gauge.

Local Diffuse Inflow: All flow inputs into the model domain other than the boundary flow. Accounts for small tributaries, local drainage and groundwater. Use daily average flows for the entire model domain.

Model Domain: The portion of the river system that is being modeled. The model domain is divided into reaches that are connected together to form a river network.

Node: Connecting point between two reaches.

Point Source: Wastewater treatment plant effluent discharged to the river system.

Probability Distribution: For the purposes of GRSM, probability distributions are expressed as a series of 11 numbers representing the range of values that a parameter may have. The 11 numbers are the minimum, 10th percentile, 20th percentile, 30th percentile, etc. up to the maximum value for that parameter.

Reach: A small section of the river which exhibits uniform physical, hydraulic, and waste assimilative characteristics. The river system to be simulated is visualized as a series of reaches connected by nodes.

2.2 Acronyms

CBOD	Carbonaceous biochemical oxygen demand
cfs	Cubic feet per second
CLAD	<i>Cladophora glomerata</i>
cms	Cubic metres per second
DO	Dissolved oxygen
GRCA	Grand River Conservation Authority
GRSM	Grand River Simulation Model
LDI	Local diffuse inflow
MIL	<i>Myriophyllum spicatum</i> , commonly known as Eurasian milfoil
NIT	Nitrate (also shown as NO ₃)
NOD	Nitrogenous oxygen demand
PAR	Photosynthetically available radiation
POT	<i>Potamogeton pectinatus</i> , commonly known as Sago pondweed. <u>Note</u> : this species was renamed <i>Stuckenia pectinata</i> and the two names are synonymous
SOD	Sediment Oxygen Demand
SS	Suspended solids
TP	Total phosphorus
UIA	Un-ionized ammonia
VBGI	Visual Basics Graphics Interface
WWTP	Waste water treatment plant

3. Model Formulation

The water quality parameters simulated by GRSM include dissolved oxygen (DO), carbonaceous biochemical oxygen demand (CBOD), nitrogenous oxygen demand (NOD), nitrate (NIT), suspended solids (SS), and total phosphorus (TP). Un-ionized ammonia (UIA), although not directly modelled, can be estimated from the simulation results based on NOD concentration, background organic nitrogen concentration, temperature and pH. The equations involved for each water quality parameter and the inter-relationships among the parameters are described in detail below.

3.1 Dissolved Oxygen

The differential mass balance equation used for the computation of dissolved oxygen was developed by O'Connor and DiToro (1970) and is an enhancement of the traditional Streeter-Phelps approach. The equation accounts for the effects of carbonaceous and nitrogenous oxygen demand, atmospheric aeration, benthic oxygen demand, and photosynthesis and respiration. Photosynthetic oxygen production and respiration of aquatic plants, as well as resulting uptake and release of nitrogen and phosphorus are predicted by the ecological subroutine of GRSM. The dissolved oxygen deficit at any downstream distance, at any specific time is related to factors affecting it by a differential equation (see Equation 1).

Equation 1: Dissolved oxygen deficit

$$\frac{\partial D}{\partial t} + \frac{U \partial D}{\partial x} = -K_2 D + K_D L + K_N N + \frac{S}{H} - P + R$$

Where:

D = oxygen deficit (mg/L) = $C_s - C$, where C_s is the temperature-dependent dissolved oxygen saturation concentration and C is the dissolved oxygen concentration.

U = velocity of streamflow (m/s)

t = time (day)

x = downstream distance (m)

K_2 = reaeration coefficient (day^{-1})

K_D = deoxygenation coefficient (day^{-1})

L = carbonaceous biochemical oxygen demand (mg/L)

K_N = nitrogenous oxidation coefficient (day^{-1})

N = nitrogenous oxygen demand (mg/L)

S = benthic bacterial respiration or sediment oxygen demand ($\text{g/m}^2\text{-day}$)

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P = photosynthetic oxygen production rate (mg/L-day)

R = algal and plant respiration rate (mg/L-day)

H = depth (m)

The terms for photosynthesis and respiration are given in volumetric units (mg/L-day). If the terms are in aerial units of g/m²-day as for attached macrophytes, then they must be divided by depth, H, in metres, to convert to volumetric units.

The deficit D, is found by integrating Equation 1. The analytical solution presented in O'Connor and DiToro (1970) is used, with the exception that the authors used a time series expansion to estimate the P term, while GRSM uses P and R values from the ECOL subroutine.

The reaeration coefficient in Equation 1 is adjusted for water depth, velocity and temperature according to Equation 2.

Equation 2: Reaeration coefficient adjustment

$$K_2 = \frac{a \times U^b}{H^c} \times 1.028^{(T-20)} + \varepsilon$$

Where:

a, b and c = user-specified constants based on stream velocity in feet per second and depth in feet. This equation gives the O'Connor-Dobbins formula when a = 12.8, b = 0.5 and c = 1.5. Adjustment of these parameters, especially the pre-exponential factor a, may be warranted for calibration to observed data. Increasing the value of a will cause the reaeration rate to increase, typically resulting in lower daily maximum DO values and higher daily minimum DO values. Additional information on reaeration rate equations can be found in numerous reference documents, including US EPA (1997).

T = water temperature in °C

ε = a random error component added to the reaeration coefficient at each timestep. The magnitude of this component is specified by the user, who must input the standard deviation for this random component.

In-stream weirs can have a significant effect on downstream dissolved oxygen levels due to enhanced aeration as water falls over the weir. Weir aeration is included in GRSM in the form of a weir aeration coefficient. In terms of the computational process, weir aeration is calculated at the head of each reach, prior to all other sinks and sources of oxygen. Equation 3 is used to account for weir aeration in GRSM:

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Equation 3: Weir aeration

$$\text{DO downstream of weir} = \text{DO}_{\text{SAT}} - K_{\text{WEIR}} (\text{DO}_{\text{SAT}} - \text{DO upstream of weir})$$

Where:

DO_{SAT} = the dissolved oxygen saturation concentration (mg/L)

K_{WEIR} = the weir aeration coefficient, read from Block J14 of RATEFILE

This approach moves the downstream dissolved oxygen concentration closer to saturation by reducing the dissolved oxygen deficit by $(1-K_{\text{WEIR}})$. Thus, if $K_{\text{WEIR}} = 1$, there is no weir effect and $K_{\text{WEIR}} = 0$ means that the dissolved oxygen level downstream of the weir is always at saturation.

3.2 Carbonaceous, Nitrogenous and Sediment Oxygen Demand

Oxygen demand traditionally has been determined by the five-day biochemical oxygen demand (BOD₅) test. The BOD₅ measurement may contain both carbonaceous (CBOD) and nitrogenous oxygen demand (NOD), although typically the nitrogenous portion is suppressed. In GRSM, the oxygen demand in the water column is separated into its component CBOD and NOD parts, utilizing CBOD₅ and total Kjeldahl nitrogen (TKN) data. GRSM also contains a sediment oxygen demand component that is specified for each reach for each month of the simulation period in the RATEFILE input file. SOD rates can be based on field monitoring as described in CH2M Gore & Storrie (1996) or from standard reference sources such as US EPA (1985) or US EPA (1997). SOD rates used in GRSM are input by the user in Block J9 of RATEFILE.

The **CBOD** has been observed to decay exponentially downstream from a point source according to a first-order differential equation. The resultant equation utilized in GRSM to calculate the concentration of CBOD is given by Equation 4.

Equation 4: Concentration of carbonaceous oxygen demand

$$L_x = L_0 e^{\left(-K_R \frac{x}{U}\right)}$$

Where:

L_x = concentration of CBOD at distance x downstream (mg/L)

L_0 = concentration of CBOD at distance x=0 (mg/L)

K_R = CBOD removal coefficient (day⁻¹) = $K_D + K_S$, where K_D is the deoxygenation coefficient and K_S is the settling removal rate. K_R and K_D are specified in RATEFILE. These rates can be based on site-specific measurements or taken from standard references such as US EPA (1985) or US EPA (1997).

U = stream velocity (m/day)

The **NOD** in the stream is calculated utilizing the same first-order decay equation as used for CBOD (Equation 4) except that concentrations and rate coefficients are for NOD rather than CBOD. NOD decay rates, K_N , are specified in RATEFILE and initial values can be based on field measurements (e.g., as described in Gowda (1980)) or taken from standard references such as US EPA (1985) or US EPA (1997).

Each decay rate is adjusted for temperature using an Arrhenius-type correction, as shown in Equation 5.

Equation 5: Decay rate adjustment for temperature

$$K(T) = K(20^\circ\text{C}) \times \Theta^{(T-20)}$$

Where:

$K(T)$ = decay rate at the current water temperature (d^{-1})

$K(20^\circ\text{C})$ = decay rate at 20°C (d^{-1})

T = water temperature ($^\circ\text{C}$)

$\Theta = 1.065$ for K_R and K_D , 1.080 for K_N and 1.040 for SOD. These values are read from RATEFILE and default values can be found in Chapra (1997), US EPA (1997), US EPA (1985), etc.

3.3 Mass Balance Calculation

GRSM divides the system into river reaches which include unequally spaced elements. For each reach, the model calculates a water balance and a mass balance for the modelled parameters. In calculating the mass balance, advective transport and reaction mechanisms are considered.

Initial conditions at the head or upstream end of each reach are calculated by mass balance equations for each parameter by Equation 6.

Equation 6: Concentration of measured parameter at each node

$$C_s = \frac{Q_1 C_1 + Q_2 C_2 + \dots + Q_n C_n}{Q_1 + Q_2 + \dots + Q_n}$$

Where:

C_s = concentration parameter after mixing

C_1 = upstream concentration of the parameter

C_2 , etc. = concentration of the parameter in the WWTP discharge, local diffuse inflow, urban runoff and/or tributary

Q_1 = upstream flow

Q_2 , etc = WWTP discharge, local diffuse inflow, urban runoff and/or tributary flow

3.4 Ecological Subroutine

ECOL is a deterministic model subroutine which simulates the seasonal and daily growth of three aquatic plant types, specifically, *Cladophora glomerata*, *Potamogeton pectinatus* and *Myriophyllum spicatum*. The ECOL subroutine incorporates a variety of processes, including: uptake and release of dissolved oxygen resulting from the photosynthetic and respiratory activity of the plant community, the uptake and release of soluble nitrogen and phosphorus associated with the plant growth and death, and luxury storage and utilization of phosphorus. The effects of various physical processes such as: incident light variations, turbidity, self-shading, temperature, and changes in river depth and velocity associated with changing hydrologic conditions are also accounted for by ECOL.

Densities of the three plant types are separately determined for each reach. Streamflow and water quality parameters routed from the upstream reach are instantly mixed, as described in Section 3.3. GRSM is capable of simulating any user-specified time interval, providing that the time interval does not exceed the hydraulic residence time of the reach. Experience gained during the development and calibration phases of GRSM indicates that a two-hour time step was adequate for the requirements of the Grand River Study.

Refer to Technical Report #14 (Walker et al 1981) for further information regarding the derivation of model algorithms, as well as the calibration and validation procedures. A review of the ECOL subroutine was carried out in 1998 and several algorithms were updated. The updated ECOL subroutine is described in Humphries (1998). Additional information regarding the interaction of the ECOL subroutine with other subroutines and functions of GRSM are further discussed in this document, under Section 6.18.

3.4.1 Photosynthesis and Respiration

The photosynthetic rate at any time (P) of aquatic plants has been replaced by a term dependent on the growth of macrophytes derived from the ECOL subroutine according to Equation 7.

Equation 7: Photosynthetic rate of aquatic plants

$$P = \frac{\mu_{\text{CLAD}} A_{\text{CLAD}} O_{\text{rat}}}{H} + \frac{\mu_{\text{POT}} A_{\text{POT}} O_{\text{rat}}}{H} + \frac{\mu_{\text{MIL}} A_{\text{MIL}} O_{\text{rat}}}{H}$$

Where μ is the growth rate of each aquatic plant species, as shown in Equation 8.

Equation 8: Aquatic plant growth rate

$$\mu = \mu_{\max} \times F_T \times F_R \times F_P \times F_I$$

Where:

μ = plant growth rate for each species of aquatic plant (day⁻¹)

A = density of plant biomass for each species (g/m²)

O_{rat} = oxygen assimilation ratio (gO₂/g-biomass), input from MAINFILE as O2ASS

μ_{\max} = maximum plant growth rate for each plant species (day⁻¹), input from MAINFILE as CGMEW for *Cladophora*, PPMEW for *Potamogeton* and EPMEW for *Myriophyllum*

F_T = temperature limiting factor (unitless)

F_R = solar radiation limiting factor (unitless)

F_P = phosphorus limiting factor (unitless)

F_I = growth inhibition factor (unitless), read from MAINFILE

H = depth (m)

The temperature limitation factor, F_T, for each aquatic plant species is calculated using the Thornton and Lessem approach as recommended by Humphries (1998) according to Equation 9.

Equation 9: Temperature limitation factor

$$F_T = K1 \times \frac{e^{(GAMMA1 \times (T - TMIN))}}{(1 + K1 \times (e^{(GAMMA1 \times (T - TMIN))} - 1))} \times K4 \times \frac{e^{(GAMMA2 \times (TMAX - T))}}{(1 + K4 \times (e^{(GAMMA2 \times (TMAX - T))} - 1))}$$

Where:

$$GAMMA1 = \left(\frac{1}{(TO2 - TMIN)} \right) \times \log \left(\frac{K2 \times (1 - K1)}{K1 \times (1 - K2)} \right)$$

$$GAMMA2 = \left(\frac{1}{(TMAX - TO3)} \right) \times \log \left(\frac{K3 \times (1 - K4)}{K4 \times (1 - K3)} \right)$$

	TMIN	TO2	TO3	TMAX	K1	K2	K3	K4
CLAD	4	7	23	28	0.1	0.98	0.98	0.1
POT	10	24	31	37	0.1	0.98	0.98	0.1
MIL	10	30	35	54	0.1	0.98	0.98	0.1

These values are read from MAINFILE in the section labelled “Temperature Growth Relationship Coefficients”. For further detail on the temperature limitation factor, see Humphries (1998).

The solar radiation limiting factor, F_R , is calculated using a Michaelis-Menten type relationship, as shown in Equation 10.

Equation 10: Solar radiation limiting factor

$$F_R = \frac{PAR_D}{PAR_D + K_{ML}}$$

Where:

PAR_D = photosynthetically available radiation at the depth of the aquatic plants

K_{ML} = half-saturation coefficient for light limitation of each plant species. K_{ML} is read from MAINFILE in the section called “Ecological Parameters”.

PAR_D is estimated using Equation 11, which takes into account light attenuation through the water column due to suspended solids and self-shading within the weedbed. For further detail on the radiation limitation factor, see Humphries (1998).

Equation 11: Estimation of photosynthetically available radiation

$$PAR_D = WATI \times e^{-(K_E \times (H - PLANT_DEPTH) - K_W \times A)}$$

Where:

WATI = solar radiation at the water surface (depends on total daily solar radiation, time of day, latitude, month, etc.)

K_E = light attenuation coefficient based on suspended solids concentration and is equal to $KE_SLOPE \times SS - KE_CONSTANT$. The KE_SLOPE and $KE_CONSTANT$ are read from MAINFILE in Block Q28.

H = water depth (m)

PLANT_DEPTH = cutoff depth for light attenuation and is read in from MAINFILE. At water depths less than PLANT_DEPTH, there is no attenuation of light due to suspended solids.

K_W = weedbed attenuation coefficient and the value depends on the dominant plant type. $K_W = 0.024$, if *Cladophora* or *Potamogeton* are the dominant plants. $K_W = 0.0083$, if *Myriophyllum* is the dominant species.

A is the total biomass of all three aquatic plant species (g/m^2)

Two different approaches are used to calculate the phosphorus limiting factor, F_P , depending on the aquatic species. For *Potamogeton* and *Myriophyllum*, F_P is calculated

using simple Michaelis-Menten kinetics based on total phosphorus in the water column according to Equation 12.

Equation 12: Phosphorus limiting factor (*Potamogeton* and *Myriophyllum*)

$$F_P = \frac{TP}{TP + K_{MP}}$$

Where:

TP = water column total phosphorus concentration.

K_{MP} = half saturation coefficient for either *Potamogeton* or *Myriophyllum*, these values are read from MAINFILE in Block Q24.

The phosphorus limiting factor for *Cladophora* is more complicated and is based on both external water column phosphorus and internal phosphorus in the plant tissues. The phosphorus limiting factor for *Cladophora* is calculated according to Equation 13. For further detail on the phosphorus limitation factor for *Cladophora*, see Humphries (1998).

Equation 13: Phosphorus limiting factor (*Cladophora*)

$$F_P = 1 - \frac{Q_0}{Q_2}$$

Where:

Q_0 is the minimum phosphorus concentration in *Cladophora* tissue (%P). This value is read from Block Q24 of MAINFILE.

Q_2 is calculated according to:

$$Q_2 = Q_1 + (P_{UP} - PHOTO_{MAX} \times Q_1) \times \Delta t$$

Where:

Q_1 = phosphorus concentration in *Cladophora* tissues from the previous timestep

$PHOTO_{MAX}$ = maximum photosynthesis/growth rate for *Cladophora* (read from MAINFILE)

Δt = length of the timestep (i.e., 2 hours in GRSM)

P_{UP} = phosphorus uptake rate calculated according to:

$$P_{UP} = P_{UP,MAX} \times \frac{TP}{TP + K_{MP}} \times \frac{K_{QP}}{(Q_1 - Q_0) + K_{QP}}$$

Where:

TP = water column total phosphorus concentration

K_{MP} = half saturation coefficient for *Cladophora* response to water column total phosphorus, this value is read from MAINFILE in Block Q24

K_{QP} = half saturation coefficient for *Cladophora* response to internal phosphorus concentration in plant tissue; this value is read from MAINFILE in Block Q24

The rate of respiration (R) at any time of aquatic plants is calculated by Equation 14 and Equation 15.

Equation 14: Rate of respiration

$$R = B \times \frac{A}{H} \times O_{rat}$$

Equation 15: Specific plant respiration rate (day⁻¹)

$$B = B_{20} \Theta^{(T-20)} \times \frac{C_{DO}}{C_{DO}^{0.8} + K_{DO}}$$

Where:

A = density of plant biomass (g/m²)

B_{20} = specific plant respiration rate at 20°C (day⁻¹); read from MAINFILE as CGR20 for *Cladophora*, PPR20 for *Potamogeton* and EPR20 for *Myriophyllum*

Θ = Arrhenius equation temperature constant for respiration for each plant species; read from MAINFILE as TC for *Cladophora*, TP for *Potamogeton* and TE for *Myriophyllum*

T = temperature (°C)

C_{DO} = dissolved oxygen concentration (mg/L)

K_{DO} = dissolved oxygen half-saturation constant (mg/L) = 1.5 mg/L

3.4.2 Nutrient Uptake and Release

Aquatic biomass is a function of nutrient concentrations (i.e., total phosphorus, ammonia, and nitrate), water temperature and solar radiation.

Only **total phosphorus** concentration is simulated by GRSM. The phosphorus taken up and released by plant biomass is subtracted or added to the instream total phosphorus concentration. The algorithm currently used by GRSM relates phosphorus limitation to aquatic plant growth using Michaelis-Menten kinetics, rather than the linear relationship that was used historically.

The computation for **nitrogen**, however, is more complex because of the different forms of nitrogen and the fact that nitrogen transformations affect both the oxygen dynamics directly (i.e., nitrification) and nitrogen is taken up by plants as a nutrient. A detailed procedure for the computation of the nitrogen components is given below.

Nitrogen species in GRSM include nitrogenous oxygen demand (NOD, consisting of organic nitrogen and ammonia), un-ionized ammonia and nitrate. Originally, GRSM included a simplified nitrogen cycle that only considered uptake/release by aquatic biomass and oxidation of NOD to nitrate. Organic nitrogen is not modeled as a state variable, rather it is assumed to be a constant concentration in each reach of the model. Nitrite is not included in GRSM as nitrite conversion to nitrate is rapid in aerated surface water systems and nitrite levels in the Grand River are generally less than 0.1 mg-N/L.

Nitrogen uptake by aquatic plants is simulated in GRSM assuming preferential uptake of ammonia over nitrate. The following approach is taken to model nitrogen uptake:

Case I: Excess Ammonia Available	If the amount of ammonia available exceeds the required plant demand, then 90% of the demand is supplied from the ammonia pool and 10% is supplied from nitrate.
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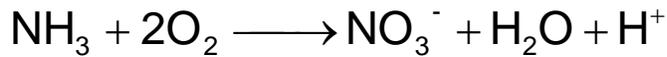
Case II: Limited Ammonia Available	If the amount of ammonia available is not sufficient to meet the entire nitrogen demand of the plants, then 90% of the ammonia is taken up by the plants and the remaining demand is met by nitrate.
---	--

Case III: No Ammonia Available	When there is no ammonia available, nitrate supplies all of the nitrogen required by the plants.
---------------------------------------	--

Nitrogen released by the aquatic plants during respiration (e.g., at night) is assumed to be in the form of ammonia. As part of the Kitchener WWTP Assimilative Capacity Study initiated in 2009, Stantec Consulting Ltd. (Stantec) recommended that GRSM be modified to take into account two important nitrogen cycle processes: loss of un-ionized ammonia by volatilization, and loss of nitrate by denitrification.

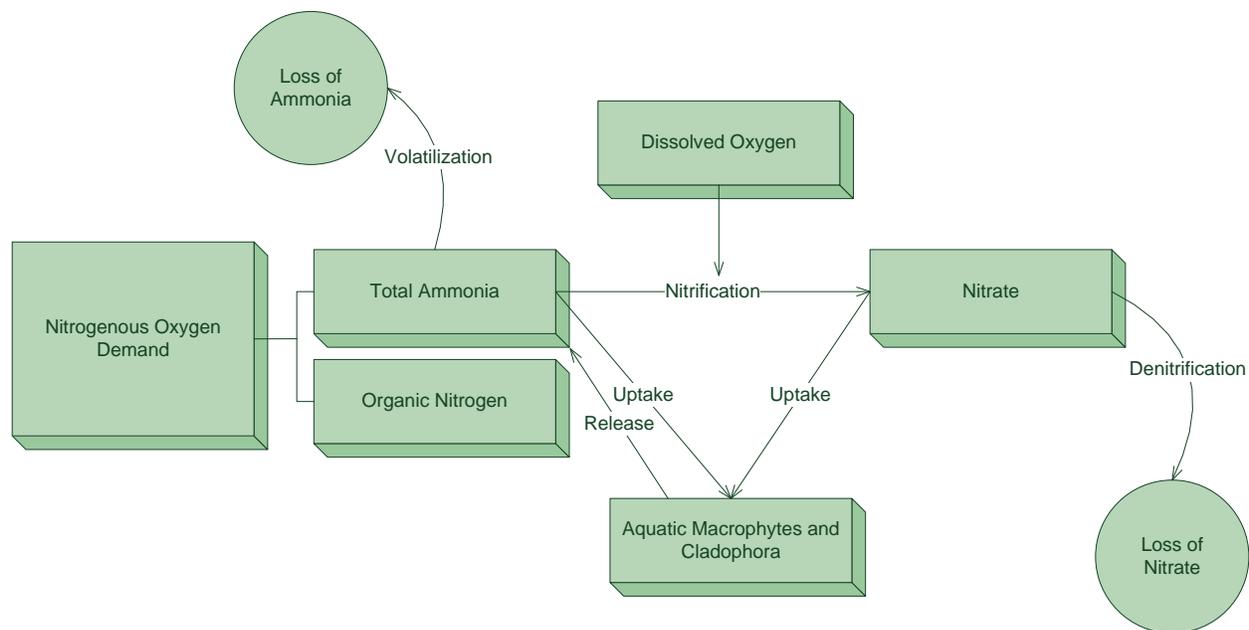
Figure 3 shows the nitrogen cycle as it is currently modeled with the modified GRSM code. NOD is the sum of organic nitrogen and total ammonia, which is expressed as the amount of oxygen required to nitrify ammonia to nitrate according to Equation 16.

Equation 16: Nitrification of ammonia to nitrate



Based on the stoichiometry of this reaction, 4.57 mg of dissolved oxygen are consumed for every mg of ammonia-N nitrified. As mentioned above, the concentration of organic nitrogen in each reach is assumed to be constant (i.e., does not contribute to oxygen consumption) and is estimated using measured TKN and total ammonia concentrations. For the purposes of GRSM, it has been assumed that nitrification occurs as a single step and the intermediate reaction product, nitrite, is considered to be negligible.

Figure 3: Updated nitrogen cycle



NOD and nitrate loads from point and non-point sources are added to each reach in GRSM. Uptake of nitrogen by aquatic biomass during photosynthesis is estimated assuming preferential utilization of ammonia resulting in a loss of NOD from the system. If there is not enough ammonia to satisfy the nitrogen required by the aquatic biomass, nitrate is removed from the system. During respiration, ammonia is excreted by the aquatic biomass and released back into the NOD pool.

In-stream nitrification is modeled as a first order decay process whereby NOD and dissolved oxygen concentrations are depleted and nitrate is produced. The first order reaction rate constant at 20°C is user specified for each reach and month of the simulation period (see GRSM User Manual section on RATEFILE). The rate constant is

adjusted to the ambient temperature according to the following simplification of the Arrhenius equation:

Equation 17: In-stream nitrification

$$k(T) = k(20^{\circ}\text{C}) \times \Theta^{(T - 20)}$$

Where:

T = ambient temperature (°C)

k(T) = rate constant at the ambient temperature

k(20°C) = rate constant at 20°C

Θ = constant equal to 1.080 for nitrification (Martin and Wool 2002, US EPA 1985); this value is also read from RATEFILE

NOD loss can also occur due to volatilization of un-ionized ammonia to the atmosphere. This mechanism has recently been added to GRSM. Un-ionized ammonia is a soluble gas, thus simple film theory can be used to estimate gas transfer of ammonia from the water column to the atmosphere. According to the film theory, the rate of un-ionized ammonia loss can be modeled as shown in Equation 18.

Equation 18: Volatilization of un-ionized ammonia

$$\frac{\partial C}{\partial t} = \frac{v}{H} \times (C_s - C)$$

Where:

C = concentration of un-ionized ammonia in water (mg/L)

C_s = saturation concentration of un-ionized ammonia in water (mg/L)

v = mass transfer velocity coefficient (m/s)

H = depth of the water column in (m)

GRSM has been modified such that the mass transfer velocity can be user-specified for each month at each reach (see User Manual section on RATEFILE). The mass transfer velocity is temperature dependent and is adjusted to the ambient temperature using the Arrhenius relationship provided in Equation 17 and using Θ = 1.045. The average water depth in each reach is estimated by GRSM based on flow for each timestep. The saturation concentration is estimated according to Equation 19 (Chapra *et al.* 2008).

Equation 19: Saturation concentration

$$C_s = 14 \frac{\text{mg N/L}}{\text{mol/m}^3} \times \frac{p_{\text{NH}_3}}{H_e}$$

Where:

p_{NH_3} = partial pressure of ammonia gas in ambient air (atm)

H_e = Henry's law constant for ammonia, calculated according to Equation 20 (atm·m³/mol)

Equation 20: Henry's law constant for ammonia

$$H_e = 1.3678 \times 10^{-5} \times 1.052^{(T - 20)}$$

For the Grand River watershed, the partial pressure of ammonia is assumed to be 5 ppb, given typical concentrations range from 1 to 10 ppb in rural and moderately polluted areas (Chapra *et al.* 2008). Therefore, the saturation concentration of un-ionized ammonia in water at 20°C is approximately 0.005 mg/L using Equation 19.

Integrating the differential equation for ammonia loss over time yields Equation 21.

Equation 21: Ammonia loss over time

$$C_{t+\Delta t} = C_t e^{-\frac{v}{H} \Delta t} + C_s \left(1 - e^{-\frac{v}{H} \Delta t} \right)$$

Where:

$C_{t+\Delta t}$ = concentration of un-ionized ammonia at the end of the timestep

C_t = concentration of un-ionized ammonia at the beginning of the timestep

Δt = length of the timestep in seconds

GRSM has been modified to calculate the loss of un-ionized ammonia according to Equation 21. Un-ionized ammonia concentrations are estimated for each reach at each timestep of the simulation. GRSM calculates **total ammonia** concentration by subtracting organic nitrogen from NOD. The **un-ionized fraction** is estimated using the ambient temperature and pH according to Equation 22.

Equation 22: Estimation of un-ionized ammonia

$$f = \frac{1}{1 + 10^{\text{pK}_a - \text{pH}}}$$

Where:

Equation 23: Acid dissociation constant

$$\text{pK}_a = 0.09018 + \frac{2729.92}{T + 273.15}$$

GRSM uses the water temperature specified by the user for every timestep of the simulation period for each reach. These inputs are based on continuous monitoring records where they are available or interpolated between adjacent monitoring locations. The pH is calculated for each timestep based on average monthly pH measurements with a variable component that depends on the time of day to mimic observed diurnal changes. As with temperature, pH inputs to GRSM are based on continuous monitoring records where available, otherwise interpolation is used for reaches between monitoring stations.

In-stream denitrification has also been recently added to the GRSM and is assumed to be a first order decay process that accelerates at low dissolved oxygen concentrations. The same approach is used by other common water quality models such as QUAL2K, EPD-RIV1 and WASP. Denitrification results in a decrease in nitrate in the water column according to Equation 24.

Equation 24: Nitrate concentration at the end of the timestep

$$C_{\text{nitrate}, t+\Delta t} = C_{\text{nitrate}, t} \times f_{\text{ox}} \times e^{-k_{\text{denit}}\Delta t}$$

Equation 25: Factor limiting the denitrification rate

$$f_{\text{ox}} = \frac{K}{K + \text{DO}}$$

Where:

$C_{\text{nitrate}, t}$ = nitrate concentration at the beginning of the timestep

f_{ox} = factor limiting the denitrification rate at higher dissolved oxygen concentrations according to Equation 25

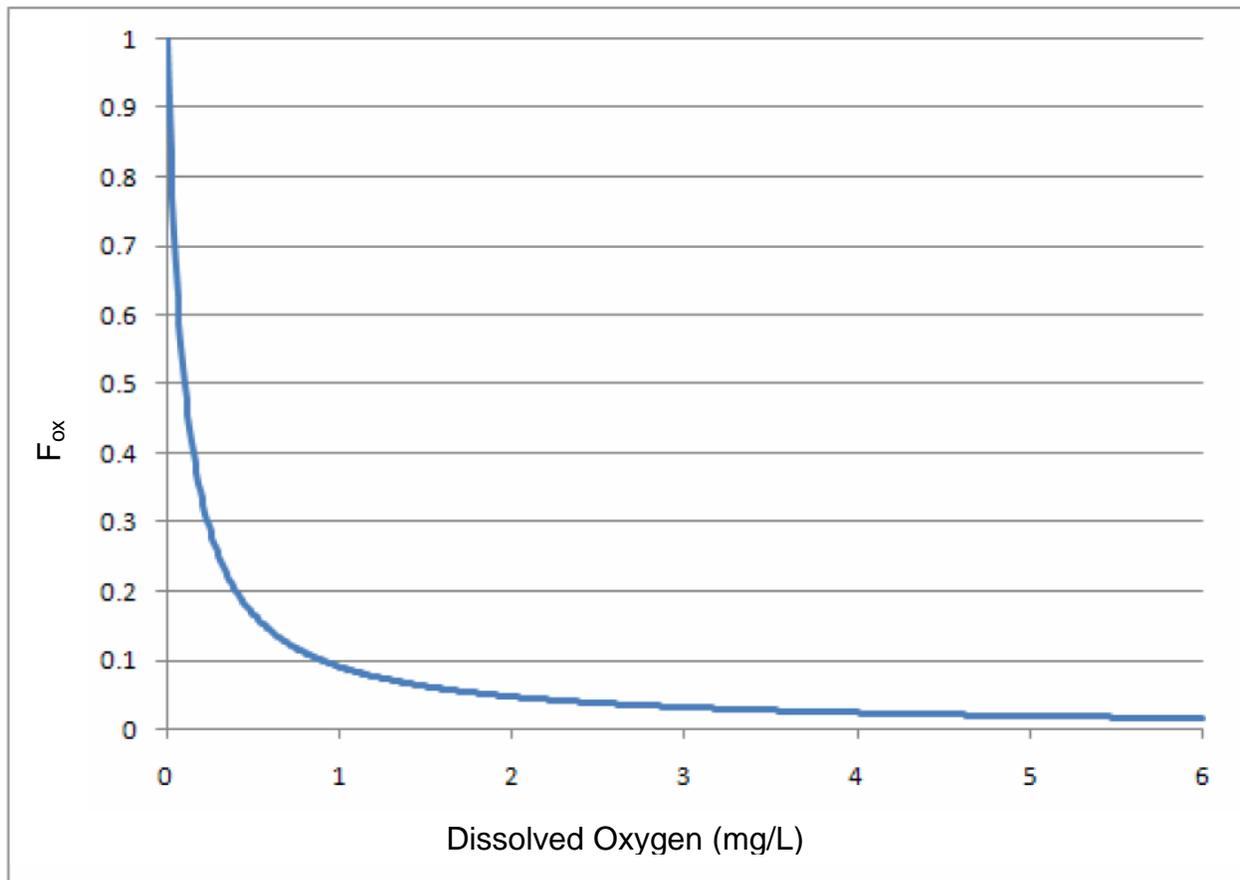
k_{denit} = first order decay rate constant; read from RATEFILE

Δt = timestep

The first order rate constant is corrected to the ambient temperature at each timestep using the Arrhenius relationship provided in Equation 17 and using $\Theta = 1.045$ (Martin and Wool, 2002).

Oxygen dependence of the denitrification reaction is estimated using a half-saturation constant (i.e., K in Equation 25) of 0.10 (Martin and Wool 2002, US EPA 1985). This means that the factor f_{ox} approaches 1 as dissolved oxygen approaches zero, as shown in Figure 4.

Figure 4: Relationship between f_{ox} and dissolved oxygen



3.5 Flow Calculation

In GRSM, the river system is represented by a series of reaches joined by node points. At the upstream boundaries of the simulation area, data representative of the river hydrology and water quality are entered as boundary conditions. Local inputs, which include WWTP effluents, urban point-source storm runoff and local inflows may be entered into each reach. At each node point, upstream and local inputs are mixed, water is withdrawn where applicable and the effects of atmospheric and weir aeration are calculated. Pollutants and streamflow are then routed through the system and the concentration of each water quality constituent is calculated at the end of each reach, according to the instream processes associated with that reach. Calculations are made for each node in the river system on a 2-hour time step.

The Muskingum method (Linsley and Franzini, 1964) of flow routing is used to calculate flows downstream at each node as shown in Equation 26:

Equation 26: Muskingum method of flow routing

$$O_2 = c_1 I_1 + c_2 I_2 + c_3 O_1$$

Where:

O_2 = Outflow at lower end of reach at timestep 2

I_2 = Inflow at head of reach at timestep 2

I_1 = Inflow at previous timestep

O_1 = Outflow at previous timestep

c_1 , c_2 , c_3 are empirically derived coefficients that represent temporary storage and flow attenuation within each reach. Current default values are $c_1 = 0$, $c_2 = 1$ and $c_3 = 0$, which simulates no transient storage or flow attenuation (i.e., inflow = outflow in the same timestep). These coefficients are read in from MAINFILE, Block F11.

4. Parameters

GRSM is a complex model that requires a large quantity of input data to characterize the major processes affecting water quality. The main input parameters that vary with time are provided to the model in two forms: a continuous time series of data (e.g., daily flow from each WWTP) or a cumulative frequency distribution (e.g., boundary water quality parameters). Table 1 provides a listing of the time variable input data required to run GRSM and identifies which inputs are provided as time series or frequency distributions. For inputs that can be provided as both a time series and a frequency distribution, the user must specify in the MAINFILE which input data type is being provided to the model. Refer to the GRSM User Manual for additional guidance.

Table 1: Time Series Input Data Required for GRSM

Input as Time Series	Frequency of Data
Boundary flow	Daily
WWTP effluent flow	Daily
Local diffuse inflow	Daily
Water withdrawal rate	Monthly
Urban stormwater flow	Every timestep
Urban stormwater quality	Every timestep
Sediment oxygen demand	Monthly
BOD decay rates	Monthly
NOD decay rates	Monthly
Water temperature	Every timestep
Solar radiation	Every timestep
Base reaeration coefficients	Monthly, adjusted for depth and velocity at each timestep
Biomass inhibition factors	Monthly
Weir aeration coefficients	Monthly

Table 2: Cumulative Distribution Input Data Required for GRSM

Input as Cumulative Distribution
Boundary water quality
WWTP effluent quality
Local diffuse inflow quality

The model relies primarily on time series inputs, although there are some data that are read in as cumulative frequency distributions. For those inputs that are specified as cumulative frequency distributions, the model randomly selects values for each input parameter for each timestep of the simulation from the given distribution. GRSM assumes a uniform distribution for the random selection of values from the cumulative distribution. This generates a set of input parameters with the same distribution and statistical properties as the original data (e.g., same average, standard deviation, etc.). The following example illustrates this approach.

GRSM variables that are input as cumulative frequency distributions require 11 data points representing the minimum, 10th percentiles and maximum values of the variable, typically based on historical monitoring records. For example, GRSM input values based on historically measured nitrate levels in Irvine Creek have the cumulative frequency distribution shown in Figure XX. GRSM selects values from this distribution for use in the simulation using a uniformly distributed random number between 0 and 1. Linear interpolation is used to interpolate between percentile values.

For illustration purposes, say the random number generator returns a value of 0.843. Based on the cumulative frequency distribution given in Figure 5, this corresponds to a nitrate concentration of 3.453 mg/L. This number is derived by interpolating between the 80th percentile (3.066 mg/L) and the 90th percentile (3.966 mg/L).

4.1 Hydrology

This section of the Technical Guidance Document presents additional information regarding the input requirements for data pertaining to hydrology, urban stormwater runoff, boundary water quality, WWTP effluents, meteorological conditions, reaction rates and continuous monitoring data.

GRSM is not a hydrologic model; therefore the flow coming into each reach from tributaries, groundwater, urban and rural non-point source runoff must be specified. Major tributaries entering the model domain are referred to in the model as boundary flows. For example, in the case of the Grand River watershed, major tributaries include the mainstem of the Grand River downstream of Shand Dam, the Conestogo River, the Speed River at Guelph Dam, the Eramosa River and the Nith River. Model input for each of these boundary flows is based on daily average measured flow at the nearest flow gauge.

The model utilizes the daily streamflow from two consecutive days and applies a linear interpolation technique to calculate the streamflow at each time step (12 time steps per day). This procedure avoids sudden increases or decreases in streamflow at any particular time step.

4.2 Urban Stormwater Runoff

Urban point-source stormwater runoff data must also be entered in GRSM. The quantity and quality of urban runoff is difficult and impractical to measure due to the large number of storm sewer outfalls contributing directly or indirectly. For this reason, the quantity and quality of urban runoff contributing to the GRSM model domain must be estimated using hydrologic models. In the case of the Grand River watershed, this data was estimated using the Guelph All-Weather Sequential-Events Runoff (GAWSER) hydrologic model, which predicts streamflow based on snowmelt and rainfall. Output from GAWSER is used to develop a 2-hour time series for urban runoff flow and water quality parameters.

Sediment washoff is calculated by GAWSER and this information was used to estimate the quality of urban runoff for input to GRSM. The sediment load from urban areas is used to estimate the concentration of other water quality parameters required by GRSM including total phosphorus, nitrate, NOD, and BOD by assuming a constant proportionality between these parameters and suspended sediment. For some parameters, such as total phosphorus and BOD, this assumption is likely valid since these parameters tend to have a significant component that is associated with sediment. However, this approach is not expected to produce reliable estimates for parameters such as nitrate, which tend to be in the dissolved phase. Fortunately, urban runoff does not appear to be a major source of nitrate or TKN, therefore this assumption has little impact on GRSM results.

Local diffuse inflow is the term used to describe all other flow inputs into the model domain to account for small tributaries, local drainage and groundwater. This term is also estimated using GAWSER to develop a daily time series for flow and a cumulative

distribution for the quality of this drainage for the entire basin. The total amount of local diffuse inflow is input to the model in the BASINFLOW input file. The fraction of this flow that enters each reach of the model is specified in Block D1 of FLOWFILE (note: not all reaches have to have local diffuse inflow). As noted above for urban runoff, local diffuse inflow has not been demonstrated to be a major source of flow or pollutants and therefore it has little effect on the overall results.

4.3 Boundary Water Quality and Flow

GRSM has the capability to define the water quality at each reach boundary of the study area using two methods. One method involves the input of continuous historical water quality data, and the other approach is to use cumulative frequency distributions of the water quality parameters. Typically, water quality data is collected infrequently and therefore the preferred method is to input data as a cumulative frequency distribution. The calculation method using cumulative frequency distributions is described in Section 4.

If the former procedure is employed, water quality associated with the model boundaries would be based on measured data collected on a frequent basis (e.g., daily or weekly). Model inputs for dissolved oxygen, total phosphorus, nitrate, total Kjeldahl nitrogen (TKN, which is converted to a nitrogenous oxygen demand), BOD and total suspended solids (TSS) would be developed using data from high frequency grab samples collected over a defined period. The input file would contain a continuous series of daily average values for each water quality parameter.

Changes in boundary water quality associated with changes in land use patterns and agricultural practices under future projected scenarios can be incorporated into GRSM by generating new water quality distributions. These distributions would be derived by factoring the existing condition distributions either up or down to reflect expected increasing or decreasing water quality parameter concentrations.

4.4 Wastewater Treatment Plant Effluent

GRSM has two input options available for wastewater treatment plant (WWTP) **effluent flow data**. One method involves the compilation and use of a continuous historical effluent flow record data set; the second method involves the use of a set of multivariate regression equations to calculate effluent flows. Typically, historical records of daily effluent flows are available and can be used to generate the input files for each WWTP. The preferred approach is to use historical records to generate a continuous input dataset. The second method is of limited use but may be employed to simulate future scenarios.

The regression equations, which were derived from existing historical flow records, account for the seasonal variation within-week variation observed at the sewage treatment plants. There is also the option to include a random error component to account for other sources of variation in WWTP effluent flows. The user must specify the standard deviation (i.e., magnitude) of this error component. Details of the

formulations of the regression model equations are given in MOE (1972). The regression model included in GRSM is given below, in Equation 27 and

Equation 28.

Equation 27: Regression model for Saturday (day number, I = 7)

$$WWTPQ = WWTPQ_{avg} \times (A_1 + A_2 IDY + IDY^2 - B_1 - B_2 - B_3 - B_4 - B_5 - B_6 + RANDT)$$

Equation 28: Regression model for Sunday to Friday (day number, I = 1 to 6)

$$WWTPQ = WWTPQ_{avg} \times (A_1 + A_2 IDY + IDY^2 + B_1 + RANDT)$$

Where:

WWTPQ = daily average wastewater treatment plant flow (cfs)

WWTPQ_{avg} = average wastewater treatment plant flows (cfs), as specified in Block C21 in STPFLOW

IDY = Julian day

A1, A2, A3 = regression coefficients, read from Block C1 of STPFLOW input file

B1, B2, B3, B4, B5, B6 = coefficients for Sunday through Friday respectively, read from Block C1 of STPFLOW input file

RANDT = a random error component with a user specified standard deviation read from Block C2 of STPFLOW input file.

The daily average effluent flows are further modified to account for within-day variations by multiplying the daily average value by a scaling factor for each timestep. The scaling factors are read from Block C3 of the STPFLOW file.

The WWTP **effluent quality data** can be entered in GRSM using either of two methods. One method involves the input of continuous historical quality data for DO, BOD, NOD, NO₃, SS, TP where high frequency (e.g. daily) effluent quality data is available. The alternate method involves the construction and use of cumulative frequency distributions for the effluent quality parameters. Typically, effluent quality data is collected infrequently and therefore it is advisable to input the data as a cumulative frequency distribution. The calculation procedure used in GRSM for model inputs using cumulative frequency distributions was described previously in Section 4.

Model calibration and validation would be performed using continuous historical records of flow from WWTPs within the simulation boundaries. The regression equations would be used to produce effluent flows for the longer term simulations and the simulations involving future population projections.

Parameters

WWTP flow and effluent quality data can also be based on reported values from each WWTP in the model domain. For most facilities, daily flow and monthly average effluent quality is available. In this case, the preferred approach is to use the daily time series of flows for each WWTP and a cumulative distribution for effluent quality. In the event daily average flows are not available, the monthly average flow can be assumed to be equally distributed on each day of the month.

4.5 Meteorological Conditions

Two of the most important factors which affect aquatic plant growth and the instream reaction rates of many water quality parameters are **sunlight intensity** and **water temperature**.

Water temperature was historically estimated using a multiple regression equation based on flow and air temperature. This approach was found to be crude and could not account for changes in water temperature from reach to reach due to groundwater input, riparian shading, heat input from wastewater treatment plants and stormwater outfalls, etc. Since GRSM is sensitive to water temperature, this approach was abandoned in favour of using 2 hour time series data for each reach based on field measurements of water temperature. For example, in the case of the Grand River watershed, continuous water temperature measurements are available at up to eight locations within the model domain at the permanent real-time water quality monitoring stations operated by the GRCA. This temperature data is augmented by deploying temporary temperature loggers at additional locations. For those reaches that are not directly monitored, the water temperature used for model input is estimated by linearly interpolating between adjacent monitoring sites.

Solar radiation input data for the model domain are based on measurements of total incident radiation recorded by Environment Canada. This data is entered as a daily time series. An internal subroutine distributes the total daily radiation value over the day depending on the time of year and latitude of the model domain.

4.6 Reaction Rates

The major reaction rate coefficients included in the GRSM model are CBOD decay (K_D), NOD decay (K_N), CBOD removal (K_R), reaeration coefficient (K_2), denitrification rates (k_{denit}), ammonia mass transfer velocity (v), weir aeration coefficient (K_{WEIR}), and sediment oxygen demand rate (SOD). GRSM requires a value for each of these coefficients and rate for each reach for each month.

CBOD decay, NOD decay and CBOD removal rate coefficients, reaeration coefficients, weir aeration coefficients and SOD rates were previously discussed in Sections 3.1 and 3.2. Denitrification rate constants and ammonia mass transfer velocity coefficients were described in Section 3.4.2.

The reaeration coefficient for each reach is adjusted by the model throughout the simulation to account for changes in average depth and velocity due to increasing or decreasing flow. The relationships between flow and depth, and flow and velocity are modelled using the power relationships (see Equation 33 and Equation 34 in Section 6.11.3) described by Leopold and Maddock (Chapra, 1997). Leopold-Maddock coefficients were estimated using hydraulic models such as HEC-2 or HEC-RAS, which is based on measured channel profiles. The development of the hydraulic coefficients is described in CG&S (1996).

All rate coefficients in GRSM are adjusted to account for variations in stream temperature. Equation 5 is used to modify the rate coefficients.

5. Calibration and Validation

The methodical application, testing and evaluation of a water quality model to predict observed field data is referred to as model calibration and validation. In general, the calibration process is an organized procedure to select model coefficients and improve unknown or poorly characterized model inputs such that model predictions are in the best possible agreement with measured data. The process of model validation, which can be described as a verification of the calibrated model, requires the comparison of another independent set of observed data with the results of a simulation set up to model the second set of conditions.

5.1 Selection of Model Variables and Input Data

Prior to commencing model calibration, you should select the model variables of interest. These selected parameters of interest should correspond with the variables that will be used for validation of the model. For example, in the case of the Grand River watershed, parameters of interest include dissolved oxygen, un-ionized ammonia, TKN, total phosphorus, and nitrate.

Once you have selected your parameters of interest, assess the availability of historical data. Ideally, calibration/validation data should be available for all parameters of interest in key locations, which would include upstream (i.e., background conditions) and highly impacted areas. Data used for model calibration and validation should be representative of the conditions being modeled. For example, if GRSM is being used to model low flow summer conditions, it would be calibrated with data collected during summer low flow. Calibration of the GRSM for dissolved oxygen is particularly important as this parameter varies quite dramatically over a very short period. In this case, it is desirable to have continuous monitoring data available for calibration purposes.

Due to the variation of watercourse conditions in different seasons, you should organize your data sets by season. Ideally, you should have more than one period of data at a particular location for your parameter, so you can use one set for calibration and a second set for validation at the same location. It is also beneficial to select data sets for various years to represent different environmental conditions against which GRSM would be calibrated and validated (e.g., climatically dry, wet, and average conditions).

Data quality should be confirmed, where possible, to ensure that the calibration/validation data is the best available. Where issues with data quality are identified, it may be possible to correct or adjust the data. Any corrections, adjustments or omission of data due to quality assurance or quality control reasons should be noted and taken into account when assessing model calibration/validation.

5.2 Parameter Sensitivity

GRSM is a complex dynamic model that requires a large number of input parameters to describe the river system. Prior to calibration, carry out an assessment of the model's sensitivity to determine which input parameters have the greatest influence on the model output and gain a better understanding of the model's behaviour.

5.2.1 Methods

Assess the sensitivity of GRSM by systematically varying each input parameter independently. General modeling practice is to use a low flow summer period to conduct the sensitivity analysis since most water quality issues are observed during summer low flow.

Typically, increase and decrease inputs by 10 to 50% from the original value, depending on the input parameter. Then compare the resulting output with a base case using the original input value. Since GRSM produces an estimate of dissolved oxygen, total phosphorus, biochemical oxygen demand (BOD), nitrogenous oxygen demand (NOD), nitrate and un-ionized ammonia for each timestep in the simulation period (i.e., 1,464 values for each output variable), comparing the output from the base case and sensitivity runs is challenging due to the large volume of output data produced. One approach to determine differences between the base case and sensitivity runs is to summarize the output using two statistical measures for each model output variable: the root mean squared error and the relative error.

5.2.1.1 The Root Mean Squared Error

The root mean squared error is calculated according to Equation 29.

Equation 29: Root mean squared error

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (C_{bc,i} - C_{sr,i})^2}{n}}$$

Where:

$C_{bc,i}$ = the predicted or modeled concentration at timestep i for the base case

$C_{sr,i}$ = the corresponding predicted or modeled concentration for the sensitivity run

n = the number of timesteps in the simulation period (e.g., number of pairs of base case and sensitivity concentrations)

The root mean squared error is a quantitative estimate of the absolute difference between paired data sets from two model runs that is expressed in mg/L, the same units as the concentrations. However, because it is based on the sum of squared residuals, it

does not indicate whether the sensitivity run is consistently higher or lower compared to the base case.

5.2.1.2 The Relative Error

You can use the relative error to determine if there is a consistent increase in the output variable compared to the base case. Relative error is calculated according to Equation 30.

Equation 30: Relative error

$$RE = \frac{\sum_{i=1}^n (C_{bc,i} - C_{sr,i})}{C_{bc}}$$

Where:

$C_{bc,i}$ = the predicted or modeled output variable concentration for the base case

$C_{sr,i}$ = the corresponding predicted or modeled concentration for the sensitivity/calibration run

C_{bc} = the average output variable concentration for the base case

n = the number of timesteps in the simulation period (e.g., number of pairs of base case and sensitivity concentrations)

Relative error can be positive or negative and is expressed as a percentage of the average base case concentration. Positive values of the relative error suggest that the sensitivity run is predicting lower concentrations relative to the base case and conversely, a negative value means the sensitivity run is higher than the base case on average.

5.2.1.3 Acceptable RMSE

In the case of the Grand River watershed, an acceptable RMSE has been established for each constituent, giving consideration to the expected order of magnitude of environmental concentrations in the central Grand River, model output resolution (i.e., GRSM does not predict concentrations less than 1 µg/L) and errors associated with measuring environmental concentrations such as sampling error, analytical or measurement error, etc. Table 3 provides a summary of these values for each water quality constituent predicted by GRSM. If the RMSE associated with a sensitivity run exceeds these acceptable values for a particular constituent, you can then consider the model to be relatively sensitive to that input parameter.

Table 3: Acceptable Values for RMSE

Water Quality Variable	Acceptable RMSE
BOD	0.5 or less
NOD	0.5 or less
Nitrate	0.3 or less
Total Phosphorus	0.010 or less
Un-ionized Ammonia	0.005 or less
Dissolved oxygen	0.5 or less

5.2.2 Sensitivity Relationships

This section of the Technical Guidance Document outlines parameter relationships derived from the application of the GRSM in the Grand River watershed. You may need to perform further analysis if you plan on applying the GRSM to a watershed that is significantly different from the Grand River watershed.

It is useful to group input parameters according to categories. For example:

- Boundary loadings describing the flow and water quality of tributary flows into the system
- Point source loadings describing the effluent flow and quality of wastewater discharges into the system
- Global time series, i.e., daily total solar radiation that is the same for each reach
- Reach-specific time series, i.e., water temperature must be specified for every 2 hour timestep of the simulation period but can be different for each reach
- Global constants that describe processes such as aquatic plant growth
- Reach-specific parameters that are used to specify inputs that may change from reach to reach, such as reach length, hydraulic constants, etc.

5.2.2.1 Boundary Flows

A range of 10% is the approximate measurement error generally associated with input flow and water quality. Analysis indicated that most water quality constituent concentrations are relatively insensitive to changes in boundary flow or quality. The exception to this is dissolved oxygen, which demonstrates moderate sensitivity to changes in boundary flows.

5.2.2.2 Wastewater Treatment Plant Loadings

GRSM does not appear to be highly sensitive to changes in the WWTP loadings within the range of $\pm 10\%$. Increasing either the effluent flow or concentration has the expected effect of increasing the concentration of constituents such as BOD, NOD, nitrate, total phosphorus and un-ionized ammonia, and decreasing the concentration of dissolved oxygen.

5.2.2.3 Global and Reach-Specific Time Series Inputs

GRSM uses a time series of daily total solar radiation for all reaches; therefore, this input series is considered to be global as opposed to reach-specific. Dissolved oxygen levels are quite sensitive to solar radiation as this determines aquatic photosynthesis and growth rates. Higher solar radiation results in higher dissolved oxygen levels, especially during the day when photosynthesis is at its peak.

Water temperature, on the other hand, is a reach-specific time series input as the model requires the user to generate an input file containing temperature values for each timestep of the simulation period for each reach. GRSM is somewhat sensitive to water temperature, in the case of the Grand River watershed a 0.5°C increase reduced predicted dissolved oxygen levels by about 0.3 mg/L on average. Increasing water temperature has the effect of increasing the rate of oxygen consuming reactions such as NOD decay and respiration. There is also a decrease in total aquatic plant biomass as *Cladophora* does not grow as well with warmer water temperatures. Decreasing water temperature has the opposite effect.

5.2.2.4 Global Constants

Of the 53 global constants, very few have an effect on predicted concentrations of BOD, NOD, nitrate, total phosphorus, or un-ionized ammonia but many of them have a moderate or strong influence on dissolved oxygen. BOD and NOD are not particularly sensitive to any of the global parameters.

Nitrate, total phosphorus, un-ionized ammonia and dissolved oxygen concentrations are highly sensitive to the maximum growth rate of *Potamogeton*, the half-saturation coefficient of light limitation for *Potamogeton*, the unit respiration rate for *Potamogeton*, and the unit respiration rate for *Myriophyllum*.

In addition, dissolved oxygen concentrations are also sensitive to the parameters listed below for aquatic plants.

Parameters for all three aquatic plants:

- The oxygen assimilation ratio
- The aquatic plant depth
- Optimum growth temperature ranges

Cladophora parameters:

- The washoff* temperature
*Washoff refers to the fraction of aquatic plant biomass that is removed during each timestep as a result of plant death, fragmentation, predation, etc.
- The maximum growth rate
- The half-saturation coefficient of light limitation
- The unit respiration rate

Potamogeton parameters:

- The washoff temperature
- The washoff rate
- The growth rate temperature correction coefficient
- The half saturation coefficient for external phosphorus

Myriophyllum parameters:

- The maximum growth rate
- The half-saturation coefficient of light limitation
- The unit respiration rate
- The growth rate temperature correction coefficient

5.2.2.5 Reach-Specific Input Parameters

Some input parameters have to be specified on a reach by reach basis, such as the reach length, hydraulic properties, etc. Several rate processes are included in GRSM such as reaeration, sediment oxygen demand, NOD decay, etc. and these can have different rate constants specified for each reach. This allows the model to have flexibility to define higher or lower rates for reaches that may be acclimatized to specific conditions.

Un-ionized ammonia concentrations are sensitive to some reach-specific inputs including the NOD decay rate, average organic nitrogen concentration, average pH and the Leopold Maddock hydraulic coefficients for velocity. The sensitivity to velocity, NOD decay rate and organic nitrogen concentration relates to the way the nitrogen cycle is modeled in GRSM. NOD is assumed to be composed of total ammonia nitrogen and organic nitrogen. The concentration of organic nitrogen is constant and does not contribute to oxygen consumption. Increasing or decreasing the NOD decay rate, changing the travel time by increasing or decreasing the velocity or modifying the organic nitrogen concentration changes the total ammonia nitrogen concentration, which is used to estimate un-ionized ammonia. Un-ionized ammonia is highly sensitive to pH and nitrate concentrations are sensitive to the denitrification rate constants for each reach.

Dissolved oxygen concentrations are sensitive to initial estimates of *Potamogeton* and *Myriophyllum* biomass at the beginning of the simulation period, the reaeration rate constant pre-exponential factor a (refer to Equation 2), the organic nitrogen concentration and all of the Leopold Maddock hydraulic parameters. Dependence of dissolved oxygen on biomass growth is multiplicative and starting with a higher biomass results in faster initial growth. Organic nitrogen has the effect of increasing or decreasing the amount of NOD available for oxygen consumption, which then has a noticeable impact on the predicted dissolved oxygen level.

Many of the rates in GRSM are area-based (e.g., reaeration from the river surface or photosynthetic oxygen production from biomass on the river bottom), which are then converted into volumetric rates by dividing by depth. The hydraulic parameters

determine the average depth and velocity in each reach for each timestep based on flow. Decreasing Leopold Maddock coefficient a or b results in a decrease in the average depth for a given flow. As the depth decreases, the volumetric rates increase. This produces higher predicted dissolved oxygen concentrations at shallower depths.

Decreasing Leopold Maddock hydraulic coefficients c or d has the effect of decreasing the average velocity through the reach. As the velocity decreases, travel time increases and time-dependent decay processes occur to a greater extent. This has the ultimate result of decreasing dissolved oxygen concentrations.

5.3 Methods for Calibration

The calibration process is an organized procedure to select model coefficients and improve unknown or poorly characterized model inputs such that model predictions are in the best possible agreement with measured data. The goal of calibration is to reduce predictive error as much as possible, while retaining realistic system structure and function.

The results of a sensitivity assessment identify which input parameters are most important and therefore which ones are potentially contributing to model error. With a well-calibrated water quality model, you can achieve a predictive error of approximately 10-20% (and in some cases less). Higher error is expected with validated models when parameter values have not been adjusted. It is important wherever possible to quantify model predictive error and to display simulation results with error bars, both for monitoring data and for model predictions.

Through a successful calibration, you will capture not only the estimated value of a given output parameter, but also the behaviour of that parameter over time. To give a very simple example, a dissolved oxygen model that accurately estimates daily average concentrations would not be useful unless it also captured the diurnal and seasonal patterns of oxygen in the river. If you predict a key output parameter within a reasonably realistic range of values, and its predicted behaviour accurately tracks known patterns, you can be confident that you have identified and appropriately simulated the most important processes affecting that parameter.

In GRSM, you can modify a large number of input parameters. In some cases, changing the input parameter dramatically from the existing value causes the model to produce unrealistic results. Systematically adjust these input parameters through successive iterations. Many of the global constants that are currently in the model have been established during previous studies, using field studies and/or literature values. You should not modify these global constants unless you have a very compelling reason to do so (e.g., new research or literature suggesting a “better” value) or if you are applying the model to a watershed that is significantly different from the Grand River watershed.

In the case of the Grand River watershed, the main model parameters that were modified for calibration included starting biomass at the beginning of each modeling period, river nitrification rate, river denitrification decay rate and species-specific biomass inhibition factors. Utilizing measured values for boundary flows, WWTP flows,

solar radiation and water temperature wherever possible is essential for model calibration and validation since the model can be sensitive to these inputs. GRSM produces output for the downstream node of each reach therefore measured data should be compared to the nearest upstream GRSM reach.

5.3.1 Calibration of Dissolved Oxygen

Dissolved oxygen concentrations are sensitive to many of the input parameters. Calibrate dissolved oxygen levels predicted by GRSM to the selected calibration data set in a step-wise fashion starting at the most upstream reach. If multiple seasons are being simulated, begin calibrating with the winter season, followed by the spring, summer and fall seasons. This allows you to calibrate dissolved oxygen levels in response to seasonal changes in aquatic plant growth in a sequential fashion (i.e., the “initial” biomass for the spring simulation should be based on output from the final day of the winter simulation, and so on). Try to minimize the number of parameters used for calibration. You should note that, historically, calibration has been focused on changing the reaeration rate constant pre-exponential factor a (see Equation 2) as well as the initial biomass and biomass inhibition coefficients for each aquatic plant species.

The dependence of dissolved oxygen on the reaeration rate is well established and has been used for calibration in previous studies using GRSM. You can adjust species-specific biomass inhibition factors for the seasonal model until you achieve a reasonable fit for dissolved oxygen. You can use aquatic plant biomass density at the end of a seasonal simulation as the starting point for the next seasonal simulation.

You can compare simulation results obtained from GRSM runs with the observed data in terms of daily minimum dissolved oxygen. Graphical time series of daily minimum dissolved oxygen are very useful to visualize how the model predictions and measured data compare. The RMSE can be used to provide a quantitative estimate of the difference between the two datasets. Since low DO levels are considered to be more important for the survival of aquatic life, place more emphasis on achieving adequate calibration based on minimum dissolved oxygen levels rather than on maximum levels.

5.3.2 Calibration of Nutrients

You can assess calibration for nutrient variables, such as total phosphorus, nitrate and un-ionized ammonia, by quantitatively or qualitatively comparing model output and measured data. Often quantitative assessment is not feasible due to the small number of nutrient grab samples. Instead, you can adjust model parameters to give the best fit to the observed nutrient data using all years rather than using a strict formal calibration process with validation on an independent dataset.

You can calibrate nitrate concentrations by adjusting denitrification rates constants for each reach. You can calibrate un-ionized ammonia and TKN levels by adjusting NOD decay rates.

5.4 Methods for Validation

The process of model validation can be described as a verification of the calibrated model. It requires the comparison of another independent set of observed data with the results of a simulation set up to model this second set of conditions. If the simulation results for the validation run are satisfactory (i.e. in close agreement with the observed data) the processes of model calibration and validation are said to be complete and the model is suitable for application. However, if the observed data are not reproduced by the model within acceptable limits during the process of validation, the model calibration must be further refined. This is achieved by further adjusting the most sensitive model parameters, as defined by a sensitivity analysis, and then repeating the calibration and verification runs and analysis. The refinement process is repeated until both the calibration and validation runs achieve satisfactory results.

5.4.1 Validation of Dissolved Oxygen

You can assess the model validation for dissolved oxygen using both graphical and quantitative approaches. Keep in mind that GRSM produces output for the downstream node of each reach, therefore, measured data are compared to the nearest upstream GRSM reach.

Ideally, you should compare model output from GRSM to data from a continuous water quality monitoring station. You can then compare modeled and measured concentrations for each season in each year by plotting maximum and minimum dissolved oxygen for each day of the simulation period. You can use the RMSE, as used for calibration above, to quantitatively assess the differences between modeled and measured dissolved oxygen concentrations. You can calculate the RMSE for both daily maximum and daily minimum dissolved oxygen for each season in each calibration or validation year.

GRSM frequently under predicts daily maximum dissolved oxygen levels during periods of active photosynthesis and is much more successful at matching daily minimum levels. This behaviour is possibly related to the model algorithms that describe the amount of oxygen generated during photosynthesis. Achieving a reasonable prediction of the daily minimum dissolved oxygen is more important than a better model fit to the daily maximum concentrations because the survival of aquatic organisms and quality of aquatic habitat can be affected if dissolved oxygen drops too low. It is important to ensure not only that the model produces a good estimate of the daily minima but also that predictions usually follow the general trends across and within seasons.

RMSE values for the daily minimum dissolved oxygen concentrations for the calibration can typically be around 1 mg/L, which is considered acceptable. You may observe some higher values when data quality is suspect. RMSE values for the daily maxima are usually somewhat higher, with values typically at approximately 1.5 to 3 mg/L. RMSE values for the validation years are usually slightly higher than those for the calibration year, but should still fall within an acceptable range.

5.4.2 Validation of Nutrients

You will typically carry out validation of GRSM for nutrient variables using all available data to provide the best fit. Because nutrient samples are collected at uneven, infrequent intervals and nutrient loadings in GRSM are handled probabilistically, it is not possible to match measured nutrient concentrations with model predictions on a particular day, unlike the analysis that can be performed for dissolved oxygen. This precludes rigorous, quantitative statistical analysis for nutrient variables.

You can use a graphical comparison of modeled and measured concentrations to assess model calibration and validation for nutrient variables. You will then compare nutrient variables to GRSM predictions for each season by considering the range of concentrations observed and predicted. A box and whisker plot is a common method for comparing the range of values predicted by GRSM and measured concentrations. If there are less than three samples for analysis, the interdecile range is not estimated and all measured values should be plotted as individual points.

You would then assess validation of the model by visually comparing the ranges of measured and predicted concentrations over all seasons, by giving more weight to seasons with greater numbers of samples. Due to the infrequent nature of nutrient sampling, it is possible that you may only be able to perform validation for a single season or year.

5.5 The Use of Spreadsheet Software for Analysis

Since the GRSM does not include a post-processor, processing of output data is accomplished through the use of spreadsheet software for analysis. **Spreadsheet post-processors are the responsibility of the user to develop.** Several post-processor spreadsheets have been developed by GRSM users. For your convenience, these templates have been included in the GRSM download package. It should be noted, however, that these files should only be used as a guide and that the GRCA will not provide technical support for these files.

The spreadsheets allow you to load the output from specific runs, plot output data, and compare values between two runs to assist with the evaluation of model sensitivity, calibration and validation. Each analysis year will require a separate spreadsheet file. The post-processing spreadsheets were created in Microsoft Excel 2007 and will need to be adapted if a different model structure is used other than the GRSM structure.

6. Model Functions and Subroutines

This section of the Technical Guidance Document provides details regarding the functions and subroutines currently used by GRSM. Each subsection displays information in the same format:

- The name of the function/subroutine is shown in capital letters.
- 'Type' specifies if this is a function or a subroutine.
- 'Purpose' provides a short description of what this function/subroutine does.
- 'Method' provides additional information regarding how this function/subroutine works.

6.1 MONTH

6.1.1 Type

Integer function

6.1.2 Purpose

Returns a month number (i.e., 1 to 12) given the Julian day number, or returns the Julian day number of the first day in the month.

6.1.3 Method

A vector containing the day numbers of the last day of each month is searched until the given day falls between two vector values. The vector position I is then returned as the month number.

6.2 WEEK

6.2.1 Type

Integer function

6.2.2 Purpose

Returns the weekday number (i.e., 0 = Saturday, 1 = Sunday, 2 = Monday, etc.) given the year and Julian day number.

6.2.3 Method

The weekday number is the integer remainder of the Julian day divided by 7.

6.3 RAN2

6.3.1 Type

Subroutine

6.3.2 Purpose

Computes uniformly distributed random real numbers between 0.0 and 1.0.

6.3.3 Method

Standard random number generator subroutine from “Numerical Recipes in Fortran 77: The art of Scientific Computing, 2nd Edition” (2003) by William H. Press *et al.* using the L’Ecuyer method with Bays-Durham shuffle and added safeguards to prevent serial correlation.

6.4 GAUSS

6.4.1 Type

Subroutine

6.4.2 Purpose

Computes normally distributed random numbers with a given mean and standard deviation.

6.4.3 Method

Twelve random numbers are generated using the RAN2 subroutine and are used to compute a normally distributed random number according to the central limit theorem. This number is then adjusted to match the given mean and standard deviation.

6.5 MSG1, MSGA1, and MSGM1

6.5.1 Type

Subroutine

6.5.2 Purpose

Prints error messages if various types of error conditions are encountered in the input data.

6.5.3 Method

The routine checks to determine the type of error condition. If it is a premature end of file (EOF), it writes a message indicating the last block of data successfully read and the next one expected. If it is not an EOF, it checks to determine if the data code block in

error is a major code or a sub-code and writes a message indicating the code it read and the code it expected.

6.6 INPUT

6.6.1 Type

Subroutine

6.6.2 Purpose

Inputs all the data required for a simulation run. Stores the data in the common blocks and system files. Performs error checks to determine if the input data is in the correct sequence.

6.6.3 Method

The data are read from a file in the order in which they are required. The routine checks the coding in the data to determine if any sequence errors have occurred. If an error does occur, the appropriate error message subroutine is called.

6.7 INDFLO

6.7.1 Type

Subroutine

6.7.2 Purpose

Adjusts the raw independent flows according to the flow regulation policy parameters input by the user and produces a regulated independent flow series.

6.7.3 Method

The daily independent flows are compared to the input regulation policy flows; if the raw flows are less than the regulation policy flows, the raw flows are reset to the policy flows.

6.8 STPFLO

6.8.1 Type

Subroutine

6.8.2 Purpose

Calculates the point source flows from the regression coefficients supplied by the user. The subroutine also includes a random error component in the calculated flows based on a user-specified standard deviation. This subroutine is only used when point source flows are internally calculated.

6.8.3 Method

The point source flow for each day is calculated using the methodology described previously in Section 4.5.

6.9 DEPFLO

6.9.1 Type

Subroutine

6.9.2 Purpose

Calculates the dependent (local diffuse) flows based on total local diffuse inflow read from BASINFLOW file and proportioned to each reach based on fractions specified in FLOWFILE.

6.9.3 Method

The list column of data contained in the independent flow file, BASINFLOW, is calculated by the user as the difference between the upstream and downstream flows after accounting for all point source and storm sewer inflows. This total flow is proportioned to each reach according to the fractions (e.g., the fraction of the total flow that drains to each reach is proportional to the local drainage basin area of each reach) entered by the user in Block D1 of FLOWFILE.

6.10 ROUTNG

6.10.1 Type

Subroutine

6.10.2 Purpose

Inputs the flows output by subroutines INDFLO, STPFLO, and DEPFLO. The output is first mixed and is then routed through the simulated section of the river.

6.10.3 Method

The regulated independent flows and the dependent flows are input for the day under simulation. The flows at each point are interpolated from the previous day's value and the present day's value. Point source inflows and withdrawals are added to and subtracted from these hourly flows to yield the total flow at the head of the reach. The total flow at the end of the reach is calculated according to Equation 31.

Equation 31: Total flow at the end of the reach

$$\text{ENDQ} = A1 \times \text{OHEADQ} + A3 \times \text{OENDQ} + A2 \times \text{HEADQ}$$

Where:

ENDQ = flow at end of reach

A1, A2, A3 = Muskingum flow routing coefficients

OHEADQ = flow at head of reach from previous day

OENDQ = flow at end of reach from previous day

HEADQ = flow at head of reach

6.11 AVGFLO

6.11.1 Type

Subroutine

6.11.2 Purpose

Calculates the average velocity, depth and flow at the head and end of each reach at each time point.

6.11.3 Method

The average flow is calculated by:

Equation 32: Average flow

$$Q = \frac{QHF + QEL}{2}$$

Where:

QHF = flow at the head of the reach at the first time point in the day

QEL = flow at the end of the reach at the last time point in the day

The average velocity (U) and depth (H) are calculated using the power functions given in Equation 33 and Equation 34.

Equation 33: Average velocity

$$U = cQ^d$$

Equation 34: Average depth

$$H = aQ^b$$

Where:

a, b, c, and d = Leopold Maddock coefficients read from Block G1 of RATEFILE

6.12 STRPRM

6.12.1 Type

Subroutine

6.12.2 Purpose

Prorates all stream parameters and rate coefficients to the conditions of stream flow and temperature for the day under simulation from the base flow and temperature input by the user.

6.12.3 Method

The daily channel flows, depths, velocities, sunlight and temperature for each reach are read in. The **sediment oxygen demand (SOD)** rate is calculated using Equation 35.

Equation 35: Sludge uptake

$$SOD = AGBSLU \times \Theta^{(T-20)} \times \frac{BDEP}{ADEP}$$

Where:

AGBSLU = base rate coefficient for sediment oxygen demand, read from Block J9 of RATEFILE.

Θ = temperature correction coefficient for SOD, read from Block J1 of RATEFILE

T = current water temperature in °C

BDEP = base depth (ft) for the channel, read from Block J6 of MAINFILE

ADEP = average depth (ft) based on current flow

If the ECOL subroutine is not used, the **respiration rate** is calculated using Equation 36.

Equation 36: Respiration rate

$$\text{RESP} = \text{ALBRES} \times \Theta^{(T-20)} \times \frac{\text{BDEP}}{\text{ADEP}}$$

Where:

ALBRES = base rate for respiration

Θ = temperature correction coefficient for respiration, read from Block J1 of RATEFILE

T, BDEP and ADEP = as defined in Equation 35

If the ECOL subroutine is not used, the **rate of photosynthesis** is calculated using Equation 37.

Equation 37: Rate of photosynthesis (ECOL not used)

$$\text{PHOTO} = \text{ALBPH} \times \text{AGSIF} \times \Theta^{(T-20)} \times \frac{\text{BDEP}}{\text{ADEP}} \times \frac{\pi}{2 \times \text{ALPSL}}$$

Where:

ALBPH = base rate coefficient for photosynthesis

AGSIF = sunlight intensity factor

Θ = the temperature correction coefficient for photosynthesis, read from Block J1 of RATEFILE

T, BDEP and ADEP = as defined in Equation 35

ALPSL = sunlight period for the day

The **atmospheric reaeration rate, K_2** , is calculated according to Equation 38.

Equation 38: Atmospheric reaeration rate

$$\text{AGK2} = \left(\frac{aU^b}{H^c} \times 1.028^{(T-20)} \right) \times (1 + K2F2)$$

Where:

a, b, c = user-specified constants read from Blocks J4a, J4b and J4c of RATEFILE

U = current channel velocity (ft/s)

H = current water depth (ft)

T = current water temperature (°C)

K2F2 = random error component for reaeration coefficient, the GAUSS subroutine is used to generate a random number with a mean of 0 and the standard deviation specified by the user in Block J3 of RATEFILE.

The BOD deoxygenation rate (K_D), NOD decay rate (K_N), and BOD decay rate (K_R) are corrected for temperature using the approach described previously in Section 3.2.

6.13 QUAL11

6.13.1 Type

Subroutine

6.13.2 Purpose

Calculates the quality of the boundary location (independent) flows.

6.13.3 Method

The stream water quality calculations proceed according to one of six types as specified by the user in Block K1 of FLOWFILE. The six available calculation types are:

- **Type 1:** The quality is constant and is independent of flow.
- **Type 2:** The quality is variable and is dependent on flow.
- **Type 3:** The quality is variable and is selected from a probability distribution which is dependent on flow.
- **Type 4:** The quality is variable and is selected from a probability distribution which is independent of flow.
- **Type 5:** The quality is variable and is selected from a distribution which is conditional upon the probability distribution given in Type 3.
- **Type 6:** The quality is variable and is selected from a distribution which is conditional upon the probability distribution given in Type 4.

The quality for each parameter for each reach for each day is calculated according to one of the calculation types. It should be noted that the first calculations may not be a Type 5 or Type 6 as they are conditional upon a previous quality calculation. As such, a Type 5 calculation must be preceded by a Type 3 calculation and a Type 6 calculation must be preceded by a Type 4 calculation. The quality values calculated are for the head of reach conditions.

6.13.3.1 Type 1

Equation 39: Quality of the boundary location flows (Type 1)

$$AGIFQ = ALPDI(IPD, 1)$$

Where:

AGIFQ = concentration of water quality parameter under consideration for the current boundary inflow and day of the simulation period

ALPDI = array containing the probability distributions read in from Block K7 of FLOWFILE

IPD = pointer to probability distribution for the independent boundary flow and quality parameter under consideration

1 = point within probability distribution for a TYPE 1, which is constant and independent of flow (it will always be 1 since there is only one point in the probability distribution)

6.13.3.2 Type 2

This type of calculation makes the concentration dependent on flow, with the assumption that the concentration is constant within user specified flow ranges or intervals. For example, the concentration of TP for Tributary X is set equal to 0.03 mg/L when the flow is between 0 and 1 m³/s and 0.045 mg/L when flows are between 1 and 2 m³/s, etc. Hence the program computes flow intervals and determines which interval the present flow is in. It first determines if the flow is in the proper range as specified in the input by checking it against ALLIF and ALHIF (the lowest and highest flows respectively for the independent boundary flow number and month under consideration). The width of the flow intervals is found as follows:

Equation 40: Width of the flow intervals

$$LGTH = \frac{ALHIF(IIF, IMTH) - ALLIF(IIF, IMTH)}{ISUB}$$

Where:

ALHIF = highest flow for each boundary in each month read from Block K2 of FLOWFILE

IIF = the boundary number under consideration

IMTH = the current month of the simulation period

ALLIF = lowest flow for each boundary in each month read from Block K3 of FLOWFILE

ISUB = number of intervals into which the flow is divided read from Block K5 of FLOWFILE

For each flow interval, there is a value giving the quality for that flow range. The flow interval (IVL) into which the flow being considered falls is defined in Equation 41: Flow interval.

Equation 41: Flow interval

$$IVL = \text{INTEGER} \left(\frac{AGIFLW(IIF) - ALLIF(IIF, IMTH)}{LGTH} \right) + 1$$

Where:

AGIFLW = daily independent boundary flow

IIF = the boundary number under consideration

IMTH = the current month of the simulation period

If the flow is lower than the lowest flow ALLIF, it is placed in the first range, and if it is greater than the highest flow ALHIF, it is put in the last range. The distribution number, IPD, is found in the array ALPDPR for the appropriate flow number, quality parameter and flow interval. The quality for this type of calculation is then the first and only point in that distribution, as shown in the equation below.

Equation 42: Quality of the boundary location flows (Type 2)

$$AGIFQ(1, IQP, IIF) = ALPDI(IPD, 1)$$

Where:

IPQ = the water quality parameter number

6.13.3.3 Type 3

This type of calculation is similar to the TYPE2 except that the quality is found from a distribution (rather than a single value) that is dependent on flow. The flow interval is calculated the same as in a TYPE2 calculation. The distribution number IPD for the quality values is found from array ALPDPR for the appropriate quality parameter (IQP), independent boundary flow (IIF) and flow interval (IVL). The point in the distribution is found by linear interpolation between adjacent points in the discrete distribution as follows.

Equation 43: Random point in the distribution (Type 3)

$$XM1 = RN \times (AGPPDD(IPD) - 1)$$

Where:

RN = a random number between 0 and 1 calculated by the RAN2 subroutine

AGPPDD = number of points in the distribution

The value of XM1 is integerized to get M2. The quality is found by interpolating between two points in the distribution: $M3 = M2+1$ and $M4 = M2+2$ to get the point $XM1+1.0$ as defined in Equation 44.

Equation 44: Quality of the boundary location flows (Type 3)

$$AGIFQ(1, IQP, IIF) = ALPDI(IPD, M3) + \\ (ALPDI(IPD, M4) - ALPDI(IPD, M3)) \times (XM1 - M2)$$

6.13.3.4 Type 4

This type of calculation is similar to the TYPE3 except the probability distribution for the quality is not dependent on flow. Thus the probability distribution is found from ALPDPR knowing the flow number and quality parameter number. The point within the distribution is found using the same linear interpolation method as described above for the TYPE3.

6.13.3.5 Type 5

In order to calculate a TYPE5 quality one of the other qualities calculated previously must have been a TYPE3. The distribution number for the quality values is then found from the array COND knowing the quality parameter number (IQP), the probability distribution number used in the previous TYPE3 calculation (IPDT3), and the point below XM1 in that distribution ($M3 = M2 + 1$). This gives a new probability distribution number IPD which is used to locate the distribution in the array ALPDI. The quality value is then calculated as in TYPE3 by finding a random point $XM2 + 1$ between two points M6 and M7 in the distribution and interpolating as shown in Equation 45.

Equation 45: Random point in the distribution (Type 5, T2)

$$T2 = ALPDI(IPD, M6) + \\ (ALPDI(IPD, M7) - ALPDI(IPD, M6)) \times (XM2 - M5)$$

Where:

XM2 = a random number calculated using the same approach as XM1 described above

M5 = the integer part of XM2

M6 = M5 + 1

M7 = M5 + 2

The procedure is repeated for the second point in the TYPE3 calculation ($M4 = M2 + 2$) to give another quality value and the step above is repeated with a new value of $XM2$ to come up with a second value from the TYPE5 distribution, $T3$. The quality is then found by interpolating between $T2$ and $T3$ to Equation 46.

Equation 46: Quality of the boundary location flows (Type 5)

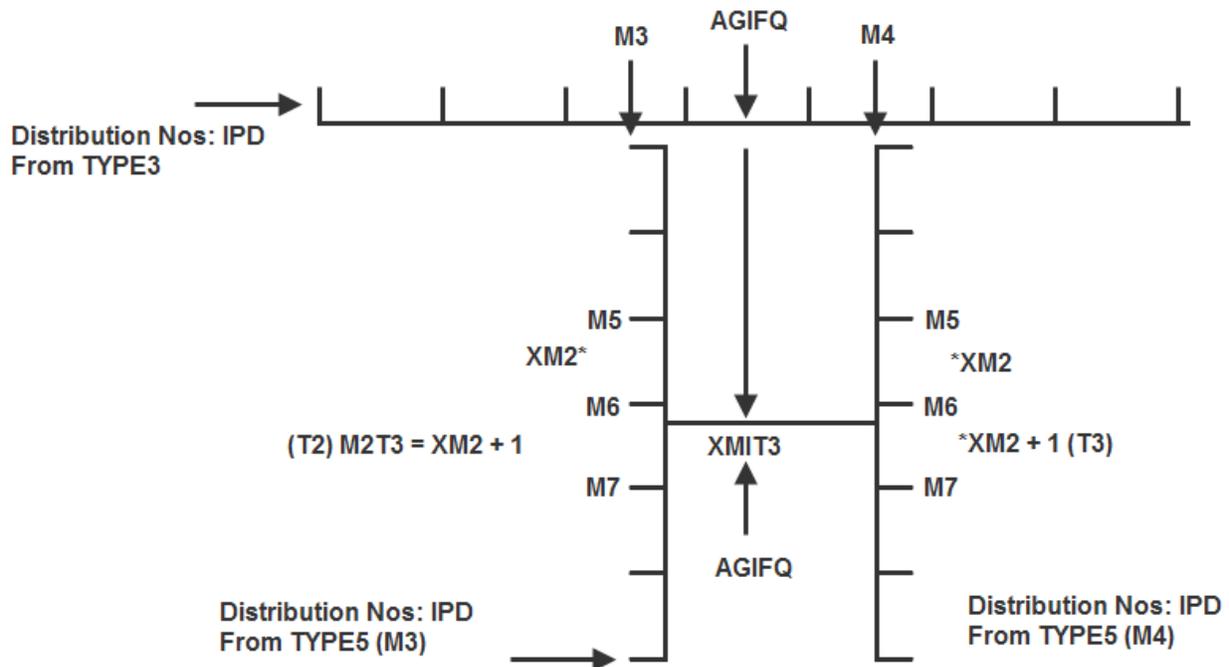
$$AGIFQ(1,IQP,IIF) = T2 + (T3 - T2) \times (XM1 - M2)$$

Where:

$XM1$ and $M2$ = the values used in the previous TYPE3 calculation

Figure 6 provides an overview of how these procedures relate to each other.

Figure 6: Type 5 procedures



6.13.3.6 Type 6

This calculation is performed the same as TYPE5 except that the previous calculation must have been a TYPE4 and the information regarding the distribution number and points within it are carried forward to this type of calculation.

6.13.3.7 Within Day Variation in Boundary Quality

The within day variation for each time point is calculated as shown in Equation 47.

Equation 47: Quality of the boundary location flows (Type 6)

$$AGIFQ(ITP, IQP, IIF) = AGIFQ(1, IQP, IIF) \times AGWIFQ(IIF, IQP, IITP)$$

Where:

AGIFQ = independent flow quality at time point ITP

IQP = quality parameter number

AGIFQ(1, IQP, IIF) = average independent flow quality calculated using one of the calculation types described above

AGWIFQ = within day variation factor read from Block K4 in FLOWFILE.

$IITP = ITP \times \frac{12}{N}$ gives the location of point ITP in array AGWIFQ according to the number of timesteps in each day (i.e. N = 12 in the current GRSM setup).

6.14 QUAL12

6.14.1 Type

Subroutine

6.14.2 Purpose

Calculates the quality of the point source inputs.

6.14.3 Method

The method of calculation and the types of calculation proceeds as per those performed in subroutine QUAL11 except that variables pertaining to independent boundary flows are replaced by those pertaining to waste water treatment plants.

6.15 QUAL13

6.15.1 Type

Subroutine

6.15.2 Purpose

Calculates the quality of the local diffuse inflows.

6.15.3 Method

The calculation of the quality for local diffuse inflow is carried out in subroutine QUAL11 along with the calculations for boundary inflows. The calculation type used is the same as that used for the boundary inflows. The quality calculated in QUAL11 apply equally to all reaches in the simulated system. QUAL13 allows you to customize the quality of local diffuse inflow to each reach. The method used is shown in Equation 48.

Equation 48: Quality of local diffuse inflow

$$QUAL_I = (A + B \times PDQ + C \times PDQ^2) \times Y_I$$

Where:

QUAL = diffuse inflow quality for each parameter for reach

A, B, and C = empirically derived “customizing” coefficients read in from Block M1 of FLOWFILE

I = current time step

PDQ = local diffuse inflow quality determined in QUAL11

Y = within day quality variation factor read from Block M2 of FLOWFILE

6.16 PHOSYN

6.16.1 Type

Subroutine

6.16.2 Purpose

Calculates the sunlight factors for each time point during the day.

6.16.3 Method

The time of sunset is determined from the time of sunrise and photo period. The sunlight factors, which are used to proportion the total daily solar radiation to each time step, are calculated by integrating the sinusoidal photosynthetic curve as described in Equation 49.

Equation 49: Sunlight factors

$$ALPHF(K) = \frac{ALPSL}{\pi \times H} \times (\cos(SM1) - \cos(SM2))$$

Where:

ALPHF = sunlight factor

K = time step during the day

ALPSL = sunlight period as a fraction of a day

H = time step as a fraction of a day

$$SM1 = \frac{\pi}{ALPSL} \times ((K - 1) \times H - ALSR)$$

$$SM2 = \frac{\pi}{ALPSL} \times (K \times H - ALSR)$$

ALSR = time of sunrise

6.17 STORM

6.17.1 Type

Subroutine

6.17.2 Purpose

Inputs the data from each of the individual storm sewer inflow files and produces one temporary file containing all the storm flow quality and quantity data.

6.17.3 Method

The quality and quantity data is read from the data files one day at a time. Nonexistent data (i.e., days with no storm events) is blank, with zeroes. The data is loaded into an array in the correct sequence so that the sequence of data matches the sequence of storm inputs defined by the user. The final array containing all the data is then output to a temporary vertical storage file.

6.18 SIM

6.18.1 Type

Subroutine

6.18.2 Purpose

Mixes all inputs at the head (i.e., upstream node) of each reach, routes them through the reaches and allows all processes affecting the concentration of each water quality parameter to occur.

6.18.3 Method

For each day of the season, the following values are read from previously created temporary files:

- The average regulated independent boundary flow for the day
- The average wastewater treatment plant flow for the day
- The average dependent local diffuse flow for the day
- The channel flows for each time point of the day
- The average velocities for each time point of the day
- The rate coefficients for the day
- The independent boundary flow quality for each time point in the day
- The wastewater treatment plant flow quality for each time point of the day
- The dependent local diffuse flow quality for each time point of the day
- The photosynthetic factors for each day (only one per month)

If there is **one upstream channel flow** then the flow being added to the node is calculated according to Equation 50.

Equation 50: Upstream channel flow added to the node

$$\text{FLOW} = \text{AGCFLW}(\text{ARNO}, \text{MIX1}, 2) \times \frac{\text{ALMIXC}(\text{IJPT}, 1, 2)}{2}$$

Where:

AGCFLW(ARNO, MIX1, 2) = channel flow at the end of the previous upstream reach

ALMIXC(IJPT, 1, 2) = percentage of upstream flow routed to the present node

This flow is added to TFLOW, which is used to accumulate the flow input to or taken away from the node.

The **pollutant loading** due to the upstream flow for each quality parameter is calculated as follows:

Equation 51: Pollutant loading from upstream channel

$$\text{POLUT} = \text{AGRFQ}(\text{ARNO}, \text{MIX1}, 1, \text{IQP}) \times \text{FLOW}$$

Where:

AGRFQ = regulated flow quality at the end of the previous upstream reach

FLOW = see Equation 50

If the parameter is dissolved oxygen (DO), then the loading is recalculated to take into account the effect of weir reaeration as follows:

Equation 52: Pollutant loading for dissolved oxygen

$$\text{POLUT} = [\text{AGCS}(\text{INDAY}, \text{MIX1}) - (\text{AGKW}(\text{IJPT}, \text{MONZ}) \times (\text{AGCS}(\text{NDAY}, \text{MIX1}) - \text{AGRFQ}(\text{ARNO}, \text{MIX1}, 2, \text{IQP})))] \times \text{FLOW}$$

Where:

AGCS = saturation DO concentration

AGKW = weir reaeration rate coefficient read from Block J14 of RATEFILE.

AGRFQ = regulated flow quality at the end of the previous upstream reach

FLOW = see Equation 50

The loadings are then added to the vector POLL (see Equation 54 below) which is used to accumulate the loadings input to the node. This procedure is repeated if the switch MIX2 indicates that there is a second upstream flow input to the node.

The program then checks MIX5 to see if there is any independent boundary flow input to the node. If there is, the flow is calculated from:

Equation 53: Independent flow input to the node

$$\text{FLOW} = \left(\frac{\text{AGRFLW}(\text{MIX5}) - \text{OLFLO}(\text{MIX5})}{\text{NTP}} \times \text{ITP} + \text{OLFLO}(\text{MIX5}) \right) \times \text{CMULT}$$

Where:

AGRFLW = regulated independent flow for the day

OLFLO = regulated independent flow for the previous day

ITP = time point of the day

NTP = number of time points in the day

$$\text{CMULT} = \frac{\text{ALMIXC}(\text{IJPT}, 5, 2)}{100}$$

ALMIXC = percentage of independent flow input to this node

Equation 53 is used to interpolate between today's flow and yesterday's flow to give values at each time point of the day. It is assumed that the flows occur at midnight on the end of a day. The day preceding the first day is arbitrarily assigned a flow the same as the first day's flow.

The calculated flow is added to the flow accumulator TFLOW. The loadings are added to the loading accumulator POLL as follows:

Equation 54: Pollutant load attributable to independent flow input

$$\text{POLL(IQP)} = \text{POLL(IQP)} + \text{AGIFQ(ITP, IQP, MIX5)} \times \text{FLOW}$$

Where:

AGIFQ = independent flow quality at time point ITP

FLOW = see Equation 53

The program then checks MIX6 to see if there are any dependent local diffuse flows input to this node. If there is, the flow is calculated as shown in Equation 55.

Equation 55: Dependent flow input to the node

$$\text{FLOW} = \left(\frac{\text{AGDFLW(MIX6)} - \text{DOLFLO(MIX6)}}{\text{NTP}} \times \text{ITP} + \text{DOLFLO(MIX6)} \right) \times \text{CMULT}$$

Where:

AGDFLW = regulated dependent flow for the day

DOLFLO = regulated dependent flow for the previous day

ITP = time point of the day

NTP = number of time points in the day

$$\text{CMULT} = \frac{\text{ALMIXC(IJPT, 6, 2)}}{100}$$

ALMIXC = percentage of dependent flow input to this node

Equation 55 is used to interpolate between today's flow and yesterday's flow to give values at each time point of the day. It is assumed that the flows occur at midnight on the end of a day. The day preceding the first day is arbitrarily assigned a flow the same as the first day's flow.

The calculated flow is added to the flow accumulator TFLOW. The loadings are added to the loading accumulators POLL as follows:

Equation 56: Pollutant load attributable to dependent flow input

$$\text{POLL(IQP)} = \text{POLL(IQP)} + \text{AGDFQ(ITP, IQP, MIX6)} \times \text{FLOW}$$

Where:

AGDFQ = dependent flow quality at time point ITP

FLOW = see Equation 55

The program then checks MIX8 to see if there are any water withdrawals from the node. If there is, the flow is calculated as shown in Equation 57.

Equation 57: Water withdrawals from the node

$$\text{FLOW} = \text{AGWFLW(MIX8)} \times \frac{\text{ALMIXC(IJPT, 8, 2)}}{100}$$

Where:

AGWFLW = withdrawal flow

ALMIXC = percentage of the withdrawal flow assigned to the node

It should be noted that withdrawal flows have a negative value, thus the total flow TFLOW when calculated above decreases.

The pollutant load is calculated shown in Equation 58.

Equation 58: Pollutant load attributable to water withdrawal

$$\text{POLL(IQP)} = \text{POLL(IQP)} + \text{WRFQ} \times \text{FLOW}$$

Where:

WRFQ = pollutant concentration prior to water withdrawal

FLOW = see Equation 57

The program then checks MIX9 to see if there are any storm flow inputs to the node. If there is, the flow is calculated as follows:

Equation 59: Storm flow input to the node

$$\text{FLOW} = \text{STOFLW(MIX9, ITP)} \times \frac{\text{ALMIXC(IJPT, 9, 2)}}{100}$$

Where:

STOFLO = storm input flow

ALMIXC = percentage of the storm input assigned to the node

The pollutant load is calculated using Equation 60.

Equation 60: Pollutant load attributable to storm flow input

$$\text{POLL(IQP)} = \text{POLL(IQP)} + \text{STOFQ(MIX9, IQP, ITP)} \times \text{FLOW}$$

Where:

STOFQ = storm flow quality at time point ITP

FLOW = see Equation 59

The program then checks MIX7 to see if there is a wastewater treatment plant input to the node. If there is, the flow is calculated as shown in Equation 61.

Equation 61: Wastewater treatment plant input to the node

$$\text{FLOW} = \text{AGTFLW(ITP, MIX7)} \times \frac{\text{ALMIXC(IJPT, 7, 2)}}{100}$$

Where:

AGTFLW = wastewater treatment plant flow for time point ITP

ALMIXC = percentage of flow assigned to this node

The flow is added to the flow accumulator TFLOW. The loadings from the wastewater treatment plant are added to the loadings accumulators POLL as shown in Equation 62.

Equation 62: Pollutant load attributable to waste water treatment plant input

$$\text{POLL(IQP)} = \text{POLL(IQP)} + \text{AGTFQ(ITP, IQP, MIX2)} \times \text{FLOW}$$

Where:

AGTFQ = wastewater treatment plant flow quality for time point ITP

FLOW = see Equation 61

The loadings are then divided by the total flows (see Equation 63) to give parameter concentrations or qualities, and are assigned to the heads of either one or two downstream reaches depending on MIX3 and MIX4. The quality of the flow at the head of the reach at that time point could be calculated by interpolation of the qualities calculated in Equation 62. The quality at the end of the reach is then calculated based on the simulation equations using the quality at the head of the reach as a starting point.

Equation 63: Parameter concentration

$$\frac{\text{POLL(IQP)}}{\text{TFLOW}}$$

Thirty-six consecutive time points of data are stored for those variables required in the backtracking. When the next day is required, it is read into the place occupied by the first day. The subsequent day replaces the second day, and so on. The following discussion assumes 12 time points to the day. Five days of values are also stored at any one time for the rate coefficients. The data is read into arrays between INTAB and JTAB.

INTAB = 1 and JTAB = 12 for days 1, 4, 7, etc
 INTAB = 13 and JTAB = 24 for days 2, 5, 8, etc
 INTAB = 25 and JTAB = 36 for days 3, 6, 9, etc

Once the time point at which the plug left the head of the reach is determined, its quality can be determined by interpolation between the known qualities at the two time points around it. The quality at the head of the reach is found from Equation 64.

Equation 64: Quality at the head of the reach

$$\text{POLL(IQP)} = \frac{\text{DELTAT} \times \text{FLOW1} \times \text{AGRFQ(INO, IRCH, 1, IQP)}}{\text{DENOM}}$$

Where:

POLL(IQP) = quality at time when plug left head of reach

DELTAT = time difference between time when plug left head of reach and next time step, in seconds

FLOW1 = average channel flow at the head of the reach at time point before plug left head of reach

AGRFQ(KNO, IRCH, 1, IQP) = quality of flow associated with FLOW1

AGRFQ(INO, IRCH, 1, IQP) = quality of flow associated with FLOW2

DENOM = DELTAT × FLOW1 + (H - DELTAT) × FLOW2

H = time difference between two time points in seconds

The values of POLL(IQP) are then assigned as follows:

DOD = POLL(1)

BOD = POLL(2)

NOD = POLL(3)

The quality at all time points after the plug leaves the head of the reach, until it reaches the end of the reach (indicated by INDEX=0) is calculated using the following simulation equations:

Equation 65: Dissolved oxygen at the present time point

$$\text{DOD} = \text{DOD} \times \text{TERM1} + \text{BOD} \times \text{TERM2} + \text{NOD} \times \text{TERM3} \\ + \text{ALPH}(\text{NPER}) \times \text{TERM4} + \text{TERM5}$$

Equation 66: Biological oxygen demand at the present time point

$$\text{BOD} = \text{COD} \times \text{EXD}$$

Equation 67: Nitrogenous oxygen demand at the present time point

$$\text{NOD} = \text{NOD} \times \text{EXN}$$

Where:

DOD = dissolved oxygen. If the term is on the left side of the equation, it represents the DOD at the present time point. If the term is on the right side of the equation, it represents the DOD at the previous time point.

BOD = biological oxygen demand. If the term is on the left side of the equation, it represents the BOD at the present time point. If the term is on the right side of the equation, it represents the BOD at the previous time point.

NOD = nitrogenous oxygen demand. If the term is on the left side of the equation, it represents the NOD at the present time point. If the term is on the right side of the equation, it represents the NOD at the previous time point.

$$\text{EXD} = e^{(-\text{AGKR}(\text{ID}, \text{IRCH}) \times \text{TFAC})}$$

$$\text{EXN} = e^{(-\text{AGKN}(\text{ID}, \text{IRCH}) \times \text{TFAC})}$$

$$\text{TERM1} = e^{(-\text{AGK2}(\text{ID}, \text{IRCH}) \times \text{TFAC})}$$

$$\text{TERM2} = \frac{\text{AGKD}(\text{ID}, \text{IRCH})}{\text{AFK2}(\text{ID}, \text{IRCH}) - \text{AGKR}(\text{ID}, \text{IRCH})} \times (\text{TERM1} - \text{EXD})$$

$$\text{TERM3} = \frac{\text{AGKN}(\text{ID}, \text{IRCH})}{\text{AFK2}(\text{ID}, \text{IRCH}) - \text{AGKN}(\text{ID}, \text{IRCH})} \times (\text{TERM1} - \text{EXD})$$

$$\text{TERM4} = \frac{\text{AGPH}(\text{ID}, \text{IRCH})}{\text{AFK2}(\text{ID}, \text{IRCH})} \times (1 - \text{TERM1})$$

$$\text{TERM5} = \frac{\text{AGCS}(\text{ID}, \text{IRCH}) - \text{AGRES}(\text{ID}, \text{IRCH}) + \text{AGSLU}(\text{ID}, \text{IRCH})}{\text{AFK2}(\text{ID}, \text{IRCH})} \\ \times (1 - \text{TERM1})$$

AGKR = K_R for BOD removal (d^{-1})

AGKN = K_N for NOD decay (d^{-1})

AGK2 = K_2 for atmospheric reaeration (d^{-1})

AGKD = K_D for BOD deoxygenation (d^{-1})

AGPH = aquatic plant photosynthesis rate from ECOL subroutine (mg/L/d)

AGCS = dissolved oxygen saturation concentration at current water temperature (mg/L)

AGRES = aquatic plant respiration rate from ECOL subroutine (mg/L/d)

AGSLU = SOD rate (mg/L/d)

ID = the time step corresponding to when the plug left the head of the reach

IRCH = the reach number under consideration

TFAC = time difference between the time when the plug left the head of the reach and the next time step, equivalent to DELTAT above but expressed in days

The last values of DOD, BOD, and NOD represent the quality at the end of the reach and are stored in the appropriate positions in AGRFQ.

6.19 ECOL

6.19.1 Type

Subroutine

6.19.2 Purpose

Simulates the seasonal and daily growth of three aquatic plant types, specifically *Cladophora glomerata*, *Potamogeton pectinatus*, and *Myriophyllum spicatum*.

6.19.3 Method

The mass of each aquatic plant species is tracked separately according to the following equation:

Equation 68: Plant biomass

$$B(j, TS + 1) = B(j, TS) + PROD_j - RES_j - WASH_j$$

Where:

B = the mass of each aquatic plant species. The subscript j indicates one of three species of aquatic plants. In the ECOL equations, j is replaced with one of three letters corresponding to one of the species:

- C – Cladophora
- P – Potamogeton
- E – Myriophyllum

TS = the current time step

PROD = production or growth over the previous timestep (g/m^2), refer to Section 3.4 for additional detail on biomass response to temperature, PAR, nutrients, etc.

RES = respiration over the previous timestep (g/m^2), refer to Section 3.4 for additional detail on biomass response to temperature, PAR, nutrients, etc.

WASH = biomass washoff over the previous timestep (g/m^2)

The washoff term in Equation 68 represents loss of biomass by fragmentation or other physical removal of the biomass from the reach. The washoff term is initially set to a constant value specified in Block Q26 of MAINFILE. The washoff term is handled slightly differently, depending on the plant species, as described in Table 4. For *Cladophora*, washoff is assumed to accelerate when the water temperature increases beyond a specific threshold, which is specified in Block Q27 of MAINFILE. *Potamogeton* washoff is assumed to accelerate at temperatures below a particular threshold value, which is also specified in Block Q27 of MAINFILE. The washoff factor for *Myriophyllum* is assumed to be constant and independent of water temperature.

Table 4: Washout factor

Aquatic Plant Species	Initial value	Temperature Dependence
<i>Cladophora</i>	$WASH_C = 0.0005 * B_C$	IF (T > WASHOFF_T _C) THEN... $WASH_C = \left(\frac{(T - WASHOFF_T_C)}{WASHOFF_T_C} \right)^2 + 0.0005) * B_C$
<i>Potamogeton</i>	$WASH_P = 0.0005 * B_P$	IF (T < WASHOFF_T _P) THEN... $WASH_P = (0.03 - 0.002 * T) * B_P$
<i>Myriophyllum</i>	$WASH_E = 0.0005 * B_E$	Not temperature dependent, $WASH_E = 0.0005 * B_E$

The effects of plant biomass on dissolved oxygen (i.e. PlantP and PlantR) are handled by the ECOL model, as described in Section 3.4 and shown in Equation 69 and Equation 70. **Error! Reference source not found. Error! Reference source not found.**

Equation 69: Effect of plant biomass on DO (photosynthesis)

$$O2P = TPROD \times O2ASS$$

Where:

O2P = aquatic plant photosynthesis rate (g/m²)

TPROD = total production or growth of aquatic plants over the previous timestep (g/m²), refer to Section 3.4 for additional detail on biomass response to temperature, PAR, nutrients, etc.

O2ASS = oxygen assimilation ratio used for photosynthesis and respiration (g DO produced or consumed per g of biomass)

Equation 70: Effect of plant biomass on DO (respiration)

$$O2UP = TRES \times O2ASS$$

Where:

O2UP = aquatic plant oxygen uptake or respiration rate (g/m²)

TRES = total respiration of aquatic plants over the previous timestep (g/m²), refer to Section 3.4 for additional detail on biomass response to temperature, PAR, nutrients, etc.

When ECOL is called from GRSM, intermediate data is written to a data file in CSV format (XXXX_1 e.csv). The first line of the file describes the order in which the data is listed. Refer to Appendix D of the GRSM User Manual for a description of the data included in this file.

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