

**A Review and Comparison of Dissolved Oxygen Models  
Appropriate for the Grand River Watershed**

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## EXECUTIVE SUMMARY

The Grand River, Ontario, experiences periodic dissolved oxygen depletion as a result of eutrophic conditions that cause excessive nuisance attached algae and macrophyte growth, especially in its middle reaches. The Grand River Conservation Authority has for many years used a purpose-built dynamic continuous simulation model, the Grand River Simulation Model (GRSM), to study the impacts of alternative water management strategies on nutrient and dissolved oxygen concentrations in the river. As part of ongoing evaluation of GRSM's utility in the current water management context, GRCA commissioned a review of four widely used models appropriate for dissolved oxygen simulation in the Grand River. These were QUAL2K, WASP7, HSPF/BASINS (all of which are free, open-source tools), and MIKE11 (also available with a GIS interface, as MIKE-BASIN), a proprietary model developed by DHI. These four models were evaluated against a range of criteria, and compared with GRSM.

The strong seasonal and diurnal influences on the river indicate the need for a dynamic, continuous model. In particular, it is necessary to predict changes in dissolved oxygen in the Grand River in response to changes in loadings from municipal wastewater treatment plants and non-point sources. Modeling of dissolved oxygen in the Grand River is required to determine:

- the possible impacts of upgrades to a single wastewater treatment plant (e.g. as part of an application for Certificate of Approval);
- the possible impacts of changing loads from several wastewater treatment plants resulting from proposed upgrades, population growth, etc. or changing loads from non-point sources related to implementing BMPs (e.g. as part of a watershed-scale assessment)

The results of this evaluation demonstrate that no other model currently available simulates species-specific plant/algae growth dynamics in the way that GRSM does. In addition, no other model employs the detailed light limitation kinetics that were incorporated into GRSM in the late 1990s; most instead use very simplistic relationships that are likely to be much less accurate than those in GRSM. On the other hand, some models employ much more detailed heat budget calculations (e.g., HSPF) or sediment-water interactions (MIKE11), and several incorporate much shorter reach lengths than does GRSM. WASP7 offers good 3-dimensional simulation capability, and is therefore well suited to the modeling of lakes and reservoirs, but that feature is less important for a river like the Grand, which is generally well-mixed through the growing season. Furthermore, while WASP has a powerful hydrodynamic model, it is limited in its ability to simulate

photosynthesis/respiration, nutrient dynamics, and dissolved oxygen accurately, and (like MIKE11) can become unstable in simulation of water quality constituents, especially at low concentrations.

QUAL2K, WASP7, and HSPF in particular are highly complex tools with extensive user training requirements. This review demonstrated that the features of these models are not sufficiently better than those in GRSM to justify a change from the existing approach. Indeed, greater model complexity does not confer greater predictive accuracy. In fact, a highly complex model like WASP7 or HSPF may be much less accurate because of the need to calibrate a very large number of state variables, and accurately reflect hundreds of thousands of state variable interactions across many model components.

Cost is also an important consideration. MIKE11, a very well-supported and easy to use tool, has the disadvantage of very high cost, typically in the \$25,000 range even for a very basic configuration. A MIKE11 configuration appropriate for the Grand, especially if coupled with the GIS interface (MIKE-BASIN) would more likely cost much more; cost alone may therefore preclude use of this proprietary tool.

We can therefore conclude that while individual models may simulate certain components more effectively than GRSM (for example, MIKE11's sediment-water dynamics, or HSPF's land-water linkage), GRSM is a highly effective, well understood, and well tested model appropriate for dissolved oxygen modeling in the Grand.

Over the longer term, GRCA should however review individual model components in the models reviewed here, and others, to determine areas where GRSM could be updated or strengthened for future applications. In particular, it will be important to reflect recent hydrogeologic and geomorphology field data in the model and improvements to low-flow hydraulic modeling capability. The challenge here will be to collate the considerable quantity of recent field data and bring it to bear on GRSM, to determine which changes may be most appropriate. For example, this review has shown that GRSM's simulation of sediment-water interactions may require strengthening, especially with respect to nutrient dynamics. These improvements may be especially important in the Central/Middle Grand reaches, where the urbanized core and associated effluent discharges has resulted in a more organic bed sediment load, with higher nutrient concentrations, than elsewhere in the basin. Similarly, GRSM does not currently simulate phytoplankton growth or nutrient dynamics, but those components may be important in certain reaches. Finally, GRSM is currently configured around very long reaches, originally established to conform to field data collection stations. These reach lengths (and reach configuration) may no longer be appropriate, especially in light of significant improvements in understanding of river hydraulic, chemical, and biological phenomena, and

extensive land use changes that have occurred in the watershed in the 30 years since the model was first developed.

**RECOMMENDATION 1:** GRCA should collate and review available data on the Grand River, and use it, possibly in a workshop setting with knowledgeable participants, to update the conceptual representation of the river. The revised conceptual model should reflect the considerable land use, geomorphic, and water quality changes that have occurred in the river over the last 30 years.

**RECOMMENDATION 2:** GRCA should use the revised conceptual model to review GRSM's current capabilities, especially with respect to reach length, reach configuration, sediment-water interactions, and detailed simulation of nutrient species (e.g., nitrate/nitrite; orthophosphorus, etc.), to determine where changes would be appropriate.

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# 1. INTRODUCTION: WATER QUALITY IN THE GRAND RIVER BASIN

The Grand River watershed encompasses some of the most productive agricultural land in Southwestern Ontario, and some of the fastest growing urban areas in Canada. The tensions between these two uses have become particularly acute in the last decade, and development pressure now places unprecedented demands on the area's pollution control infrastructure.

The river itself is an important cultural, aesthetic and recreational resource. In 1994, it was recognized as a Canadian Heritage River, because of its historical importance in regional transportation and community economic development.

In the late 1970s, in response to flooding and water quality impairment issues that had plagued the Grand for many years, the Grand River Conservation Authority, in partnership with the Ontario Ministry of the Environment, established a Grand River Basin Water Management Study. That initiative involved a comprehensive examination of river geomorphology, hydraulics, and water quality, and concluded in 1982 with a number of recommendations aimed at reducing flood frequency and improving water quality. Among these were proposals to enhance wastewater treatment at area sewage treatment plants. A key component of this analysis was the development and application of a water quality model for the river, the Grand River Simulation Model, a dynamic, continuous model focusing on nutrient dynamics, dissolved oxygen concentrations, and nuisance aquatic plant and algae growth.

In the years since the study concluded, GRCA has undertaken several reviews and revisions to GRSM, and continues to use it in the evaluation of water management options for the river. But over the years, the watershed itself has also changed dramatically, with rapid population growth and associated urbanization. Channel morphology has altered over time, pollutant sources have declined in volume and quality, and fisheries are improving in diversity and population health. Yet water quality problems continue to challenge the river, and remain a focus of GRCA's modeling efforts. Much of the data now available comes from the Provincial Water Quality Monitoring Network (PWQMN), which tracks the concentrations of nutrients, suspended sediment, metals, and major ions at 36 long-term monitoring sites in the basin. A variety of other water quality, geomorphic, hydrologic, and biological data are collected by GRCA and other partners. The following summary of river water quality is drawn largely from Cooke (2006).

## **Watershed Characteristics**

The Grand River watershed occupies a land area of 6,965km<sup>2</sup> in southern Ontario, much of it rich agricultural land (76%) and forested areas (17%), with urban areas (5%) located mainly in the central portion of the watershed.

In addition to the main stem of the Grand, the river has eight major tributaries that carry flows and associated pollutants: the Speed/Eramosa Rivers, Fairchild Creek, Boston/McKenzie Creek, Whiteman's Creek, Nith River, Canagagigue Creek, Conestogo River, and Irvine Creek, in addition to many other smaller tributaries. In 2008, almost 1 million people live in the Grand River basin, with about 80% of that population served by 28 sewage treatment plants; the remainder are serviced by on-site wastewater treatment systems (e.g., septic systems). Sewage treatment technology varies across the basin, ranging from traditional secondary treatment to advanced tertiary treatment (including advanced nitrogen removal), depending on location.

The river can be divided into three distinct areas based on geology and land use. The **Upper Grand**, including the Upper Conestogo River, is characterized by extensive agricultural areas on a till plain. The surficial geology of this region, combined with the agricultural activity, contribute to the significant runoff that enters the river there. Two of the river's four major reservoirs, Belwood and Conestogo, capture most of that runoff, providing flood protection during high flows and low-flow augmentation during low flow periods. Generally speaking, water quality in the Upper Grand is good to excellent.

In the centre of the basin lie the major areas of urban growth. The **Central Grand** region is characterized by highly permeable sands and gravels, part of the Waterloo and Paris-Galt moraine systems, and significant groundwater reserves, which are used to supply drinking water to area residents and industries. Where groundwater discharges into the river, it creates coldwater or coolwater conditions suitable for sport fish species. The Central Grand is characterized by water quality that is fair at best, and often marginal to poor.

South of Paris, the Lower Grand traverses a clay plain, also supporting extensive agriculture and, like the Upper Grand, also generating significant runoff. South of Dunnville, the Grand discharges into Lake Erie. Water quality in the Lower Grand tends to be marginal, but generally not as poor as in highly urbanized sections of the Central Grand.

The following paragraphs describe observed water quality patterns for specific constituents.

**Total phosphorus** concentrations exceed Provincial Water Quality Objectives throughout the basin, with few exceptions: Irvine Creek in the Upper Grand; the Speed/Eramosa River in the Central Grand; and Whiteman's Creek in the Lower Grand. Levels range from a low of about 0.005 mg/L in the Eramosa River to a high of 0.822 mg/L in Canagagigue Creek. Every sampling station showed some exceedance of the PWQO values. Values tend to be highest in Canagagigue Creek and the Nith River, and highest in the spring, presumably because of high runoff from agricultural lands. While the overall trend is toward increasing phosphorus concentrations from upstream to downstream, there are exceptions,

especially between dams, for example between the Shand Dam and West Montrose, where levels decrease significantly.

Unlike phosphorus, which appears to arise mainly from nonpoint sources in agricultural portions of the basin, nitrogen species tend to be highest in the Central Grand, although upper Canagagigue Creek also experiences high levels of ammonia, possibly from manure management activities. Exceedances of PWQO values for **ammonia** are common through the Central Grand, although the timing of exceedances varies with location in the basin. **Nitrate** levels are high throughout the basin, except for the headwaters of the Grand and Speed, and in lower Fairchild's Creek and MacKenzie Creek. As with ammonia, while there is generally a trend toward increasing nitrate concentrations from upstream to downstream, there are "hot spots" throughout the basin, for example between the Shand Dam and West Montrose, that suggest specific sources or phenomena affecting those reaches.

**Nitrite** concentrations vary widely through the basin, from undetectable levels to concentrations as high as 0.840 mg/L, 14 times the Canadian Environmental Quality Guideline of 0.060 mg/L. Concentrations tend to be highest in the Central Grand.

**Total kjeldahl nitrogen (TKN)**, the sum of total organic nitrogen plus total ammonia, is a good measure of organic pollution. TKN levels also vary widely throughout the basin, with low values in the lower Nith and Eramosa Rivers, and higher values downstream of sewage treatment plants.

**Total suspended solids** concentrations are relatively constant in the Upper Grand down to Glen Morris, but increase significantly downstream of Brantford and again between York and Dunnville. Portions of the lower Speed River also show elevated solids concentrations.

**Dissolved oxygen and temperature** fluctuate widely in response to sunlight and (in the case of dissolved oxygen) photosynthesis. In some locations, especially in the Central Grand, the normal diurnal oxygen fluctuation is more pronounced than in others, suggesting that aquatic organisms are experiencing a wide range of dissolved oxygen conditions, with associated physiological stress. In the Central Grand, aquatic macrophytes and attached algae dominate the system, although this is less true in other parts of the basin, especially in the Lower Grand where planktonic algae and sediment oxygen demand may be a more significant influence on dissolved oxygen.

These brief comments illustrate the complex interplay between geomorphology, land use, point sources such as sewage treatment plants, and nonpoint sources such as agricultural and urban runoff, in the Grand River Basin. While this report seeks to investigate models appropriate for dissolved oxygen simulation in the

Grand, it is clear that an appropriate model must also incorporate consideration of nutrient dynamics (which can affect photosynthesis and therefore dissolved oxygen), suspended solids (which can reduce photosynthetically available light), and temperature (an important consideration in the simulation of parameters like oxygen and ammonia). It is also clear that the timing of PWQO exceedances varies widely depending on basin location and water quality parameter, so it is not possible to say, for example, that ammonia is always highest in the summer months, at a particular station.

The complexity of this system therefore demands careful thought in the choice and application of a water quality model. The following sections discuss these issues in more detail.

## 2. SELECTING AN APPROPRIATE WATER QUALITY MODEL

A model, simply put, is a representation of a natural or artificial system. Models may be of many types, including physical (scale) models, statistical models that represent mathematical (but not necessarily mechanistic) relationships between variables, and mechanistic models that attempt to approximate physical, chemical, or biological phenomena using mathematical equations. Models allow the user to explore system mechanics and predict outcomes before costly infrastructure is built. In water resources management, models are particularly useful when:

- Pollutant sources are numerous and/or highly variable in quantity and quality, making it difficult to predict their behavior in space and/or time using simple computational tools;
- The dynamics of the receiving water are complex, for instance, in a large river or lake, requiring assessment of impacts in two or three dimensions as well as over time;
- There is a need to optimize the behavior of a complex system such as a storm or sanitary sewer system, or a sewage treatment plant, where several unit processes or steps may be involved between influent and effluent;
- There is a regulatory requirement present, for example to produce accurate loading or concentration estimates for specific pollutants.

The mid- to late 1970s and early 1980s saw the development of dozens, perhaps hundreds, of sophisticated computer simulation models for use in water management. Many of these were based on the Stanford Watershed Model, developed by Crawford and Linsley (1966) from Crawford's doctoral thesis research (Crawford 1962)<sup>1</sup>. These models were costly to develop and costly to run, requiring the use of minutes or hours of processing time on a mainframe computer. Through the later 1980s some of these models were converted for use on desktop microcomputers, although most remained Fortran-based and, to a large extent, inconsistent with newer software technology. Many models were developed for a given task and/or geographic location and may have limited application in other systems.

Models are not always used singly. It is not uncommon to find several models, perhaps of different types, linked together in the modeling process.

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<sup>1</sup> The Stanford Watershed Model is the basis for the current HSPF (Hydrologic Simulation Program-Fortran), which is the dynamic computational mechanism underlying US EPA's Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) modeling system.

Clearly, the challenges involved in building, calibrating, and validating a model increase substantially when more than one model is in use. Nevertheless, use of linked models allows the analyst to tailor simulation tools to the particular task at hand. Computer simulation models are also routinely linked to GIS data nowadays, for a wide variety of applications. Digital elevation models (DEMs) are a digital representation of terrain stored in GIS form. They are useful in developing geographically precise models of flow patterns, for example for erosion potential.

There are now hundreds, if not thousands, of models available, covering virtually every aspect of water resources management. Simulation models may be of several types. These include:

- **Stochastic** (i.e., outputs are determined by random or probabilistic inputs) vs. **deterministic** (i.e., outputs are determined by specific user-input values) models
- **Steady-state** (i.e., single condition) vs. **dynamic** (i.e., varying outputs in response to varying inputs, sometimes on a very short time step)
- **Continuous** (i.e., employing continuously recalculated differential equations to change the system over time) vs. **discrete** (i.e., using step changes to jump the model condition from one state to the next)

Water managers are therefore faced with a bewildering array of choices. Conventional wisdom holds that the best choice is the simplest model that will adequately represent key processes in the area of concern. Generally speaking, model choice begins with a question or problem of interest. Examples of such questions include:

- What land-based pollutant loading reductions would be necessary to achieve a specific instream concentration? (or, alternatively, how much instream water quality improvement will a certain level of loading reduction “buy”?)
- What are the range of flow or water quality conditions that could reasonably be expected in the river under extreme and typical precipitation, temperature, or loading scenarios?
- Under what flow and loading conditions will critical pollutant threshold concentrations be exceeded?

For problems involving estimation of pollutant loadings and/or concentration, the goal is to close a mass balance for the system using known or estimated inputs of water and pollutant mass, while moving both water and pollutant through the river system.

The general equation for mass balance in any given volume of water or sediment, or in any area of land (for plants and animals) is:

$$\begin{aligned} \text{Rate of mass increase} &= \text{rate of mass entering} - \text{rate of mass leaving} \\ &+ \text{rate of mass created internally} - \text{rate of mass lost internally} \end{aligned}$$

with each term expressed in units of mass per unit time.

Transport processes are of two kinds, (1) advection, or transport of material by the flow of water into or out of a control volume, and (2) diffusion, or transport of the constituent by turbulence in the water. Advection may be estimated in one, two or three dimensions; diffusion is almost always a three-dimensional calculation, and may be neglected in systems where transport is dominated by a single dimension (e.g., a well-mixed river system where downstream flow is the most important transport mechanism).

Transformation processes, i.e., those that change the form or mass of a pollutant in a given model compartment, may be of many types. For dissolved oxygen, the most important target parameter in the Grand River system, key transformation processes include BOD oxidation (consumption of available oxygen by oxygen-demanding compounds, a first-order process in which oxidation rate is proportional to the amount of BOD present); sediment oxygen demand, which may be particularly important in systems with high loadings of organic matter, for instance downstream of sewage treatment plant discharges; surface reaeration, which occurs when ambient DO is below saturation and oxygen from the atmosphere enters the water surface (flux proportional to the oxygen deficit); and photosynthesis and respiration. The latter two processes are highly species-specific and may be affected by optimal and typical growth rates, "luxury" uptake of excess nutrients for storage in the plant, plant crowding, tissue ageing, death, and washout. Other parameters that may be of interest, depending on the system and question, include sediment transport and settling; bacterial growth and die-off; adsorption to and desorption from solids; volatilization; and photolysis.

Once the question or problem is clear, the analyst should proceed to a more detailed list of questions (adapted from James 1992):

### **1. What processes must be modeled?**

- What flow, water quality or other parameters will be used to make decisions; i.e., what parameters must be modeled?
  - What kinds of information will be useful in making decisions (e.g., load reductions from land sources? in-stream water quality? average contributions from a given source, etc.)?
  - Identify all the hydraulically-, hydrologically-, chemically- and biologically-significant elements and processes in the basin so that the model(s) selected can be shown to include all relevant processes; develop study objectives that relate objective functions to design options
  - Identify important performance criteria so that minimum modeling effort can be used to select the best option.

## **2. What time period(s) must be modeled?**

- Over what time period (days, hours, seasons, years) would predictions be helpful? In other words, is it enough to know that average annual phosphorus will decline by 0.2 ppm under a given management strategy? Or is it necessary to know the maximum and minimum phosphorus concentrations that are likely to occur during a particular rainstorm?
- Is it enough to simulate a “snapshot” condition? Or is it necessary to simulate realistic variability, including consecutive events or cumulative impacts, in system conditions?

## **3. What spatial dimensions must be modeled?**

- Do the performance criteria need to be evaluated in one, two, or three dimensions?
- Can the water body be considered “well mixed” over some or all of its range?

## **4. What tools are available?**

- What computer models or other predictive tools are available for the parameters that must be evaluated? Do available models predict the variable(s) of interest in a realistic fashion? (i.e., are the algorithms upon which the model is based sufficiently realistic to represent the system, and its response to management intervention, accurately?)
- What are the input data requirements for each model that could be used?

## **5. What data are available to drive the model?**

- What data have already been collected for the watershed system of interest? Is the existing data consistent with the needs of available models to produce a reasonable prediction? Does additional data need to be collected?
- What hardware/software does each model require? Is the required system available? Is sufficient memory, hard disk space, etc. available? Is an experienced user available to operate the model or to advise a novice user?

## **6. What predictive error is expected? Acceptable?**

- How accurate do model predictions need to be? What level of error is acceptable?

The answers to these questions will guide the selection of an appropriate model or set of models. There is also a need to balance many competing

factors in selecting a model, e.g., choosing a less complex model that can be set up with existing data vs. collecting additional field data to set up a more complex model.

A model is only useful as a planning tool if the user understands how, and how well, it represents the natural world. To gain this understanding, the analyst must go through four steps:

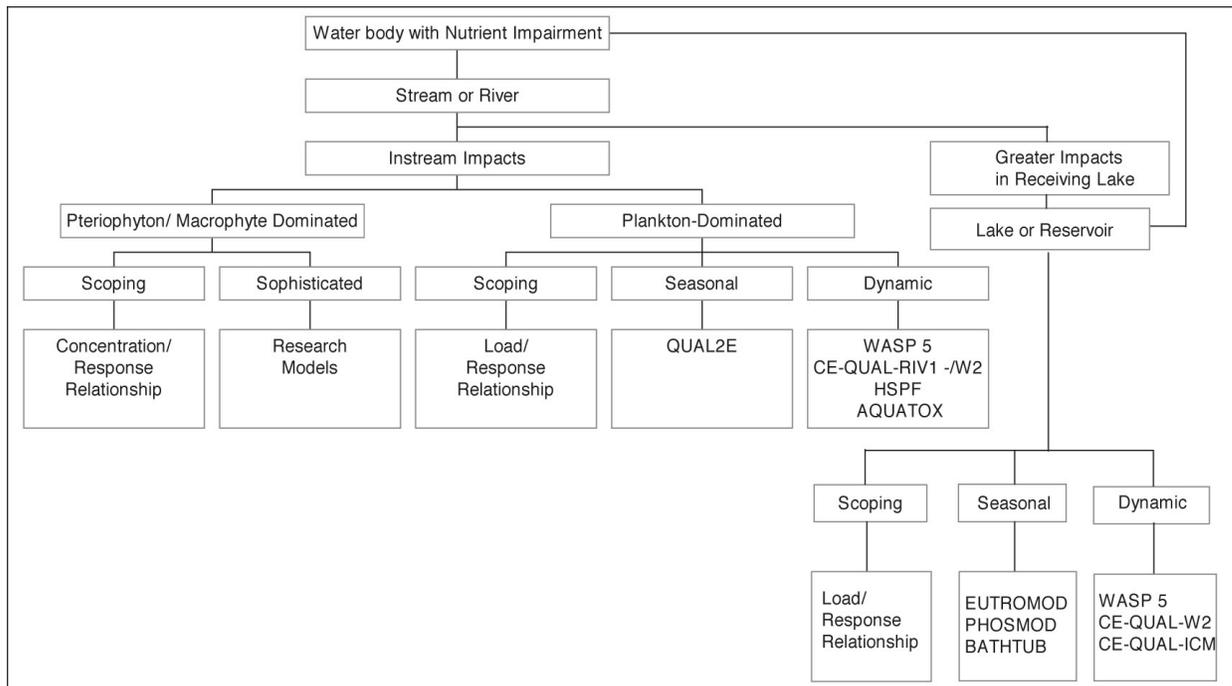
- *Model verification*—Determining whether the algorithms used by the model are appropriate for the system, or should be replaced with others more suitable. Verification also tests whether the algorithms have been correctly used and are free from bugs or other errors.
- *Model calibration*—Tuning the model so that it simulates a set of observed conditions with a high degree of accuracy.
- *Model validation*—Seeing how well the tuned model predicts a different data set, without changing any input variables or rate kinetics.
- *Sensitivity analysis*—To determine which input variables most influence model output and must therefore be chosen with great care.

It should be clear from this discussion that, in general, there is no single right answer as to which river water quality model is best. Rather, the analyst must choose from a wide (and growing) variety of models of all kinds and complexities. McIntyre (2004) makes the point that model complexity, especially the number of modeled variables and the spatial refinement of models, has been increasing exponentially since the 1970s, in response to improved computing power and better understanding of the physical, chemical and biological processes that drive water quality change. Modellers have increasingly realized that water quality cannot easily be explained or predicted on the basis of a handful of variables, as might have been contemplated 50 years ago. And as the number of modeled state variables and the number of spatial compartments in a given model increase, so do the number of interactive components. McIntyre (2004) estimates that while the number of state variables modeled in the 1960s was probably less than 10, it now is over 100 in most current models. Similarly, 40 to 50 years ago, the number of spatial compartments modeled was typically 10 to 20; now it may approach 500,000. As a result, the number of interactions between variables and compartments may approach 10 million in a given model!

Certainly, advances in computing technology do not rule out such a computational challenge, but as Reckhow (1994) points out, such immense model complexity demands vast quantities of data and a very high level of technical expertise and experienced with the preferred model—both increasingly scarce in a time of government “downsizing” and fiscal constraints. Perhaps in

response to these forces, the literature reflects what might be termed a backlash against highly discretized, mechanistic models, in favour of more lumped and conceptual approaches. Yet, as Irvine et al. (2005) point out, such simplified models may not be sufficient to meet policy requirements when pollutant sources are complex, unknown, or otherwise in dispute. Greater model complexity does not necessarily confer more predictive accuracy. Indeed, the reverse may be true, in that it is vastly more difficult to calibrate (and diagnose calibration problems) a model with 100 state variables than one with 10.

US EPA (1999) provides a helpful diagram illustrating the main choices to be made in model selection. The diagram demonstrates that different models are useful in different contexts, and that “research models” may be required for the simulation of specialized processes or constituents. The Grand River Conservation Authority’s Grand River Simulation Model (GRSM) is a specialized model designed to simulate macrophyte growth and associated nutrient dynamics in a macrophyte-dominated system, and therefore would be categorized as a “research model” in the following scheme.



**Figure 1. Decision tree for selecting an appropriate model technique (US EPA 1999)**

### 3. MODELLING DISSOLVED OXYGEN PROCESSES IN THE GRAND RIVER, ONTARIO

Water quality and streamflow models have many applications in the Grand River, including flood forecasting, sediment transport, assessment of water quality dynamics and associated assimilative capacity, and mixing zone evaluation.

As discussed in Section 1, the Grand is a macrophyte-dominated river, especially in its middle reaches, where nutrient enrichment causes excessive plant growth and exaggerated diurnal dissolved oxygen fluctuations. Remedial actions to address these issues include land-based practices such as bank protection, buffer strips and conservation tillage, designed to control nonpoint sources of nutrients; point source controls, such as advanced treatment of sewage treatment plant effluents; and instream measures, such as channel modification and nuisance plant harvesting. Some of these sources (e.g., sewage treatment plant effluents) are relatively constant in time, while others (e.g., agricultural and urban runoff) are strongly dependent on rainfall and (because of the implications of saturated soils for runoff) on pre-existing soil moisture conditions. It is therefore important to simulate real or realistic sequences of rainfall and dry weather conditions. Simulation of a single rainfall event could lead to serious predictive error, for example in the case of several consecutive large storms. Simulation of just one of these events would assume a relatively low level of soil saturation, and consequently lower runoff, than would likely be the case with saturated soils. Yet such conditions are increasingly common in recent years and cannot be neglected, given the infrastructure cost and water quality implications of an inaccurate prediction.

Water managers therefore require a diverse toolbox, including land-based pollutant loading models; hydrodynamic models (for flood forecasting); near-field multi-dimensional mixing zone models; and far-field one-dimensional models for the assessment of plant growth and nutrient/dissolved oxygen dynamics in reaches downstream of point sources such as sewage treatment plant effluents.

The purpose of the current review is to examine models for the prediction of far-field dissolved oxygen levels in the river. In particular, it is necessary to predict downstream changes in dissolved oxygen in the Grand River in response to changes in loadings from municipal wastewater treatment plants and non-point sources. (Near-field assessment of such changes would require more complex models, almost certainly including three-dimensional simulation, but such dimensional complexity is not necessary outside the mixing zone, where the river is usually well-mixed.)

Modeling of dissolved oxygen in the Grand River is required to determine:

- the possible downstream impacts (i.e., downstream of the mixing zone) of upgrades to a single wastewater treatment plant (e.g., as part of an

application for Certificate of Approval) (again, note that near-field assessment of impacts, within the mixing zone, would require different and probably three-dimensional modeling tools); and

- the possible cumulative downstream impacts of changing loads from several wastewater treatment plants resulting from proposed upgrades, population growth, etc. or changing loads from non-point sources related to implementing BMPs (e.g., as part of a watershed-scale assessment)

Dissolved oxygen is a critical consideration in the maintenance of healthy fisheries and the invertebrate community that supports the fishery.

In light of this requirement, we can propose answers to the questions posed in the previous section:

### **1. What processes must be modeled?**

- Streamflow must be modeled, but not necessarily in three dimensions (fish are mobile, so the main consideration is average dissolved oxygen within a river reach). Geomorphic and hydraulic relationships between flow, velocity and depth are critical for predicting advective transport and oxygen reaeration.
- Structures such as online weirs must be modeled because of their potential to increase reaeration
- Flow and concentration from point and non-point pollutant sources, especially of nutrients and oxygen-demanding substances
- Instream dissolved oxygen sources, sinks, and concentrations; these include carbonaceous and nitrogenous BOD oxidation, reaeration, sediment oxygen demand, photosynthesis, and respiration at minimum
- Sources, sinks and concentrations of nutrients (P, N) that are likely to have an indirect effect on dissolved oxygen levels as a result of aquatic plant and algae growth; these include uptake/release of nutrients by plants, nitrification, denitrification, volatilization, sediment exchange (e.g. settling or resuspension of TP).
- Instream dissolved oxygen concentration is the principal output (i.e., not P loadings from the land surface or kg/sq m of biomass)
- Plant growth dynamics, including washout, die-off, and growth kinetics, ideally tailored to the three species of concern in the Grand River: *Cladophora*, *Myriophyllum*, and *Potamogeton*.

### **2. What time period(s) must be modeled?**

- Ice-free period, especially the growing season for aquatic plants (approximately April to October)

- Daily average concentrations are not sufficient; minima must be modeled accurately; it is less critical to have accuracy in maxima
- Diurnal oxygen fluctuations are important so dynamic simulation is important, preferably on a two-hour time step or less
- It is not enough to simulate a single “snapshot” condition; a range of conditions (best to worst) must be simulated to give an indication of the frequency of low dissolved oxygen conditions. Cumulative impacts, for example of consecutive storms or warm temperatures coupled with low flows, may be important in determining DO levels, and so must be modeled

### **3. What spatial dimensions must be modeled?**

- Downstream of effluent discharge mixing zones, the river is shallow and narrow enough in most locations that two- or three-dimensional modeling is likely unnecessary and would significantly add to computational complexity; the river is well-mixed over most or all of its length for the ice-free period. Three-dimensional mixing zone modeling may be required for toxic contaminants such as ammonia or chlorine to determine zone of passage requirements but, as noted previously, this level of complexity is not considered necessary for dissolved oxygen, and is not further considered in this report.

### **4. What tools are available?**

- Few readily available water quality models simulate aquatic plant growth and associated nutrient and dissolved oxygen dynamics. The following models have been identified as appropriate for this purpose. The remainder of this report considers the attributes of each of these models in detail, including data requirements, hardware/software requirements, flexibility, rigour, and user experience.
- The models to be evaluated are:
  1. GRSM (Grand River Simulation Model)
  2. WASP
  3. QUAL2K
  4. HSPF
  5. MIKE11

### **5. What data are available to drive the model?**

- GRCA and the Ontario Ministry of the Environment have been collecting data on the Grand River system for decades. Data on all conventional parameters (DO, SS, and various forms of phosphorus and nitrogen) are available over a very long time period, although some parameters such as

nutrient data have not been collected at high frequency in most years. Extensive and reasonably continuous dissolved oxygen, water temperature, streamflow and meteorological data are available for several decades. This data can be used to characterize the model boundary conditions and calibrate/validate the model.

- Streamflows and flows from point- and nonpoint sources are either known or can be calculated. Meteorological data must be accurate and appropriate to the date and time of day; i.e., cannot be input on a random basis. A deterministic model is therefore preferred over a stochastic model, although some aspects of the model could be input on a probabilistic basis (e.g., storm frequency, size and duration).
- A large amount of hydraulic cross-sectional survey data has been collected and hydraulic models have been constructed to estimate flood stage in the Grand and Speed Rivers. Additional field survey data has been collected in priority areas to characterize low flow hydraulics and geomorphology.

## **6. What predictive error is expected? Acceptable?**

- DO minima must be simulated with a high degree of accuracy, preferably 20% error or less. Higher error rates could reduce the model's utility in simulating water conditions suitable for fish and other aquatic biota.

The next section reviews five major models in light of these considerations. Section 5 provides some discussion of the relative strengths and weaknesses of these models, and draws some conclusions about their suitability for modeling dissolved oxygen in the Grand River.

## 4. REVIEW OF KEY MODELS

This review will begin with an examination of QUAL2E/QUAL2K, which is considered by many authors to be the “industry standard” in assimilation capacity modeling.

### 4.1 QUAL2E and QUAL2K

While not the oldest water quality model available (certainly the Streeter-Phelps model predates it by at least 50 years, and the Stanford Watershed Model by at least a decade), QUAL2E has been called the most widely-used water quality model in the English-speaking world (Chapra, 1997, Rauch et al. 1998, Shanahan et al. 1998). It has been adapted and modified to address a huge range of problems and conditions in every part of the world, and remains a mainstay in the modeller’s toolbox.

QUAL2E grew out of the pioneering work of Streeter and Phelps (1925) on the mathematical representation of oxygen dynamics downstream of a source of organic matter. Its origins lie in work conducted by the Texas Water Development Board in the late 1960s, which was later adopted by US EPA. In the earliest days of its administration, US EPA recognized the need for a predictive tool that would allow the assessment of wasteload allocations for permitting purposes (Brown and Barnwell 1987). Its first form, QUAL1, was developed in the early 1970s and was required by EPA as the basis for developing new, more advanced basin-specific models (the QUAL2 series which followed several years later). QUAL1 incorporated nitrogen processes, especially nitrification (Rauch et al., 1998; Orlob, 1982). In the mid-1970s, phosphorus cycling and phytoplankton were added, creating a second generation of the model, QUAL2. QUAL2 had the capacity to simulate rivers under steady or unsteady flow. Phosphorus cycling and algae were added to this generation of the model (Brown and Barnwell, 1987). Several versions of QUAL2 were available, although QUAL2E (released in 1987) became the most popular and widely used, and was the basis on which a version with explicit uncertainty analysis (QUAL2E-UNCAS) was later developed (Brown and Barnwell, 1987).

QUAL2E was and remains a highly versatile one-dimensional, steady-state model with the capability to model major nutrient reactions, planktonic algae production, sediment and carbonaceous oxygen demand, reaeration, and resulting impacts on dissolved oxygen. Options within the model include heat- and mass-balance modeling for conservative constituents, coliform bacteria, and non-conservative substances such as radionuclides. The basic form of the model has not changed since 1987, although there have been recent modifications to the user interface. QUAL2E has been a component of EPA’s comprehensive modeling/data suite, BASINS, since the latter was introduced in the mid-1990s.

As a wasteload allocation assessment tool, QUAL2E examines only steady-state conditions for streamflow and discharge as specified in regulatory requirements. In these applications, dissolved oxygen is usually the main variable of concern, and the model has been widely used for that purpose, but it has also been applied in nonpoint source loading situations and for a range of other variables.

QUAL2E has in some applications been replaced by more complex, continuous models such as WASP and HSPF but the user expertise and data challenges of those more complex tools make QUAL2E a perennially popular choice for water quality simulation at steady state. QUAL2E should not in any sense be considered a “simple” model, however; more than 100 separate input variables are required and user experience is therefore important in model construction and calibration. Rauch et al. (1998) observed that the documentation for QUAL2E basically consists of a description of model formulation and input formats for a model user who is assumed to be experienced and knowledgeable. They observe that one weakness of QUAL2E is therefore that its ready availability encourages use by individuals who lack the necessary technical understanding to apply the model properly.

In early 2003, QUAL2E was replaced with a reformulated version of the model, QUAL2K, which is written in Visual Basic for Applications. This was a major improvement over QUAL2E, which was written in FORTRAN with a Windows interface. In March 2007, the most recent version of the QUAL model series was released, QUAL2K version 2.07 (Chapra et al. 2007). The documentation for QUAL2K is significantly improved over that for QUAL2E, but the model is no less complex than its predecessor.

The basic features of QUAL2K are as follows:

**Streamflow:**

- One dimensional. The channel is well-mixed vertically and laterally. Not designed for temporal variations in streamflow or for where major discharges fluctuate over diurnal or shorter time periods (Shanahan *et al.*, 1998)
- Steady state hydraulics. Flow is uniform within a reach or element, but may be varied from reach to reach or element to element. The model does not however capture the impact of diurnal flow variations or consecutive rainfall events. (Such simulation would require multiple runs using different flow input conditions. It would therefore be preferable and more realistic to use a continuous model with realistically varying flow inputs.)
- QUAL2K divides the river into reaches that can be of varying length. Individual reaches can then be divided into a series of equally-spaced “elements”. For each element, the model calculates a water balance, a heat balance, and a mass balance for pollutants (both advective and

dispersive transport mechanisms are considered in calculating mass balance).

- The model can accommodate multiple loadings and abstractions in any reach.
- Effects of weirs and waterfalls on reaeration are included.
- The model has the capacity to simulate a branching stream system; the stream is typically divided into “headwaters”, “reaches” and “junctions”
- Not appropriate for simulating highly variable wet weather sources such as nonpoint-source runoff from urban or agricultural areas

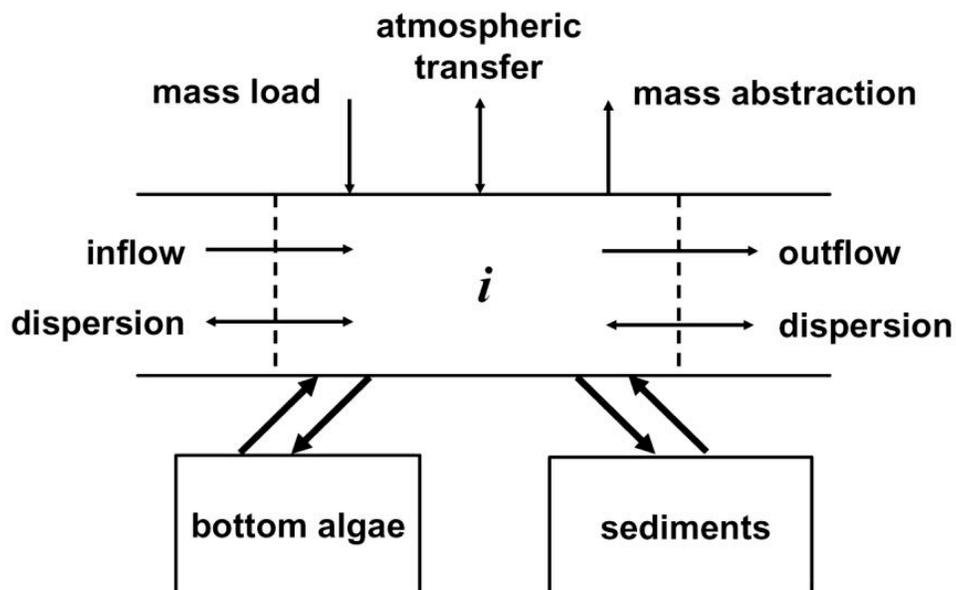
**Temperature:**

- Diurnal heat budget. The heat budget and temperature are simulated as a function of meteorology on a diurnal time scale.
- QUAL2K incorporates options allowing the modeler to simulate bulk heat transfer by advection, dispersion, extractions and pollution sources; long wave radiation to/from the atmosphere, sky and surrounding land; effective short-wave radiation from the sun; convection to and from the atmosphere; and evaporation losses and condensation gains

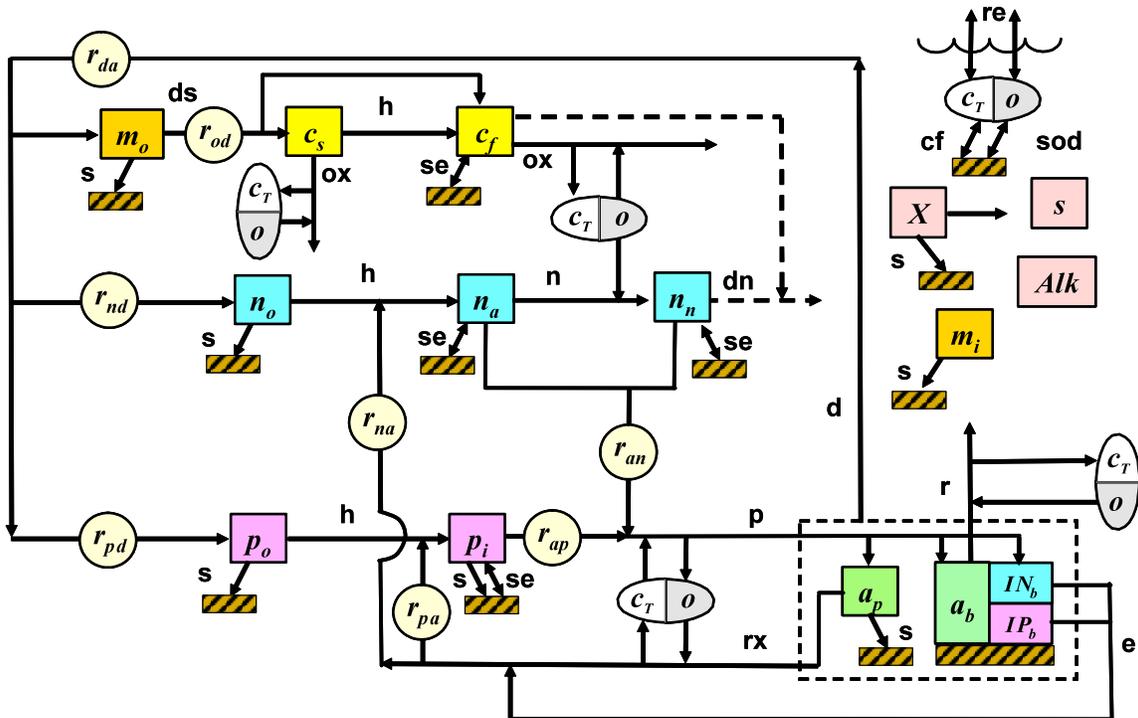
**Water Quality Constituents (General):**

- Diurnal water-quality kinetics: All water quality variables are simulated on a diurnal time scale with a user-defined timestep. That is, the model incorporates unsteady-state water quality computations (but steady-state flows).
- Simulates point and non-point heat inputs and mass loads and abstractions
- Simulates dissolved oxygen and associated water quality variables and incorporates degradation of organic matter, growth and respiration of algae, nitrification, hydrolysis of organic nitrogen and phosphorus, reaeration, sedimentation of algae, organic phosphorus and organic nitrogen, sediment uptake of oxygen, and sediment release of nitrogen and phosphorus
- QUAL2K : Sediment oxygen demand and nutrient flux are simulated explicitly as a function of settling particulate organic matter, reactions within sediments, and concentrations of soluble forms in overlying waters, rather than being prescribed as model inputs.
- Simulation of anoxia and denitrification, neither of which was incorporated in QUAL2E
- Simulates diurnal variation in plant growth, nutrient dynamics and dissolved oxygen where those parameters are related to photosynthesis. Not effective for simulating transient temperature or water quality conditions related to dynamics flow or pollutant source conditions (flow is steady-state).

- Does not partition organic matter into dissolved, suspended and sedimented fractions, and so does not allow changes in sediment quality to be simulated
- Sediment-water fluxes of dissolved oxygen and nutrients are not input but are simulated internally as a function of settling particulate organic matter, and sediment and water chemistry
- Capacity to simulate one non-conservative constituent and three conservative constituents
- Rauch et al. (1998) observe that it can be difficult to close mass balances in QUAL2E because of incomplete consideration of sediment-water exchange of heat and mass; this situation may be improved by the improved carbonaceous BOD speciation and sediment-water interactions in QUAL2K.
- Simulation of pH, based on alkalinity and inorganic carbon levels
- Simulation of a generic pathogen, whose removal from the system is determined on the basis of temperature, light and settling.



**Figure 2. Schematic illustrating mass balance calculations in QUAL2K** (Chapra et al. 2006). (Note that *i* = stream element "i")



**Figure 3. Model kinetics and mass transfer processes used in QUAL2K** (Source: Chapra et al. 2007). The state variables are defined in Chapra et al. (2007). Kinetic processes are dissolution (ds), hydrolysis (h), oxidation (ox), nitrification (n), denitrification (dn), photosynthesis (p), respiration (r), excretion (e), death (d), respiration/excretion (rx). Mass transfer processes are reaeration (re), settling (s), sediment oxygen demand (SOD), sediment exchange (se), and sediment inorganic carbon flux (cf).

### Nitrogen:

- QUAL2E models organic nitrogen, ammonia, nitrates, and nitrites explicitly (two-step nitrification) but neglects denitrification altogether (note however that QUAL2K incorporates denitrification; see below)
- QUAL2E also incorporates provisions for sedimentation and mineralization of N and release of N from sediments
- Nitrification rates can be corrected to take into account inhibition at low DO concentrations

### Phosphorus:

- Like many major models, QUAL2E represents the numerous and inter-related fractions of phosphorus by two mutually exclusive conceptual fractions, organic P and dissolved P
- Modeled like the nitrogen cycle but in a more simplistic fashion
- P balance incorporates settling and mineralization, regeneration from sediment, and uptake and respiration from planktonic algae

### ***Suspended Solids:***

- QUAL2E does not model bed or suspended sediment movement, although light extinction as a function of suspended sediment (and other variables) in QUAL2K

### ***Light:***

- Three light limitation factors available:
  - Half-saturation (Michaelis-Menten), where phytoplankton growth light limitation is calculated as an exponential function of depth
  - Smith's function, which modifies phytoplankton growth in response to the Smith parameter (the photosynthetically available radiation at which growth is 70.7% of maximum growth); and
  - Steele's equation, which modifies phytoplankton growth relative to an optimal incident light condition.
- Incorporates diurnal and climatic changes in radiation, and light extinction in the water column due to turbidity (detritus, inorganic solids) and self-shading
- Photosynthetically available light at the water surface is assumed to be a fixed fraction of solar radiation; below the surface, light extinction is calculated as a simple function of water depth, colour, inorganic suspended solids, particulate organic matter, and chlorophyll, all of which are input by the user as separate light extinction coefficients.

### ***Dissolved Oxygen***

- Like most other major models, the dissolved oxygen processes are based on the Streeter-Phelps model, but also include:
  - implicit calculation of reaeration rate (nine methods available)
  - temperature effects for both BOD decay and aeration
  - some representation of sediment oxygen demand
  - phytoplankton photosynthesis and respiration
- BOD (ultimate) is modeled as a first-order degradation process
- Carbonaceous sediment oxygen demand (CSOD) is input as a user-specified constant for each reach (QUAL2K expands this by using two forms of carbonaceous BOD to represent organic carbon, a slowly-oxidizing form and a rapidly-oxidizing form, and the ability to simulate non-living particulate organic matter).
- QUAL2E does not simulate anoxia, although this function has been added in QUAL2K (see below) by reducing oxidation reactions to zero at low oxygen levels. In addition, in QUAL2K, denitrification is modeled as a first-order reaction that becomes pronounced at low oxygen concentrations.
- The major sources of dissolved oxygen in QUAL2E are algal photosynthesis and atmospheric reaeration.

**Plant Growth:**

- QUAL2E can model the role of phytoplankton in carbon and oxygen dynamics but does not model macrophytes (QUAL2K has added some capacity to model “bottom” algae; see below)
- Chlorophyll ‘a’ is used as the surrogate variable for planktonic algal biomass
- Assumes a first-order reaction to describe the accumulation of algae biomass
- Accumulation of biomass is calculated as a balance between growth, respiration, and settling of algae
- Maximum growth rate is modeled as being light and nutrient limited (three options available to simulate N and P limitations)
- For algal N uptake, the model favours ammonia over nitrate by using an algal preference factor
- **NOTE:** It should be noted that the temperature-, light-, and nutrient-limitation equations used in QUAL2K appear to be similar to or the same as those used in early versions of ECOL but are not as precise or effective as those developed by Alison Humphries (Humphries 1998) and incorporated into GRSM. QUAL2K also does not accommodate species-specific growth, death, or washout functions.

Data input requirements for QUAL2K include the following (from Birgand, undated and Capacasa 2008).

Class	Parameters
Geographic information and temporal information	Number of reaches, reach length, junction locations, headwater or not, latitude, longitude, standard meridian, basin and reach elevation, period of simulation within the year calendar
General variables	steady state or quasi-dynamic simulations, units, type of simulation to be performed (regular simulation, uncertainty analysis, type of uncertainty analysis), state variables to be modeled, maximum iteration number, in case of dynamic simulations: time step, total simulation length, time increment for intermediate summary reports of concentration profiles,
Compartment and flow characteristics	compartment size and flow type, dispersion coefficient, coefficient and exponent of the velocity for flow calculation, coefficient and exponent of the flow for stream depth calculation, Manning's coefficient, incremental inflow per reach, headwater flows, water quality characteristics of point sources
Climatic data for light limitation	Dust attenuation coefficient, solar radiation factor, light averaging factor, criteria for light average from solar radiation, fraction of cloud cover, absolute solar radiation shading (fraction of solar radiation that is blocked because of shade from topography and vegetation)
Climatic data for temperature calculations	Two evaporation coefficients, dry and wet bulb temperatures, barometric pressure, wind speed, air and water temperature, dew-point temperatures, cloud cover (% of sky covered)

Temperature	Temperature coefficient for: BOD decay, BOD settling, reaeration, SOD uptake, organic N decay, organic N settling, ammonia decay, ammonia source, nitrite decay, organic P decay, organic P settling, Dissolved P source, algal growth, algal respiration, algal settling, coliform decay and three arbitrary non-conservative constituents, initial temperature per reach, mean, minimum, and maximum temperature
Nitrogen cycle (values per reach)	Ammonia oxidation coefficient, nitrite oxidation coefficient, nitrogen content in algae coefficient, benthos source rate for ammonia nitrogen, organic nitrogen settling rate, rate constant for the hydrolysis of organic nitrogen to ammonia, nitrification inhibition coefficient, initial values per reach for the four components of the nitrogen cycle and at the headwater
Phosphorus cycle (values per reach)	Organic phosphorus settling rate, benthos source rate for dissolved phosphorus, rate constant for the decay of organic phosphorus to dissolved phosphorus, initial values per reach for the four components of the phosphorus cycle
Algae	Maximum specific algae growth rate, respiration rate, Michaelis-Menten nitrogen half saturation constant, Michaelis-Menten phosphorus half saturation constant, Michaelis-Menten half-saturation constant for light, non-algal light extinction coefficient, linear algal self-shading coefficient, non-linear algal self-shading coefficient, algal preference factor for ammonia, algal settling rate, ratio of chlorophyll-a to algal biomass, fraction of algal biomass that is nitrogen, fraction of algal biomass that is phosphorus, light saturation coefficient, initial Chl. A values per reach and at the headwaters, types of nutrient and light limitation functions, bottom algae coverage (%), bottom SOD coverage (%)
Dissolved Oxygen	O <sub>2</sub> production per unit of algal growth coefficient, O <sub>2</sub> uptake per unit of algae respired, benthic oxygen demand, carbonaceous deoxygenation rate constant, criteria for the type of reaeration, type of reaeration calculations, reaeration coefficient and associated coefficient and exponent, initial DO value per reach and at the headwater
BOD	Rate loss of BOD due to settling, initial BOD values per reach and at the headwater, type of BOD: BOD-5 or ultimate BOD, TSS, alkalinity (mc CaCO <sub>3</sub> /L)
Arbitrary non-conservative constituent	Arbitrary non-conservative settling rate, benthic source rate for arbitrary non-conservative settling rate, arbitrary non-conservative decay coefficient
Coliforms	Coliform die-off rate

## 4.2 WASP

The WASP series of models originated in the early 1983 as part of US EPA's framework for modeling contaminant fate and transport in surface waters. The latest version of the model is WASP7.

WASP is a generalized framework, designed for easy substitution of user-written routines, rather than a fixed model structure. The model incorporates three submodels, the toxics model, TOXI-WASP (which combines the EXAMS2 kinetic structure with WASP's transport structure and sediment balance algorithms); the dissolved oxygen/eutrophication model EUTRO (adapted from the Potomac Eutrophication Model developed by Thomann and Fitzpatrick, 1982); and the WASP hydrodynamic model, DYNHYD. WASP has been constructed in such a way that inputs are easily read from other stand-alone models, and outputs can be easily read and used by external models.

WASP essentially represents a body of water as a series of boxes (control volumes), with environmental properties and chemical concentrations considered to be uniform within each box or element. A Windows-based user interface simplifies the significant challenge of parameter estimation and data input.

The consensus from the literature is that WASP offers considerable spatial resolution and flexibility, but is limited in its ability to simulate photosynthesis/respiration, nutrient dynamics, and dissolved oxygen accurately. Numerous studies point to the limitation of the model for various kinds of problems and settings. But the overwhelming message in the literature is that the model is simply so complex that it is inaccessible to all but the most experienced users. Even analysis of uncertainty is limited because of the model's complexity (McIntyre 2004). While unquestionably a powerful tool for the three-dimensional simulation of lakes and reservoirs, WASP is much less commonly used than QUAL2K, MIKE11, or even HSP-F for one-dimensional water quality dynamics. To put this another way, WASP incorporates a powerful hydrodynamic model, but less effective, and often unstable, water quality routines, making it a less satisfactory choice for many river water quality applications.

Much of the following description is drawn from the USGS Surface Water and Water Quality Models Information Clearinghouse at [http://smig.usgs.gov/cgi-bin/SMIC/model\\_home\\_pages/model\\_home](http://smig.usgs.gov/cgi-bin/SMIC/model_home_pages/model_home).

### ***Streamflow and Transport:***

- Six mechanisms for describing transport:
  - Advection and dispersion in the water column
  - Advection and dispersion in the pore water
  - Settling, re-suspension, and sedimentation of up to three classes of solids; and
  - Evaporation or precipitation

- Internal kinematic wave flow routing for one-dimensional branching streams or rivers; calculates flow wave propagation and resulting variations in flows, volumes, depths, and velocities through the stream network
- Each inflow or circulation pattern requires specification of the fraction routed through relevant water column segments and the time history of the corresponding flow.
- Dispersion requires specification of cross-sectional areas between model segments, characteristic mixing lengths, and the time history of the corresponding dispersion coefficient.
- The physical configuration of the water body can involve lateral and vertical subdivisions as well as longitudinal (reach-wise) subdivisions
- Segments may be of four types: epilimnion layer, hypolimnion layer, upper benthic layer, and lower benthic layer
- Segment volumes and simulation time step are directly related; as one increases or decreases, the other must do the same to insure stability and numerical accuracy.
- Segment size can vary from very small to very large
- Dams and spillways are not explicitly modeled, but the user can specify the location of low dams or spillways where reaeration might occur
- WASP's explicit one-step Euler solution technique has potential for instability or numerical dispersion in the user-specified computational network. These problems can usually be controlled by manipulating the time step.
- Time step is specified by the user but must be linked to the water quality time step. The default time step appears to be a day, but can be set smaller or larger if the user desires. Example applications typically show time steps of approx. 2 hours (see for example Phosphorus Modelling in the Loxahatchee National Wildlife Refuge: [http://mwaldon.com/LoxModel/WkShp1Files/Presentation\\_5\\_TP.pdf](http://mwaldon.com/LoxModel/WkShp1Files/Presentation_5_TP.pdf); note that this application found that WASP was not reliable for interior marsh simulations – was too simple; needs a storage state variable; their next step was to move to MIKE-FLOOD.)

### **Temperature:**

- Simulation of bulk transfer by advection, dispersion, extractions, and pollutant sources; long wave radiation to/from the atmosphere, sky, and surrounding land; effective short-wave radiation from the sun; convection to/from the atmosphere; evaporation losses and condensation gains

### **Water Quality Constituents (General):**

- For each state variable (termed 'system' In WASP), the user must specify loads, boundary concentrations, and initial concentrations. The dissolved

fractions of each variable also must be specified for each segment. Only dissolved concentrations are transported by pore water and only particulate concentrations are transported by solids.

- Simulated chemicals undergo several physical or chemical reactions as specified by the user in the input dataset. Each variable is advected and dispersed among water segments, and exchanged with surficial benthic segments by diffusive mixing. Sorbed or particulate fractions may settle through water column segments and deposit to or erode from surficial benthic segments. Within the bed, dissolved variables may migrate downward or upward through percolation and pore water diffusion. Sorbed variables may migrate downward or upward through net sedimentation or erosion. Rate constants and equilibrium coefficients must be estimated from field or literature data in simplified toxic chemical studies.
- WASP has the capacity to model temperature, salinity, coliform bacteria, nitrogen, BOD, algae, phosphorus, silica, DO, cohesive sediments, noncohesive sediments, sediment diagenesis, conservative tracers, user-defined constituents, pesticides, and synthetic organic compounds.
- The transport and transformation of chemicals and particulate matter (up to three of each) may be independent or may be linked with reaction yields, such as a parent compound-daughter product sequence
- Transfer processes in the model are simplified and include sorption and volatilization. Sorption is treated as an equilibrium reaction.
- Transformation processes include biodegradation, hydrolysis, photolysis, and oxidation, all treated as first-order processes.
- WASP uses a mass balance equation to calculate sediment and chemical mass and concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed.
- The model has limited applicability in simulation of chemical dynamics. Chemical concentrations should be near trace levels, i.e., below half the solubility or  $10^{-5}$  molar. At higher concentrations, the assumptions of linear partitioning and transformation begin to break down. Note however that high concentrations in the natural system can be important in affecting ecosystem dynamics, such as pH or bacterial action, and thus may alter transformation rates.
- *Note: More detail is available on WASP's simulation of organic chemicals but has not been included in this review as it is not directly relevant to the simulation of DO and nuisance aquatic plant growth in the Grand River.*

**Nitrogen:**

- Simulates ammonia and nitrate; neglects nitrite

**Phosphorus:**

- Assumes that only one fraction of P is relevant at the time-scale in question (usually orthophosphates)

### ***Suspended Solids:***

- Capacity to incorporate total solids as a single variable or as up to three solids types or fractions (user-defined); these might be sand, silt, and clay, or organic solids and inorganic solids, for example. The user defines each type by specifying its settling and erosion rates and its organic content.
- WASP performs a simple mass balance on each solid variable in each compartment based on user-specified water column advection and dispersion rates, settling, deposition, erosion, burial, and bed load rates. Mass balance is performed in water column segments and in benthic segments.
- No special provisions are made for shear strength or water column shear stress, so the TOXI sediment model should be considered descriptive and must be calibrated to site data
- In a simulation, sediment is advected and dispersed among water segments, settled to and eroded from benthic segments, and moved between benthic segments through net sedimentation, erosion, or bed load.
- In WASP7, a state variable can be used to simulate TSS, non-biotic solids or a conservative substance. Sorption of ammonia and phosphate to solids has been added. Furthermore, solids concentration can be used to predict light extinction (see Light, below).

### ***Light:***

- In previous versions of WASP the user could specify up to five different light extinction time functions that could be assigned to individual segments. This functionality still exists in WASP 7, where it is accomplished by using the background light extinction function as described below:

**Background  $K_e$  = Segment Parameter (User Specified) \* Time Function (1 of 4) \* Extinction Background Multiplier**

- In WASP7, additional light extinction algorithms have been added to allow the model to predict light extinction as a function of background light extinction (water color, ligands), productivity (algal concentration), solids (total suspended solids, solids loadings), and dissolved organic carbon (detritus, CBOD). These new algorithms allow the model to predict changes in light extinction as function of management practices that reduce solids loading, nutrients and CBOD.
- Algal self-shading is included as a user-specified shade multiplier.

### ***Dissolved Oxygen:***

- WASP simulates DO using the EUTRO submodel, which can be operated at several levels of complexity to simulate some or all of the following: transport and interaction among nutrients; phytoplankton dynamics (also

- “bottom” algae in the most recent version, WASP7); carbonaceous material; and DO in the aquatic environment.
- To simulate only one of these processes, the user may bypass calculations for the others.
  - Option to include carbonaceous BOD (CBOD) and either ammonia (NH<sub>3</sub>) or nitrogenous BOD (NBOD) expressed as ammonia
  - Sediment oxygen demand may be specified
  - Photosynthesis and respiration rates may be specified
  - Four levels of complexity available:
    - Streeter-Phelps
    - Modified Streeter-Phelps
    - Full linear DO balance, and
    - Nonlinear DO balance
  - Capacity to simulate temperature effects for BOD decay and aeration
  - In WASP7, the user can specify low-head dams and spillways where oxygen would be added as a function of water quality condition and dam type

**Plant Growth:**

- Like QUAL2E/2K, WASP uses chlorophyll ‘a’ as a surrogate variable for simulation of biomass. In WASP7, “bottom” algal biomass (attached algae) is simulated separately from phytoplankton.
- WASP7 contains a new module, named “periphyton,” that includes the standard WASP7 eutrophication algorithms, and incorporates bottom algae, with three additional state variables: bottom algal biomass, bottom algal cell nitrogen, and bottom algal cell phosphorus.
- Bottom algae are not subject to advective and dispersive transport.
- Sources and sinks include nutrient uptake, growth, nutrient excretion, death, and respiration.
- Nutrient uptake rates are driven by concentrations of inorganic nitrogen and phosphorus in the water column and within algal cells, and are controlled by cell minimum and half-saturation parameters.
- Biomass growth is computed from a maximum zero or first-order rate constant that is adjusted internally by water temperature, bottom light intensity, internal nutrient concentrations, and maximum carrying capacity.
- Nutrient excretion, death, and respiration are represented by first-order, temperature dependent rates.
- Growth, respiration, and death rates affect other model state variables, including dissolved oxygen and nutrients. The algorithms for predicting bottom algal biomass and nutrient concentrations are based upon the periphyton routines included in the QUAL2K model (Chapra 2005).
- Periphyton, like phytoplankton, also excrete cell contents and die, recycling dissolved and particulate organic matter to the stream’s carbon and nutrient pools. While the modeling approaches used for phytoplankton and periphyton are similar, periphyton differ from phytoplankton in a number of fundamental ways:

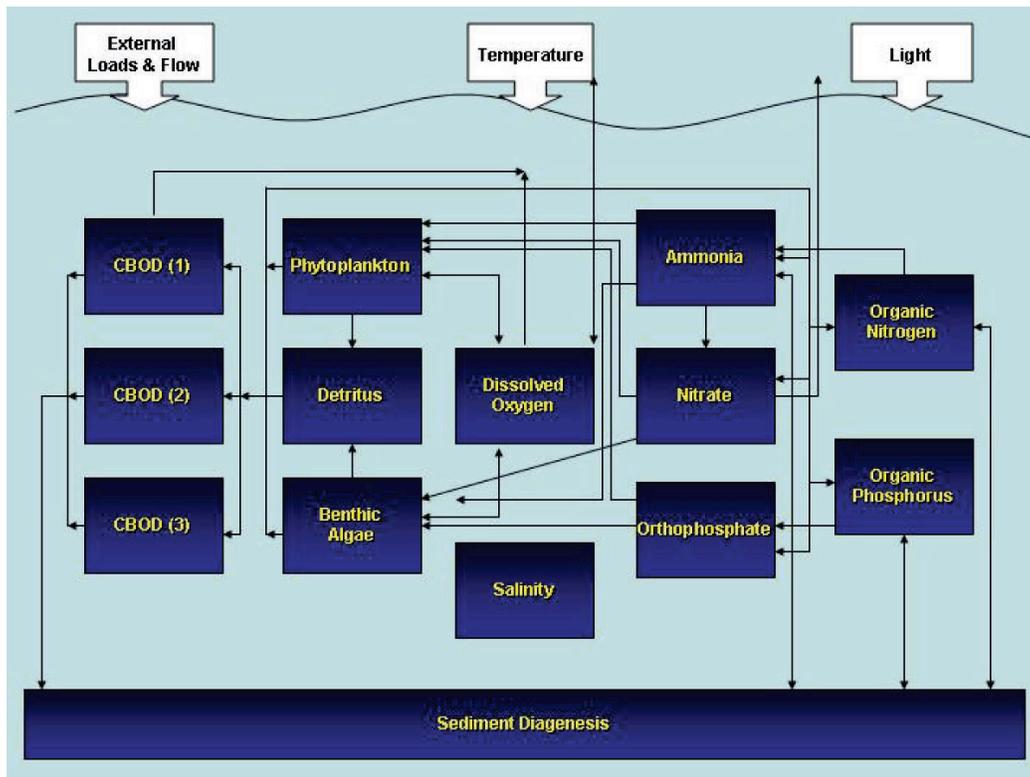
- Periphyton do not move with the water current, as do phytoplankton,
- Periphyton typically dwell on or near the bottom, so are not impacted by the average light in the water column but the light reaching the bottom (substrate).
- Periphyton are limited by the amount of substrate available for growth.
- There is typically a maximum density for attached plants.
- Maximum growth rate is typically on the order of 30 g/m<sup>2</sup>/day, with a range of 10-100.
- **NOTE:** It should be noted that the temperature-, light-, and nutrient-limitation equations used in WASP7 appear to be similar to or the same as those used in early versions of ECOL but are not as precise or effective as those developed by Alison Humphries (Humphries 1998) and incorporated into GRSM. WASP also does not accommodate species specific growth, death, or washout functions.

Section 3 of the WASP7 Benthic Algae User's Guide

(<http://www.epa.gov/athens/publications/reports/Ambrose600R06106WASP7.pdf>)

contains details about the theoretical basis for WASP's calculation of bottom algal biomass, photosynthesis, temperature and light limitation, space limitation, losses to respiration and death, nutrient uptake and release.

The WASP7.1 release notes ([http://epawasp.com/files/Release\\_Notes.pdf](http://epawasp.com/files/Release_Notes.pdf)) provide a general overview of model structure and function.



**Figure 4. Overview of WASP EUTRO Model Structure**

(from US EPA WASP Factsheet:

<http://www.epa.gov/athens/wwqtsc/WASP.pdf>)

WASP7.3 is scheduled for release in January 2009 (persistent bugs delayed the release from the scheduled date of September 2008). It is expected to include the following improvements (these notes are taken verbatim from <http://epawasp.com/node/5>):

- Improved Model Import Routine: this is a critical component of linking WASP with BASINS. This will allow the user to develop model networks in the BASINS GIS environment. Pass flow information from USGS gages to WASP. Get predicted loads and flows from watershed models (HSPF and SWAT).
- Improved Kinematic Wave Option – the built-in one-dimensional hydrodynamic model in WASP has been improved dramatically for ease of use as well as functionality. The user has the ability to specify different cross sectional assumptions, not just rectangular.
- Time Step Optimization has been drastically improved and has been integrated into the kinematic wave calculations. The timestep optimizer will

not only look at what just happened to determine the next timestep, but will look forward as well.

- Conventional Pollutant Model Updates (Eutrophication). Substantial updates have occurred in the eutrophication module. The user now has the ability to define and use up to three algal components. This enhances the model to be better capable of predicting early spring and late fall algal blooms. The user will have ability to specify one of the algal groups as a nitrogen fixing blue-green algae, so that when nitrogen levels are reduced in the aquatic environment they will have a competitive advantage and start to fix nitrogen from the atmosphere. The sediment diagenesis sub model has been linked in again, giving the user predictive capabilities for sediment oxygen demand and nutrient releases from the sediments. Averaging algorithms have been added to the output so that the user can look at daily average dissolved oxygen concentrations as well as other constituents.
- Improved Temperature Module will be released, correcting some “bugs” found in the code.
- Linking WASP Modules – methods have been added where the user can link the output of one WASP model type with another. For example, the Heat Module could be applied to a system to predict temperature. These model results can be used by the Eutrophication Model, providing the predicted temperatures.

### **4.3 HSPF and BASINS**

While there is no single model that meets all user needs throughout a watershed, US EPA's Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) package is probably one of the most comprehensive model packages currently available. It combines a number of submodels allowing the user to calculate runoff and pollutant loadings from the land surface (HSPF, ARM, NPS, SWAT, etc.), a water quality model (QUAL2E, as described in Section 4.1), national databases (for the US; not available for Canada), a range of assessment tools for the evaluation of water quality and point source loadings at a variety of scales, extensive utilities for data import, land use mapping and classification, DEM creation, catchment delineation, and so on, and a range of post-processing tools for creating and interpreting model output. Option flags allow the user to bypass whole modules if the processes involved are deemed to be unimportant and/or if data are not available.

HSPF is one of the few models currently available (and perhaps the only open-source model) that allows integrated simulation of land-based runoff and pollutant loading processes with instream water quality simulation, sediment transport, and sediment-pollutant interactions. As noted previously, HSPF is the current form of the Stanford Watershed Model developed in the early 1960s (Crawford 1962). Originally a hydrologic model only, water quality processes were added in the 1970s, and pre- and post-processing software and a variety of algorithm improvements were developed in the 1980s jointly by USGS and US EPA. The current version of HSPF is Version 12.

Data requirements for HSPF are considerable; as a result, the model usually requires a team effort for data processing, parameter estimation, calibration, validation, and post-processing. Continuous simulation requires continuous input of data to drive the simulations. For this reason the full BASINS package incorporates databases on selected regions, in addition to a range of analytical and reporting tools. Model documentation has been weak in the past (although it is improving) and the model is frequently revised, in part because of the large number of submodels, each with its own revision schedule. Application demands experienced users and significant time for model building and testing.

#### ***Streamflow and Transport:***

- Well-mixed, one-dimensional flow, therefore limited to well-mixed rivers and reservoirs; not appropriate for lakes, ponds or wetlands
- HSPF produces a time history of runoff, sediment load, nutrient and pesticide concentrations, and water quantity and quantity at any point in the watershed
- A modular system of models incorporating both watershed and channel simulation of hydrology and water quality.

- Dynamic and continuous simulation of fate and transport overland and in one-dimensional channels.
- This model allows integrated simulation of land and soil erosion processes with in-stream hydraulic and sediment-chemical interactions.
- Incorporates a wide range of watershed processes that can be combined or ignored to suit the needs of the use.
- Program can simulate channel routing, reservoir routing, constituent routing, one or many pervious or impervious unit areas discharging to one or many river reaches or reservoirs.
- Frequency-duration analysis can be done for any time series.
- Any time step from 1 minute to 1 day that divides equally into 1 day can be used.
- Any period from a few minutes to hundreds of years may be simulated.
- HSPF makes no assumptions regarding the shape of a reach and does not require that the cross-section be trapezoidal or even that the shape be prismoidal. This is one reason why both free flowing reaches and reservoirs can be handled by the same application module.
- HSPF cannot simulate reversing flow
- The flow routing technique falls in the class known as “storage routing” or “kinematic wave” methods

***Temperature:***

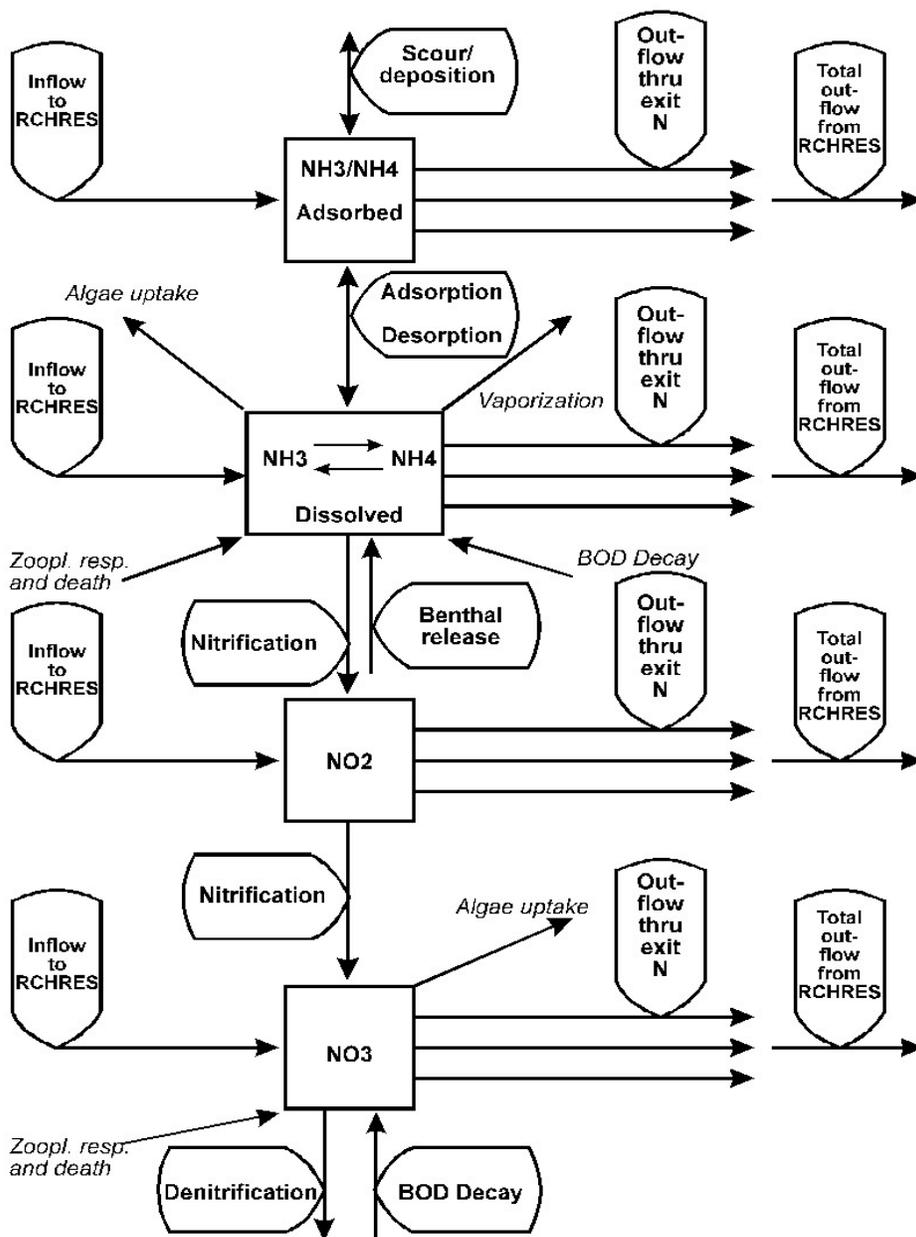
- HSPF calculates a detailed heat budget for the land segment or river reach, including simulation of bulk transfer by advection, dispersion, extractions, and pollutant sources; long wave radiation to/from the atmosphere, sky, and surrounding land; effective short-wave radiation from the sun; convection to/from the atmosphere; evaporation losses and condensation gains; soil temperature; snowmelt; and air and water temperature

***Water Quality Constituents (General):***

- HSPF simulates pH, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, organic phosphorus, phytoplankton, and zooplankton
- Transfer and transformation processes for contaminants include hydrolysis, oxidation, photolysis, biodegradation, volatilization, and sorption

***Nitrogen:***

- Capacity to simulate ammonia, nitrite, nitrate, dead refractory organic N
- Four additional quantities are estimated from simulation of these constituents. These quantities are total organic nitrogen, total organic phosphorus, total organic carbon, and potential biochemical oxygen demand
- Nitrification and denitrification simulated (see example diagram, below)

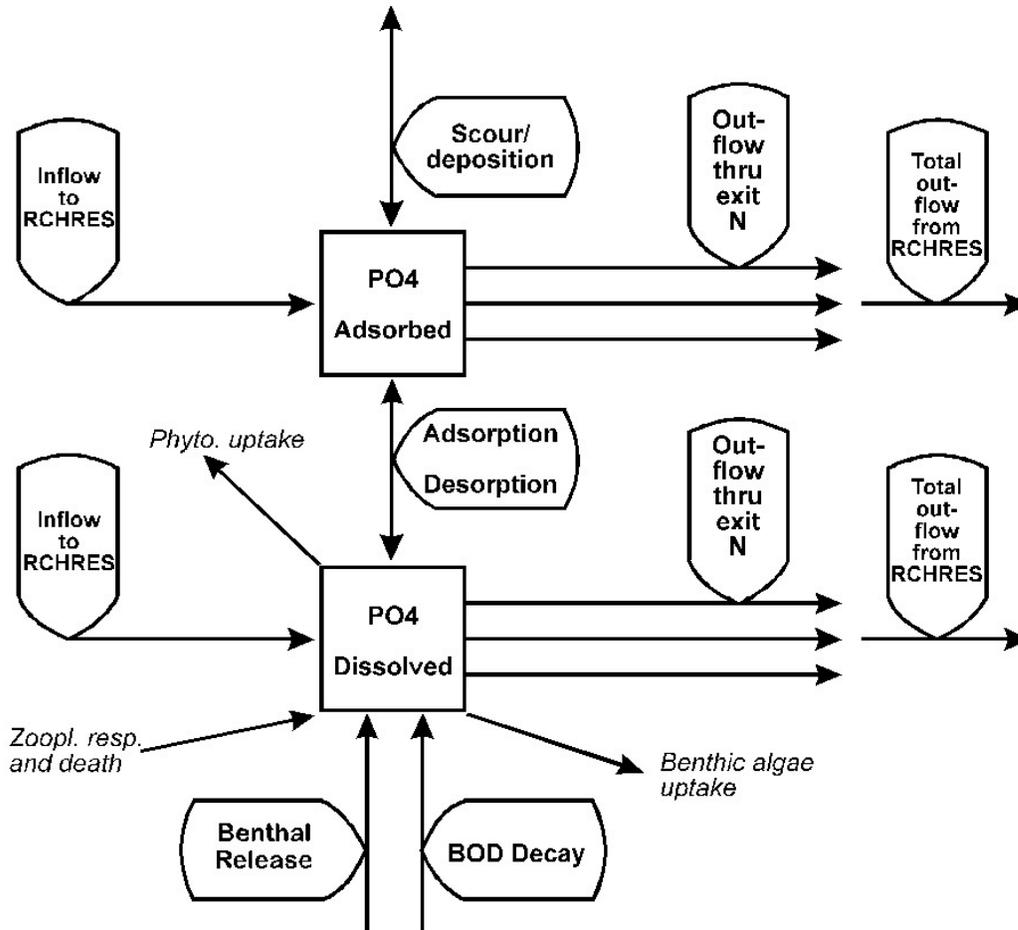


**Figure 5. Flow diagram for inorganic nitrogen transformations included in HSPF** (from HSPF user's manual: <http://www.epa.gov/waterscience/basins/bsnsdocs.html#hspf>)

**Phosphorus:**

- Capacity to simulate orthophosphorus and dead refractory organic P
- Four additional quantities are estimated from simulation of these constituents. These quantities are total organic nitrogen, total organic

phosphorus, total organic carbon, and potential biochemical oxygen demand.



**Figure 6. Flow diagram for ortho-phosphate transformations in HSPF** (from HSPF user's manual:

<http://www.epa.gov/waterscience/basins/bsnsdocs.html#hspf>)

**Suspended Solids:**

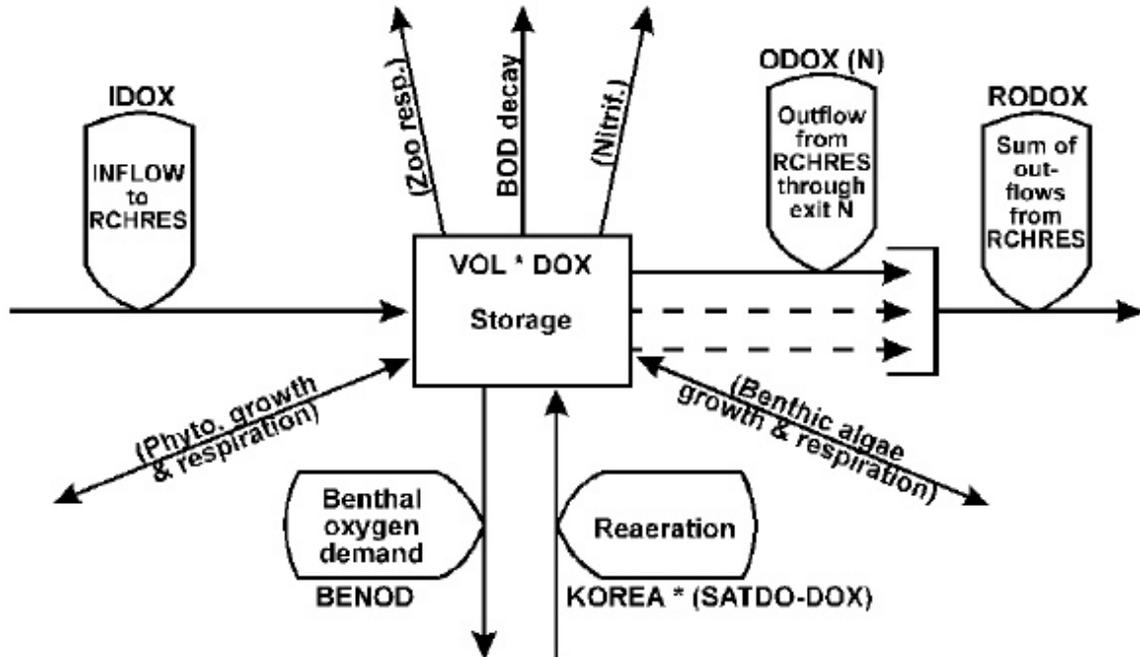
- Three sediment fractions simulated: sand, silt and clay
- Resuspension and settling are defined in terms of shear stress at the sediment-water interface
- Sediment transport capacity is calculated and resuspension or settling is defined by the difference between the sediment in suspension and the transport capacity
- Calibration requires data for all three sediment fractions
- Benthic exchange is modeled as sorption/desorption and deposition/scour with surficial sediments; deeper sediments and pore water are not modelled

### ***Light:***

- Light attenuation is incorporated when water depth exceeds 2 inches (the HSPF user's manual notes that the algorithms used to represent planktonic algae processes related to light are not accurate for very shallow waters)
- Light intensity just below the water surface is calculated as a function of incident radiation and surface reflection
- Light extinction at greater depth is calculated as a function of total suspended sediment and an optional incremental factor reflecting phytoplankton density
- HSPF assumes that algal growth occurs only in the euphotic zone, which is the distance below the water surface at which 1% of the incident light is still available.
- The equation used to calculate the amount of light available to benthic algae assumes that all benthic algae are at a common, average depth below the water surface.

### ***Dissolved Oxygen:***

- HSPF calculates dissolved oxygen through five separate subroutines as a function of water temperature, longitudinal advection of dissolved oxygen and BOD, sinking of BOD material, benthic oxygen demand, benthic release of BOD, reaeration, and oxygen depletion due to decay of oxygen-demanding materials
- The dissolved oxygen concentration below which anaerobic conditions are considered to exist is determined by a user-input value
- Nutrient dynamics (e.g., nitrification, denitrification) and plant growth dynamics (see below) are used to adjust dissolved oxygen concentrations



**Figure 7. Flow diagram for dissolved oxygen processes in HSPF** (from HSPF user's manual: <http://www.epa.gov/waterscience/basins/bsnsdocs.html#hspf>)

**Plant Growth:**

- Advective transport, growth, die-off, settling and zooplankton predation of phytoplankton
- Advective transport, growth and die-off of zooplankton
- Growth and die-off of benthic algae
- Advective transport and storage of dead refractory organics from phytoplankton, benthic algae and zooplankton die-off
- In addition to nutrient dynamics and oxygen concentrations, a mass balance for carbon dioxide is computed at every time step
- Photosynthesis and respiration are modeled with a fairly crude relationship, where dissolved oxygen is calculated as a function of TP and biomass
- Algal growth subroutines perform a series of initial checks to determine whether or not light, temperature and nutrient conditions are suitable for growth
- The user can specify temperature preferences of algae by assigning low, medium and high growth temperatures
- Phosphorus growth limitation is calculated as a function of orthophosphorus concentration, nitrate concentration, and temperature, using a Michaelis-Menten relationship; nitrogen growth limitation is calculated as a function of maximum growth rate corrected for ammonia retardation, organic and inorganic nitrogen species concentrations, and

- temperature, again using a Michaelis-Menten relationship
- Light limitation of plant growth is based on early work by Dugdale and MacIsaac (1971), and is a simple relationship in which light-limited growth is calculated as a function of temperature-corrected maximum growth rate and available light, again using Michaelis-Menten relationships. These relationships do not therefore reflect the changes incorporated in GRSM based on the work of Humphries (1998), as discussed previously in the case of QUAL2K and WASP7.

#### 4.4 MIKE11 and MIKE-BASIN

MIKE 11 is a product of the Danish Hydrological Institute (DHI), which produces a wide range of software products for water resources modeling. MIKE11 was developed in the mid-1980s and remains one of the Institute's most popular products. (Of all of the models reviewed in this report, only MIKE11 has a Wikipedia entry!).

MIKE11 is a modular one-dimensional hydrodynamic model framework including a full solution of the St. Venant equations, plus many process modules for advection-dispersion, water quality and ecology, sediment transport, rainfall-runoff, flood forecasting, real-time operations, and dam break modelling.

The model framework includes a number of separate modules, including:

- **HD module** for diffusive wave approximation and kinematic wave approximation, flow routing (Muskingum, Muskingum-Cunge and linear routing methods); provisions for adaptation to subcritical and supercritical flow; can simulate hydraulic structures such as weirs, culverts, bridges, pumps, energy loss, and sluice gates; the user is guided to choose the appropriate routing method for the time step and parameters of interest.
- **RR (Rainfall-Runoff) module** using the unit hydrograph method and a soil moisture accounting model; includes an auto-calibration tool for parameter estimation based on comparison between observed data and simulated conditions. MIKE's rainfall-runoff model, NAM, is a lumped, conceptual rainfall-runoff model simulating overland flow, interflow, and baseflow as a function of moisture content in snow storage, surface storage, root zone storage, and groundwater storage.
- **AD (Advection-Dispersion) module** for the simulation of transport and dispersion of heat, conservative pollutants and other constituents with linear decay.
- **SO (Structure Operation) module** for simulating the operation of structures like weirs, culverts, pumps, bridges, and sluice gates.
- **DB (Dam Break) module** for definition of dam geometry, breach development in time and space, and failure mode.
- **ST/GST (Noncohesive Sediment Transport) module** for the simulation of transport, erosion and deposition of non-cohesive and graded noncohesive sediments, including simulations of river morphology.
- **ACS (Cohesive Sediment Transport) module**, incorporating a 3-layer bed description and quasi-2D erosion.
- **Water Quality module**, for the simulation of steady-state reactive transport of major water quality parameters, for example to determine compliance with EU water quality standards). Parameters in the WQ module include ammonia, nitrate, oxygen, total phosphorus, E.coli, BOD, and a user-defined substance (e.g., salinity). Transformation processes are represented mechanistically with user-specified or default rate

constants. The user can specify time-varying oxygen sources and sinks including respiration, photosynthesis, sediment oxygen demand, etc. Weir reaeration is included in oxygen simulation. Both point and non-point sources of pollution can be modeled. Nonpoint source pollution includes user-specified total nitrogen and phosphorus loads, with user-specified seasonal variation. The Load Calculator function in MIKE-BASIN WQ allows the integration of GIS-based loading data with the MIKE11 WQ module.

- **Stratified module**, to simulate vertical density differences such as salinity or temperature in two-layer or multi-layered stratified water bodies.
- **Real Time module**, a simulation package and GIS interface intended for use in flood forecasting systems; includes real-time updating and Kalman filtering.
- **AUTOCAL module**: MIKE11's automatic calibration tool for a wide range of parameters, including rainfall runoff parameters, Manning's number, head loss coefficients, and various water quality parameters.
- **MIKE-BASIN GIS extension**, an interface with and extension of the GIS system ArcMap, to support catchment mapping, cross-section mapping, Digital Elevation Model data, GIS-based pollutant loading estimates, etc.; supports flood visualization/animation as 2D maps and presentation of other results using Temporal Analyst

MIKE11's popularity is based in part on its user-friendly interface and clear interactive menu system for data management, execution of model runs, and pre- and post-processing (including, as noted above, an automatic calibration tool).

The MIKE-BASIN catchment modeling package

(<http://www.dhigroup.com/Software/WaterResources/MIKEBASIN.aspx>) links the MIKE11 model with a powerful GIS tool and user interface. MIKE-BASIN includes a number of time series tools allowing the user to fill gaps, correct data based on double mass curves, modulate monthly time series by a daily reference, detect outliers and correlations, and so on. If no DEM exists for the basin, a Pseudo-DEM function in MIKE-BASIN allows the approximation of river elevations. In addition to the functions included in the above modules, groundwater processes, including aquifer water quality, can be simulated for each catchment.

MIKE11 is less stable than some other software in its calculation of water quality processes (note that WASP also has difficulties with this issue). MIKE11 is also considered superior to QUAL2K and the WASP series in its partitioning of organic matter into dissolved, suspended, and sedimented fractions, thus allowing changes in sediment quality to be incorporated explicitly in the model (Rauch et al. 1998). Some users have also found that the sediment transport components of MIKE11 are unreliable under many high flow conditions because they do not account for heterogeneity in the depth of sediment.

Calculation of heat balance is similar to that in QUAL2K and WASP; the same is true for carbon-dissolved oxygen processes. Unlike those two models, MIKE11

incorporates not only phytoplankton dynamics but also zooplankton and benthic (attached) algae.

*NOTE: I was not able to obtain details on these aspects of the model, because it is a proprietary tool, but I note that MIKE11 has been successfully applied in the simulation of estuarine salinity distributions and associated phytoplankton and benthic microalgae in South Africa (see for example <http://www.fwr.org/wrcsa/756103.htm>)*

## **4.5 GRAND RIVER SIMULATION MODEL (GRSM)**

The Grand River Simulation Model was developed in the mid-1970s by the Ministry of the Environment in partnership with the Grand River Conservation Authority. It built on similar work on the Thames River in Southwestern Ontario, in which a dynamic simulation model had been used in the evaluation of alternative management strategies for the control of eutrophication in that river. The model was the main simulation tool used by the Grand River Implementation Committee in its evaluation of water management options during the Grand River Basin Water Management Study.

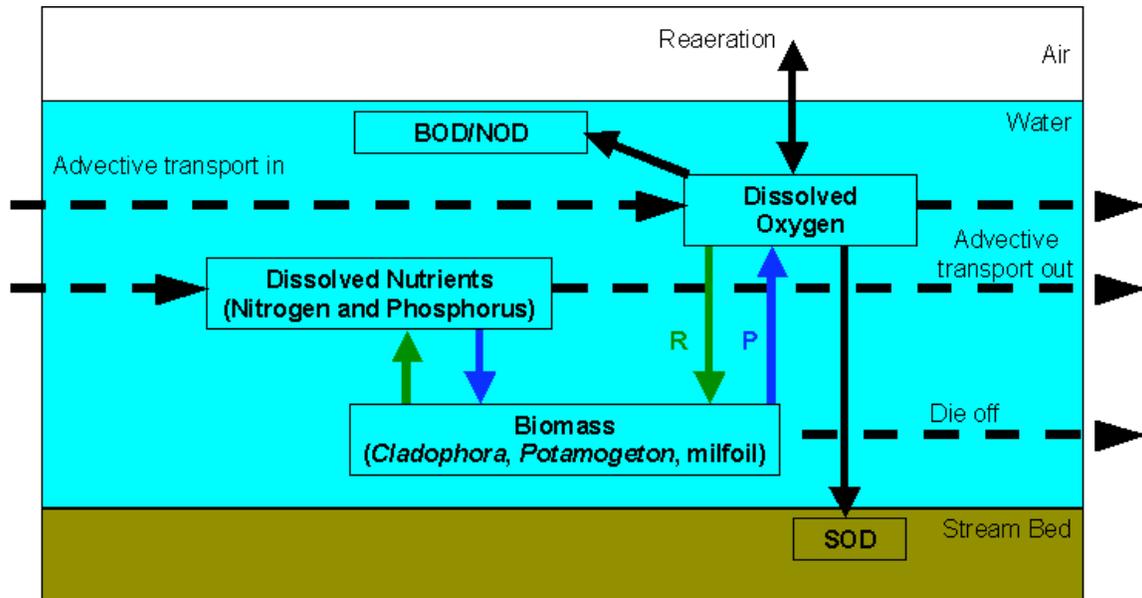
GRSM is a dynamic (non-steady state) water quality model capable of simulating up to 10 water quality parameters and three aquatic plant species for a period of up to 20 years, using a finite time step of two hours. The model simulates carbonaceous and nitrogenous BOD, nitrate plus nitrite, suspended solids, total phosphorus, un-ionized ammonia (NH<sub>3</sub>), three species of aquatic plants, *Cladophora glomerata*, *Potamogeton pectinatus*, and *Myriophyllum spicatum* (originally “periphyton”), and dissolved oxygen. The main processes influencing dissolved oxygen include BOD, NOD, and sediment oxygen demand, photosynthesis, respiration, and reaeration at the water surface. The model can incorporate input from up to 30 point sources (sewage treatment plants or industries), 30 urban storm sewer outfalls, 100 tributaries and 100 withdrawal sites. Loadings from rural diffuse runoff and groundwater inflow are also incorporated.

The model has undergone considerable scrutiny and reformulation over the past 30 years. In the mid 1990s, the model was converted to desktop format and was recalibrated for more recent conditions. Some subroutines were also modified at that time, for example in the water temperature calculation (to include a multivariate regression model based on daily and antecedent flow and air temperature), and in the turbidity-light extinction relationships. A few years later, 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. Changes recommended at that time (Humphries 1998 and Heathcote and Humphries 1997) included (GRCA 2007):

- changes to the equations governing phosphorus limitation of aquatic plants. The recommended algorithm relates phosphorus limitation to aquatic plant growth using Michaelis-Menton kinetics, rather than the linear relationship that was used historically.
- changes to the temperature-growth response to allow for a range of optimum growth temperatures based on existing literature, instead of a single optimum temperature for growth.

- modification of the light attenuation equation to include a better representation of attenuation due to the density of the weedbed.

The following summarizes how GRSM handles various processes. Figure 8 illustrates the main processes in graphic form.



**Figure 8: Overview of GRSM model structure**

**Streamflow:**

- GRSM is not a hydrologic model, therefore the flow coming into each reach from tributaries, groundwater, urban and rural non-point source runoff, etc. must be specified (GRCA 2007). Major tributaries entering the model domain are referred to as boundary flows. Where possible, model input for each of these boundary flows is based on daily average measured flow at the nearest flow gauge.
- GAWSER, a calibrated hydrologic model of the Grand River watershed, is used to predict daily average streamflow and sediment concentrations for smaller tributaries, urban catchments and local drainage that are not explicitly measured.
- One dimensional. The channel is assumed to be well-mixed vertically and laterally.
- Steady state hydraulics. Non-uniform, steady flow is simulated. Inflow to each reach (e.g. from boundary or urban catchment) can vary on a daily average basis. GRSM does not simulate rapid changes in streamflow over diurnal or shorter time period. Power equations are used to specify

- hydraulic characteristics of each reach to relate mean velocity and depth to flow.
- Large abstractions of water are specified as monthly average taking (e.g. large water takings for Region of Waterloo and City of Brantford for drinking water supply).
  - GRSM segments the system into river reaches comprised of un-equally spaced elements. For each element, the model calculates a water balance and a mass balance for pollutants (advective transport and reaction mechanisms are considered in calculating mass balance)
  - Not appropriate for simulating highly variable wet weather sources such as nonpoint-source runoff from urban or agricultural areas where flows may vary widely within a 24 hour period.

**Temperature:**

- Water temperature was historically estimated using an empirical regression equation based on either flow or air temperature and solar radiation. 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 the 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. Continuous water temperature measurements are available at 7 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 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 at the Elora Research Station 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 (in this case, approximately 43°N).

**Water Quality Constituents (General):**

- Boundary water quality inputs are based on measured data for DO, TP, NO<sub>3</sub>, TKN, BOD, and TSS using data from the Provincial Water Quality Monitoring Network. Limited data sets mean that time series input is not feasible.

- In lieu of time series input, the user creates a range of possible values (drawn from representative five-year monitoring data) for pollutant source inputs, and assigns a probability to each value. The model then draws input values from this data set for each day in the model simulation. The resulting input file therefore reflects realistic frequencies for input values.
- This approach is preferable to simulating “best”, “worst”, and “typical” snapshot conditions, because it allows the user to simulate realistic storm frequencies (including the impact of consecutive rainfall events) and associated input flow and quality values. The output therefore reflects a realistic distribution of flow and water quality conditions, and allows the user to estimate the frequency of water quality violations, not just the magnitude of a violation under a single flow/input condition.
- STP flow and quality is based on reported data from each plant in the model domain. The model requires a daily time series of flows and uses a cumulative distribution for effluent quality.
- Urban and local nonpoint source flow and concentrations are estimated using GAWSER
- Sediment oxygen demand, and BOD and NOD decay rates can be specified for each month and for each reach in the model domain. The values currently used in the model were originally based on field measurements that were made in the 1970s during the early stage of GRSM development. These values were updated in 1996 based on field monitoring carried out in 1995.
- Does not partition organic matter into dissolved, suspended and sedimented fractions, and so does not allow changes in sediment quality to be simulated.

### ***Nitrogen:***

- NOD inputs are calculated based on TKN concentrations assuming  $NOD = 4.57 * TKN$ . This conservatively overestimates NOD since there is a refractory component of TKN that does not consume oxygen. NOD decay (i.e. nitrification) consumes dissolved oxygen and produces nitrate. Reaction rates vary from reach to reach and are temperature sensitive.
- Un-ionized ammonia concentrations are estimated based on monthly average pH for each reach (assigned as input) and water temperature for each timestep.
- Nitrogen balance includes uptake by plants during photosynthesis and release during respiration. Aquatic plants and algae are assumed to preferentially take up ammonia followed by nitrate. Ammonia is assumed to be released from aquatic plants during respiration.
- Several nitrogen transformation processes are not included in GRSM such as volatilization of un-ionized ammonia, inhibition of nitrification at low DO and denitrification in sediments.

**Phosphorus:**

- Only total phosphorus is modeled. GRSM includes uptake of total phosphorus by aquatic plant biomass during photosynthesis and release during respiration.
- The 1997-1998 changes incorporated a (nonlinear) Michaelis-Menten based equation for phosphorus uptake by aquatic plants and algae.
- No accounting for uptake of P via sediment or roots (note that this was also the case with other major models studied)
- Settling of total phosphorus and release of phosphorus from sediment (either as a result of resuspension or flux of orthophosphate) are not included in GRSM.

**Suspended Solids:**

- GRSM does not model bed or suspended sediment movement, although light extinction as a function of suspended sediment (and other variables) is included.
- TSS is essentially treated as a conservative parameter.

**Light:**

- Incorporates diurnal and climatic changes of radiation, and light extinction in the water column due to turbidity and self-shading
- Light limitation equations were also modified in 1997-1998, while retaining Michaelis-Menten relationships. The modifications calculate photosynthetically available light at the top of the plant growth, where most photosynthetic activity would occur.

**Dissolved Oxygen**

- Like most other major models, the dissolved oxygen processes are based on the Streeter-Phelps model, but also include:
  - implicit calculation of reaeration rate based on water depth and velocity
  - advective transport into and out of each reach
  - weir effects are included and have the effect of increasing reaeration
  - temperature effects for both BOD/NOD decay, reaeration and aquatic biomass growth.
  - representation of sediment oxygen demand by explicitly specifying as an input for each reach
  - species-specific photosynthesis and respiration for three species of plants: *Cladophora glomerata*, *Potamogeton pectinatus*, and *Myriophyllum spicatum*
- BOD and NOD are modeled as a first-order degradation process, with the reaction rates specified by the user based on historical field monitoring data.

**Plant Growth:**

- Models three species of aquatic plants, *Cladophora glomerata*, *Potamogeton pectinatus*, and *Myriophyllum spicatum*
- Does not simulate phytoplankton (i.e., floating algae), which are not considered to be the dominant influence in this river. Phytoplankton may, however, play some role in observed dissolved oxygen dynamics, and may be an avenue for future modifications to the model.
- Biomass production is limited by solar radiation, stream temperature and available nutrients, while respiration and washout result in a loss of biomass; all three processes (production, respiration and washout) are dependent on the biomass density at the previous time step. Biomass washout is assumed to be constant below a specified flow, if flow exceeds this threshold biomass washout increases.
- Biomass inhibition coefficients were included in the model to account for processes that are not explicitly modelled, e.g. grazing of aquatic biomass by benthic invertebrates, fish, water fowl, etc. Grazing has been shown to cause significant changes in aquatic plant community and density (Humphries, 1998)
- The density of aquatic biomass at the beginning of the simulation must be specified for each of the three species included in the model.
- GRSM has been shown to be sensitive to the value of the reaeration coefficient, as well as factors related to aquatic plant growth (Willson, et al. 1982).
- The 1997-1998 changes incorporated more sophisticated temperature limitation algorithms for biomass growth, making use of both maximum and minimum temperatures and a range of optimum temperatures for each species of interest

## 5. DISCUSSION

This report has described the context for dissolved oxygen modeling in the Grand River, Ontario, and has reviewed five major models that appear appropriate for such modeling. In Section 3, we considered the major questions that confront modelers in the selection of an appropriate tool for dissolved oxygen in the Grand River. The answers to those questions are summarized in the following table. All of the models examined were able to simulate flow and pollutant sources, including temperature, solids and nutrients; all included some consideration of instream DO sources, sinks, and concentrations. The models varied widely in their treatment of sediment-water dynamics and in the treatment of plant and attached algae growth dynamics.

One other criterion should be mentioned here: cost. While QUAL2E/2K, WASP7, and HSPF are open-source models, downloadable, with support materials, free of charge from the US EPA website, MIKE11 and MIKE-BASINS are not. Waterloo Hydrologic quotes a “sale” price of \$2495 CAD for a single MIKE11 module, the SO module (normal price for the SO module is given as \$5750 CAD; see [http://www.swstechnology.com/pdfs/enews\\_archive/2006\\_archive/2006-Dec-enews.pdf](http://www.swstechnology.com/pdfs/enews_archive/2006_archive/2006-Dec-enews.pdf); Wayne Huber, a distinguished modeler based at Oregon State University, estimates the price for a reasonable but basic MIKE11 configuration at \$25,000; MIKE-BASINS would almost certainly be tens of thousands more expensive.

The following table summarizes the main operational features of the models examined in this review.

## Comparison of Model Attributes (after US EPA 1997; Rauch et al. 1998)

	DO	CBOD or Total BOD	NBOD	SOD	Temperature	Total P	Organic P	PO4	Total N	Organic N	NH3	NO2	NO3	Carbon	Phytoplankton or Chl a	Macrophytes/Att'd Algae	Zooplankton	pH	Alkalinity	TDS	Coliform Bacteria	Streamflow	Dynamic simulation	Models Weirs	Unstable water quality	Other
QUAL2E	X	X	*	#	X		X	X		X	X	X	X		X	X				X	X	1D		X		Arbitrary conservative and nonconservative substances
WASP5	X	X	*	#	#	X	X	X	X	X	X		X			X	#	#		X		3D	X	@	X	User can add own subroutines to model other substances
HSPF	X	X	X	#	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	1D	X	X		Total inorganic carbon. Complex model with many subroutine modules and submodels that can be turned on or off to suit user needs.
MIKE11	X	X		X	X	X					X		X		X						X	1D	Opt.	X	X	User can add a user-defined substance (e.g., salinity).
GRSM	X	X	X	#	#	X				X	X		X		X	X						1D	X	X		Species-specific dynamics for three algae/macrophyte spp.

X Constituent modeled

@ Dam reaeration only

\* NBOD simulated as nitrification of ammonia

# Specified by model users

DO Dissolved oxygen

Total N Total nitrogen

CBOD Carbonaceous BOD

NH3 Ammonia nitrogen

NBOD Nitrogenous BOD

NO2 Nitrite

SOD Sediment oxygen demand

NO3 Nitrate

Total P Total phosphorus

Phytoplankton Phytoplankton biomass

Organic P Organic phosphorus

Zooplankton Zooplankton biomass

PO4 Inorganic phosphorus

TDS Total dissolved solids

A review of the above table, and the individual model reviews in Section 4, reveals that model selection involves tradeoffs. We can conclude the following:

- QUAL2E/2K is probably not appropriate for the Grand River because of its steady-state formulation.
- MIKE-11 offers excellent flexibility and an outstanding user interface, especially if coupled with a powerful GIS framework as in MIKE-BASIN, but does not incorporate species-specific plant growth and is extremely high in cost. Its additional features probably would not justify switching from GRSM, especially since a switch to MIKE11 would also entail the loss of current species-specific modeling capability.
- WASP7 adds much more flexibility in terms of the physical configuration of the model, but lacks GRSM's species-specific plant growth dynamics. In addition, its plant growth kinetics appear out of date compared to those in GRSM. Its strengths, allowing two- and three-dimensional configurations, would not be of great benefit in the Grand River, and would not justify the loss of GRSM's strengths in plant growth simulation.
- HSPF is a comprehensive, extremely flexible, and highly appropriate model for the Grand. One weakness is that, like the other models, it simulates only a single generic benthic plant species. But the overriding concern about HSPF is its huge complexity and associated data requirements, and the lack of previous experience with it in the Grand River Basin. BASINS databases are not available for Canada, so required input data would have to be generated locally and probably at considerable time and expense.

We can therefore conclude that while individual models may simulate certain components more effectively than GRSM (for example, MIKE11's sediment dynamics, or HSPF's land-water linkage), GRSM is a highly effective, well understood, and well tested model appropriate for dissolved oxygen modeling in the Grand. Reference to Figure 1 suggests that GRSM probably should be categorized as a "research model" because of its highly developed plant growth dynamics, specialized for the three species of concern in the Grand River.

Over the longer term, GRCA should however review individual model components in the models reviewed here, and others, to determine areas where GRSM could be updated or strengthened for future applications. In particular, it will be important to reflect recent hydrogeologic and geomorphology field data in the model and improvements to low-flow hydraulic modeling capability. The challenge here will be to collate the considerable quantity of recent field data and bring it to bear on GRSM, to determine which changes may be most appropriate. For example, this review has shown that GRSM's simulation of sediment-water interactions may require strengthening, especially with respect to nutrient dynamics. These improvements may be especially important in the Central/Middle Grand reaches, where the urbanized core and associated effluent discharges has resulted in a more organic bed sediment load, with higher

nutrient concentrations, than elsewhere in the basin. Similarly, GRSM does not currently simulate phytoplankton growth or nutrient dynamics, but those components may be important in certain reaches. Finally, GRSM is currently configured around very long reaches, originally established to conform to field data collection stations. These reach lengths (and reach configuration) may no longer be appropriate, especially in light of significant improvements in understanding of river hydraulic, chemical, and biological phenomena, and extensive land use changes that have occurred in the watershed in the 30 years since the model was first developed.

**RECOMMENDATION 1:** GRCA should collate and review available data on the Grand River, and use it, possibly in a workshop setting with knowledgeable participants, to update the conceptual representation of the river. The revised conceptual model should reflect the considerable land use, geomorphic, and water quality changes that have occurred in the river over the last 30 years.

**RECOMMENDATION 2:** GRCA should use the revised conceptual model to review GRSM's current capabilities, especially with respect to reach length, reach configuration, sediment-water interactions, and detailed simulation of nutrient species (e.g., nitrate/nitrite; orthophosphorus, etc.), to determine where changes would be appropriate.

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