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Northeastern University**

TECHNICAL REPORT NO. 7

Review of Watershed Ecological Models

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DISCLAIMER

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Introduction

Different environmental problems like flooding, upland soil and streambank erosion, pollution from agricultural run off require the understanding of the natural processes leading to these problems. Mathematical models can be useful tools in simulating and simplifying these complex processes and help find solutions. When applied at the watershed-scale, these models can be used to assess the environmental conditions of a watershed. An ecological model is a mathematical expression that can be used to describe or predict ecological processes or endpoints such as population abundance (or density), community species richness, productivity, or distributions of organisms (Rousseau et al., 2000). Hence a watershed ecological model deals with endpoints at the watershed level, like population, ecosystem or landscape. Ecological models also serve as important tools for chemical risk assessment.

There are four basic steps (Rousseau et al., 2000) in developing ecological models. First, the problem is formulated and a conceptual model is developed. The next step is assessing the magnitude and frequency of exposure to the problem by the ecological receptors. Next, the potential effects of the problem on organisms are analyzed and exposure-response relationships are developed. The fourth step is risk characterization in which the results of the exposure to the problem and its effects analyses are combined to evaluate the likelihood of adverse effects on ecological receptors. In this step the values for all the parameters in the model are defined and parameters are adjusted in a model calibration exercise. Sensitivity analysis is performed and the ecological significance of any identified risks is also described in this final step.

This document is a review of seventeen watershed ecological models. Each of these models has been analytically reviewed and discussed along with their conceptual model, and a brief history of its development. Also, some important applications of each of these models are presented. These models are AQUATOX (release 2.1), System Impact Assessment Model (SIAM), Geography Referenced Regional Exposure Assessment Tool for European Rivers (GREAT-ER), ECOTOX, EcoWin2000, Risk Analysis and Management Alternatives Software (RAMAS), CompMech, Decision Support System for Evaluating River Basin Strategies (DESERT), Spreadsheet Tool for River Environmental Assessment Management and Planning (STREAMPLAN), Deterministic and Stochastic Matrix Models, VORTEX (version 9.58 7), Stream Reach Management, an Expert System (STREAMES), Gestion Intégrée des Bassins versants à l'aide d'un Système Informatisé (GIBSI), Contaminants in Aquatic and Terrestrial ecosystems (CATS), Green Bay Mass Balance Study (GBMBS), Across Trophic Level System Simulation (ATLSS), and Patuxent Landscape Model (PLM).

Amongst the models reviewed, AQUATOX 2.1 was chosen to run various simulations of the eutrophication problem in Clear Lake, California. AQUATOX has a very user-friendly input interface and a graphic output interface that helps the modeler to easily understand and summarize the results of the model. It is suitable to use AQUATOX where the user needs to understand the processes relating the chemical and physical environment with the biological community. This seemed a very relevant choice for the eutrophication problem of the Clear Lake in California. AQUATOX also has the capability of probabilistic modeling approaches so that the implications of uncertainty in the analyses can be considered. The different simulation scenarios for Clear Lake, detailed parameter descriptions and model outputs have been presented in the Appendix of this document.

AQUATOX (release 2.1)

Developer:

Richard A. Park of Eco Modeling and Jonathan S. Clough of Warren Pinnacle Consulting with EPA funding.

AQUATOX Model Description:

AQUATOX is the latest in a long series of models, starting with the aquatic ecosystem model CLEAN (Park et al., 1974) and subsequently improved in consultation with numerous researchers at various European hydrobiological laboratories, resulting in the CLEANER series (Park et al., 1975, 1979, 1980; Park, 1978; Scavia and Park, 1976) and LAKETRACE (Collins and Park, 1989). The MACROPHYTE model, developed for the U.S. Army Corps of Engineers (Collins et al., 1985), provided additional capability for representing submersed aquatic vegetation. Another series started with the toxic fate model PEST, developed to complement CLEANER (Park et al., 1980, 1982), and continued with the TOXTRACE model (Park, 1984) and the spreadsheet equilibrium fugacity PART model. AQUATOX combined algorithms from these models with ecotoxicological constructs; and additional code was written as required for a truly integrative fate and effects model (Park, 1990, 1993). The model was then restructured and linked to Microsoft Windows interfaces to provide greater flexibility, capacity for additional compartments, and user friendliness (Park et al., 1995). Release 1 from the EPA was improved with the addition of constructs for chronic effects and uncertainty analysis, making it a powerful tool for probabilistic risk assessment. Release 1.1 provided a much enhanced periphyton submodel and minor enhancements for macrophytes, fish, and dissolved oxygen. The latest release of 2.1 which is published in October 2005 has a number of major enhancements. To further assist in modeling nutrients AQUATOX has been significantly updated since release 2 was released. There have also been several enhancements related to toxicity, along with improvements to the user interface, including:

- a large increase in the number of biotic state variables, with two representatives for each taxonomic group or ecologic guild;
- a multi-age fish category with up to fifteen age classes for age-dependent bioaccumulation and limited population modeling;
- an increase in the number of toxicants from one to a maximum of twenty, with the capability for modeling daughter products due to biotransformations;
- computation of “chlorophyll a” for periphyton, bryophytes and phytoplankton;
- fish biomass is entered and tracked in g/m^2 ;
- options of computing respiration and maximum consumption in fish;

- respiration in fish is density-dependent;
- fish spawning can occur on user-specified dates as an alternative to temperature-cued spawning;
- elimination of toxicants is more robust;
- settling and erosional velocities for inorganic sediments are user-supplied parameters;
- uncertainty analysis now covers all parameters and loadings;
- more realistic tracking of nutrients;
- un-ionized ammonia (which may be toxic) and variable pH may now be simulated;
- the user can now get have Steinhaus¹ community similarity indices calculated and exported;
- AQUATOX is now an extension to BASINS, providing linkages to geographic information system data, and HSPF and SWAT simulations.

Purpose (decision making/academic tool/etc.):

AQUATOX is developed for simulation of aquatic systems. AQUATOX predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants. It has been implemented for streams, small rivers, ponds, lakes, and reservoirs. This model is a valuable tool for ecologists, biologists, water quality modelers, and anyone involved in performing ecological risk assessments for aquatic ecosystems.

Basic description:

AQUATOX simulates the transfer of biomass, energy and chemicals from one compartment of the ecosystem to another. It does this by simultaneously computing each of the most important chemical or biological processes for each day of the simulation period; therefore it is known as a process-based or mechanistic model. AQUATOX can predict not only the environmental fate of chemicals in aquatic ecosystems, but also their direct and indirect effects on the resident organisms. Therefore it has the potential to establish causal links between chemical water quality and biological response and aquatic life uses. AQUATOX differs from most water quality models in several ways. Most models include few if any biological components, whereas AQUATOX is an ecosystem model. It includes not only numerous types of plants, invertebrates and fish, it also treats the biota as interacting with the chemical/physical system.

AQUATOX can model numerous inter-related components in aquatic ecosystems, known as the state variables:

¹ The Steinhaus index can be used as one measure of how the predicted composition of the biotic communities varies between simulations.

- phytoplankton (multiple species)
- periphyton and submerged aquatic vegetation (multiple species)
- planktonic and benthic invertebrates (multiple species)
- forage, game, and bottom fish (multiple species)
- nutrients and dissolved oxygen
- organic and inorganic sediments
- toxic organic chemicals (up to 20 different chemicals simultaneously)

AQUATOX is not intended to include every species of plant or animal that can exist in an aquatic habitat or every ecological process, but attempts to characterize the significant factors that determine the functioning of the ecosystem.

Aquatic ecosystems represented by AQUATOX includes: vertically stratified lakes, reservoirs and ponds, rivers and streams, experimental ponds ("mesocosms"). As in many water quality models, AQUATOX assumes that the water body is uniformly mixed, except where vertical stratification occurs in lakes and reservoirs.

AQUATOX is a process-based model, meaning that it explicitly simulates the numerous biological and ecological processes that operate to link the ecosystem together. In this way it predicts the environmental fate (includes; nutrient cycling and oxygen dynamics / partitioning of organic toxicants to water, biota and sediments/ toxic organic chemical transformations/ bioaccumulation through gills and diet) and ecological effects (include: food consumption/ growth and reproduction/ natural mortality/ acute and chronic toxicity/ trophic interactions) of the various environmental stressors.

AQUATOX also provides the capability of probabilistic modeling approaches so that the implications of uncertainty in the analyses can be considered. It is possible by allowing the user to specify the types of distributions and key statistics for any and all input variables. Depending on the specific variable and the amount of available information, any one of several distributions may be most appropriate but a lognormal distribution, which is the most commonly used for environmental and pollutant loadings, is set as the default. In the uncertainty analysis, the distributions for constant loadings are sampled daily, providing day-to-day variation within the limits of the distribution, reflecting the stochastic nature of such loadings. A useful tool in testing scenarios is the multiplicative loading factor, which can be applied to all loads.

The conceptual ecosystem model represented by AQUATOX is showed in Figure 1 below.

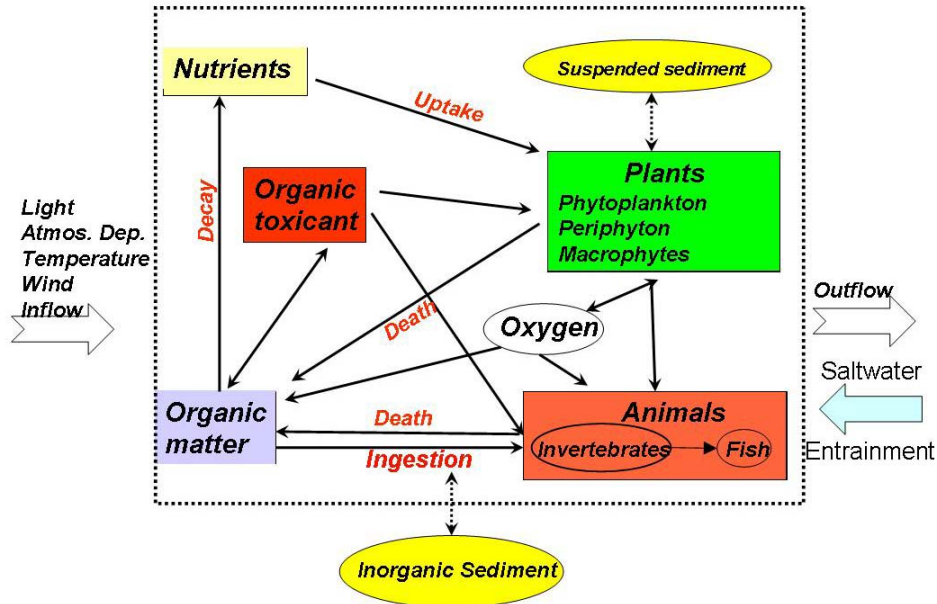


Figure 1. Conceptual model of ecosystem represented by AQUATOX.

AQUATOX Model Application:

AQUATOX has a myriad of potential applications to water management issues and programs, including water quality criteria and standards, TMDLs (Total Maximum Daily Loads), and ecological risk assessments of aquatic systems. AQUATOX can be used to predict ecological responses to proposed management alternatives. It may help to determine the most important of several environmental stressors, e.g. where there are both nutrients and toxic pollutants.

The choice of an appropriate model or other tool depends upon the kinds of questions to be answered, the complexity of the situation, and the consequences of the outcome. AQUATOX should be considered where the user needs to understand the processes relating the chemical and physical environment with the biological community.

- Where ecological and biological processes are complex
- Where indirect effects are important but difficult to monitor
- When one needs to articulate linkages between nutrients and biotic community
- Where the environmental conditions may change appreciably

The following examples are some illustrations of potential applications:

- Recovery Following PCB Remediation
- Recovery Following PCB Remediation

- Nutrient Enrichment
- Pesticides in a Pond Mesocosm
- Multiple Stressors Due To Agricultural Runoff

AQUATOX has been validated with several data sets from diverse sites and applications; however, like any complex model, it should be evaluated for the intended use. Three model validation studies performed for different environmental stressors and in different water body types. The validations were performed for;

- Version 1.66 with data from Lake Onondaga, New York,
- Version 1.66 with data from Coralville Reservoir, Iowa'
- Version 1.68 for predicting bioaccumulation of PCBs in the Lake Ontario food web.

Detailed reports on model validation, including analysis of model predictions as compared to observed data, are found in US EPA ,2000.

The AQUATOX periphyton submodel was also successfully calibrated and validated with data from Walker Branch, Tennessee. It has performed based on the weight of evidence of production of observed patterns of biomass change, concordance of maxima between predicted and observed biomass, and equivalence in predicted and observed means and variances as confirmed by relative bias and F tests.

System Impact Assessment Model (SIAM)

Developer: United States Geological Survey (USGS).

SIAM Model Description:

The System Impact Assessment Model (SIAM) was developed by the United States Geological Survey, Fort Collins Science Center. They recently released version 4.0 in October 2005 with multiple updates from the version 3.0 which include a new splash screen and help file documentation (Bartholow, J.M. and et. al, 2005). The SIAM model included multiple sets of models and data which are used to evaluate and compare the potential impacts of water management alternatives from an ecological perspective. The goal directly from the U.S. Geological Survey report on Evaluating Water Management Strategies with the Systems Impact Assessment Model: SIAM Version 4 (Revised October, 2005), “is to further the process of reaching a decisive consensus on management of water resources in order to stabilize and restore riverine ecosystems, and its meant to be used in the context of the Instream Flow Incremental Methodology (IFIM)” (Bartholow, J.M. and et. al, 2005), which is a 5 phase method developed by the U.S. Geological Survey to evaluate relationships between ecology and hydrology (Bovee, K.D., 1998).

SIAM consists of five different models that all serve different purposes. The five models are MODSIM (water quantity), HEC-5Q (water quality), PHABSIM and Time Series Library (physical habitat), and SALMOD (fish production model). The fifth model is the Ecosystem Health Model (ecological health model). Figure 2 below shows how each of the different models are linked.

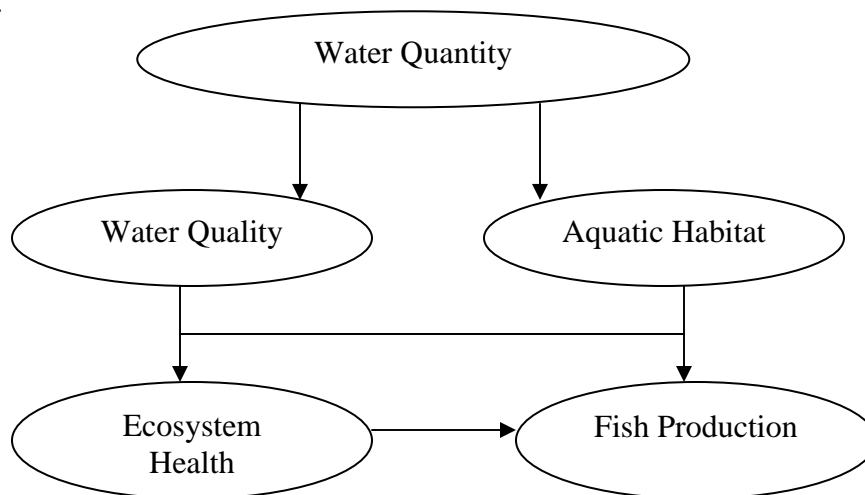


Figure 2. Schematic of the System Impact Assessment Model.

MODSIM is a deterministic dynamic model used to simulate water quantity developed by Colorado State University. MODSIM has the ability to predict stream flow and track reservoir volumes (Bartholow, J.M. and et. al, 2005). The structure of MODSIM is based on a prioritization scheme to model flows throughout the system (river) based on different constraints of flow, water allocations, and agricultural demands for irrigation. MODSIM uses a series of nodes and links where the nodes are considered storage and non-storage features (reservoirs, inflow locations, stream gage locations) and links represent water conveyance (reaches, canals, and tunnels). The temporal scale of MODSIM is on a monthly frequency for SIAM but MODSIM has the ability to operate on a weekly or daily input preparation.

Once the results have been obtained from MODSIM they are passed on to the Army Corps of Engineers program of HEC-5Q (deterministic dynamic model), which has the ability to simulate water quality parameters. HEC-5Q of SIAM has been set up for mean daily simulation for water quality. For more information about the HEC-5Q model please refer to US Army Corps of Engineers, 1986.

The components of MODSIM are inputs into the physical habitat model of PHABSIM (Physical Habitat Simulation System) and TSLIB (Time Series Library). PHABSIM and TSLIB are deterministic dynamic models where both models relate instream flow/discharge from reservoirs to indices of aquatic habitat availability through time. The theory of PHABSIM is based on the quantity and quality physical habitat is related to the environmental needs of aquatic life (Milhous, R.T., 1999). PHABSIM is a specific model designed to calculate an index to the amount of microhabitat available at different life stages at different flow levels. PHABSIM is executed in four major steps, which include the following. The first step is to simulate water surface elevations, the second is to simulate velocities, the third is to simulate the physical habitat versus stream flow relationship, and the fourth is to simulate the physical habitat when combinations of flows are involved (Milhous, R.T., 1999).

The fish production model of SALMOD (designed by the U.S. Geological Survey) is a deterministic dynamic model written in FORTRAN 90 with the graphical user interface written in C++ (Everette, L, 2003). The foundation of the SALMOD model is based on egg and fish mortality, which is directly related to the quantity of stream flow and various meteorological variables. The model simulates the dynamics of resident and anadromous (migrating up rivers from the sea to breed in fresh water) species. "Model processes are implemented such that the user (modeler) has the ability to more-or-less program the model on the fly to create the dynamics thought to animate the population. SALMOD then tabulates the various causes of mortality and the whereabouts of fish" (Everette, L, 2003). The biological time step for SALMOD is based on the spawning activities (week 1) for salmon and the variables of mortality

and growths are updated on weekly bases. SALMOD can only model one reach at a time, considered one linear segment. If a watershed model wants to be performed each segment has to be modeled separately.

The Ecosystem Health model is an internal component built into SIAM. Certain criteria are identified by “red flags” when they have exceeded criteria through time and space. It is not considered a model but a compilation of criteria, which would affect the limit of fish populations (Bartholow, J.M. and et. al, 2005). In general terms these criteria are considered flow quantity or quality, or habitat quality. The strength of this model is based on the facts it can quickly examine large amounts of data to determine if they exceeded criteria created by the user (Bartholow, J.M. and et. al, 2005).

SIAM Application:

The SIAM model was used on the Klamath River, which flows from Oregon to California and eventually into the Pacific Ocean (Figure 3). Ever since the 1950's the basin has become more populated and resulted in an increase in water demand. The increase in water demand has caused some serious drought conditions and there was concern for the anadromous population. The species of coho salmon was considered an endangered species in 1997 and there have been the conversion of natural marshes in the headwaters that have been irrigated to pasture and agricultural land use (Flug, M., and S.G. Campbell, 2005).

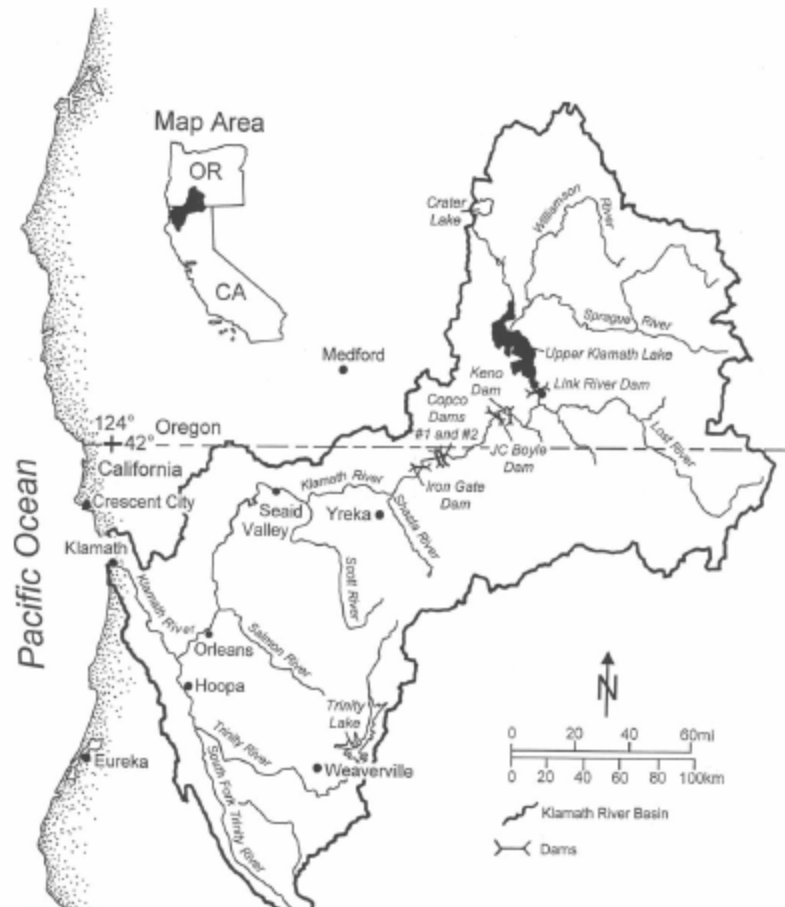


Figure 3. Map of the Klamath Basin

The water quantity model MODSIM developed for the Klamath River was considered excellent because there was only a 0.1% difference during calibration between the model and the actual U.S. Geological Survey gauge locations and a 1.0% difference for validation. Once all of the individual models that are part of SIAM are complete it was concluded that there was not adequate water in low flow years to meet target water storage levels for endangered species. It was also concluded in the simulation that increase in water quantity did not improve water quality conditions for salmonids. This was a common belief by water resource conservationists in the region. Please refer to Flug, M., and S.G. Campbell (2005) for a complete report on the drought allocations using the SIAM model on the Klamath River.

Geography Referenced Regional Exposure Assessment Tool for European Rivers (GREAT-ER)

Developer: Environmental Steering Committee of the European Union.

GREAT-ER Model Description:

Geography Referenced Regional Exposure Assessment Tool for European Rivers (GREAT-ER) is a GIS assisted model for environmental risk assessment and management of chemicals in river basins. The software is publicly available and was developed as part of the European Chemical Industry Long Range Initiative. The purpose of the model is for it to be used under the European Union regional environmental risk assessment. GREAT-ER uses the Monte Carlo method to provide a stochastic approach; as a result the number of iterations performed during the simulation has to be inputted (Koorman, F., Wagner, J.O., Boeije, G., and A. Young, 1999). The output from the model is able to provide Predicted Environmental Concentrations (PEC's). These PEC's concentrations are then able to be compared to lethal concentrations of aquatic organisms and species.

There are two models that are part of the GREAT-ER Model, a hydrologic model and a chemical fate simulator. The chemical fate and transport model is a hybrid model which uses a stochastic (Monte Carlo) method and deterministic techniques while the core of the model is deterministic. It should be noted that during the simulation the river network, flow velocity, flow volume, discharge point locations, treatment plant information. For complete details on how the chemical fate and transport hybrid model works please refer to Boeije, G.M., Vanrolleghem, P.A. and Matthies, M. (1997). Due to the facts that the model is for the European Union with a wide range of river flows across space and time estimates of the magnitude and variability of river flow velocities at ungauged river reaches are essential components of GREAT-ER. The Mediterranean region typically has dry summers (limited flash floods) with high winter flows. The main components to the hydrologic model are to have a river network level and a digital elevation level. The hydrologic model for ungauged rivers is based on long term annual rainfall, potential evaporation, and annual runoff depth.

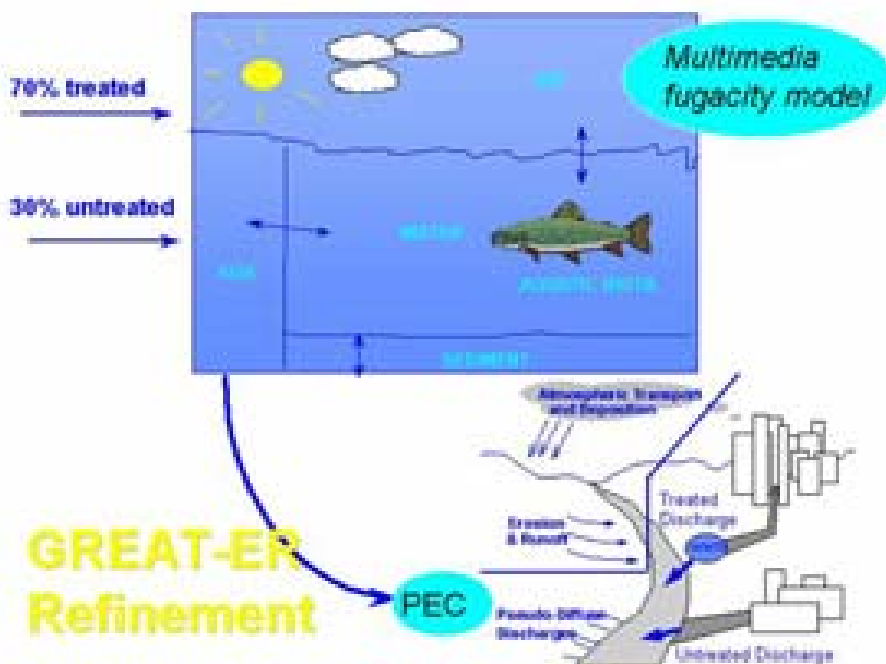


Figure 4. Schematic of how the GREAT-ER model functions.

GREAT-ER Model Application:

The GREAT-ER model was used in the Aire catchment in Yorkshire, UK to predict the environmental concentration for boron. The aim of the project is to develop a model which can be used, within the European Union, to improve the predictions of the concentrations in rivers of chemicals from household products. Measured boron concentrations were performed within 33 locations every month on two major reaches within the Aire catchment over for a two year period. The model predictions for most of the boron concentration means in the catchment were within one standard deviation of the measured values (Fox, K.K., Daniel, M., Morris, G., and M.S. Holt., 2000). Because of the model predictions were within one standard deviation of the measured values the model predictions are within the realm of error expected during actual sampling. By determining the boron concentrations known in different reaches the ecological toxicity to aquatic life could be calculated.

ECOTOX

Developer: United States, Environmental Protection Agency (EPA) and the U.S. Department of Defense's Strategic Environmental Research and Development Program (SERDP)

ECOTOX Model Description:

ECOTOX database is supported by U.S. Environmental Protection Agency and contains a broad review of toxic chemical effects on several ecologic endpoints (U.S. EPA, 2000). Even though ECOTOX is not a model itself, it contains the results of a great review of toxicological tests done with different types of chemicals and on different endpoints. The different endpoints measured are the lethal, sub lethal and residue effects of single (not mixed) chemicals on aquatic, terrestrial species or plants. ECOTOX is composed of four main databases:

- **Aquatic Toxicity Information Retrieval (AQUIRE):** created in 1981 by the Mid-Continent Ecology Division in Duluth, MN (MED-Duluth) with assistance from the Office of Toxic Substances and the Office of Water. AQUIRE was initially released to governmental users in 1987. In 1999 AQUIRE was made available to the general public via World Wide Web. AQUIRE includes the lethal, sublethal effects of different chemicals on species that are exclusively aquatic. Amphibians are also included in AQUIRE as well as in TERRETOX which will be discussed later.
- **PHYTOTOX:** the database was developed at the National Health and Environmental Effects Research Laboratory (NHEERL), West Ecology Division in Corvallis, OR (WED-Corvallis) in the early 1980. Currently PHYTOTOX is maintained at MED-Duluth. PHYTOTOX is a database that contains lethal and sublethal toxic effects data for terrestrial plants. PHYTOTOX is basically focused on agricultural chemicals and agricultural plant species. Data available in PHYTOTOX range from 1926 to present.
- **TERRETOX:** the database contains sublethal toxic effects data for terrestrial animals and amphibians. Created also at WED-Corvallis, OR. Currently maintained by MED-Duluth. The data available in TERRETOX goes from 1969 present.

ECOTOX became a unified database composed by the previous three databases in 1995. The U.S. Department of Defense's Strategic Environmental Research and Development Program (SERDP) and the U.S. EPA's Office of Research and Development funded MED-Duluth to develop a unified data retrieval interface integrating AQUIRE, PHYTOTOX and TERRETOX. In 1996 ECOTOX was released to governmental users and to general public in year 2000.

Models Using ECOTOX Data: Quantitative Structure- Activity Models (QSAR)

ECOTOX database is widely used for quantitative structure-activity relationship (QSAR) models to predict toxic effects to biota. Some regulatory programs rely in such models. Even though databases such as ECOTOX provide information about toxicity of a specific chemical on a specific species (usually an aquatic species), it would not be feasible to test each one of the chemicals available in the market on every known species. QSAR models are useful to predict toxic effects to biota (Moore et al., 2003) and can have mechanistic and/or probabilistic approaches depending on the accuracy of the data available and rely on chemical toxicity data (such as molecular size) of tested chemicals or biological parameters to model toxicity effects of a specific chemical on a specific endpoint. Deterministic approaches in QSAR models can only be used when detailed knowledge of the chemical structure and the biological receptor exist. Otherwise statistical methods are usually used. Usually probabilistic models based on concentration-exposure theories are used to assess the effects on endpoints and, hence, ecological risk assessment in the area under study. (Johnston et al., 2001; Morton et al., 2000; Sadiq et al., 2003) Some toxicological models introduce stochasticity or variability to the probabilistic calculations using Monte Carlo simulations or Bayesian methods as recommended by the U.S. Environmental Protection Agency (Lin et al.,2004; MacIntosh et al.,1994). Bayesian networks are probabilistic tools that are becoming more and more promising in ecological risk assessment and water resources management fields due to its ability to introduce uncertainty and linking a wide range of different parameters based on probabilistic dependencies (Borsuk et al., 2003; Bromley, 2005; Sadoddin et al., 2005).

ECOTOX (QSAR) Model Applications:

Some QSAR models currently available and widely used are the following (Moore et al.,2003):

- **Assessment Tools for the Evaluation of Risk (ASTER):** ASTER was developed by U.S. EPA Office of Solid waste and Emergency Response. The main goal of this model was to assist regulators in hazard ranking and development of comprehensive risk assessments. ASTER provides high quality information about toxic effects of chemicals included in the ECOTOX's AQUIRE database or deterministic estimates (simple linear regressions or bilinear regressions) if the chemicals are not included in AQUIRE. ASTER's QSAR module was developed with a set of 617 organic chemicals tested with fathead minnow in an acute 96-h bioassay with the LC50 as the calculated endpoint. The chemical inputs in the ASTER model can be introduced using the CAS code (Chemical Abstract Number) the chemical name or a Simplified Molecular Input Line Entry System (SMILE) code. ASTER is not available on the EPA web-site due to funding limitations (U.S. E.P.A. , 2002)

- **Ecological Structure Activity Relationships (ECOSAR):** this model is extensively used by U.S. EPA Office of Pollution Prevention and Toxics. The computer program is used to estimate the toxicity of chemicals used in industry and discharged into water. The program predicts the toxicity of industrial chemicals to aquatic organisms such as fish, invertebrates, and algae by using Structure Activity Relationships (SARs). ECOSAR relies on deterministic approaches (linear regressions) that usually relate toxicity to some specific characteristic of the chemical (such as octanol/water partition coefficient, K_{ow} and molecular weight). ECOSAR is able to determine the chemical's acute toxicity (short-term) and the chronic toxicity, if available. The chemical inputs are also entered with the SMILE code. The software is available in the EPA's web-site (U.S. EPA, 2000). The latest version is ECOSAR v.099g.
- **TOPKAT:** this program uses multiple regression analysis to develop quantitative predictions of toxicity. TOPKAT has the capability to determine whether the structure of the chemical under study is within the optimal prediction space (OPS) of the multiple regression model. This is useful to determine the confidence interval in a toxicity prediction.

TOPKAT's latest version is TOPKAT 6.2 and can calculate up to 16 endpoints such as LC50, mutagenicity, carcinogenicity etc. and also uses the SMILES code for input entry. TOPKAT also assigns structural descriptors to the chemicals contained in the database. Databases such as AQUIRE, using toxicity (96-h LC50) on fathead minnow can be used. The comparison between the chemical under study structural descriptors and those stored in the database will determine the toxicity of the chemical. TOPKAT can be obtained in the developer web-page (Accelrys[®], 2006). Some current applications of TOPKAT are the following:

- Chemical tests based on toxicity.
 - Determining toxicity of chemical compounds and providing manufacturers with early decision-making capabilities for changing the process or compound
 - Responding to constantly emerging regulatory standards and requirements quickly and cost-effectively
- **Neural Networks: Probabilistic Neural Nets (PNN) and Computation Neural Nests (CNN)**

Neural networks are designed to learn from data in a way that emulates a simple brain and are usually used when insufficient knowledge exists to write a mechanistic model or design an expert system. Many Neural networks use a back-propagation algorithm to

learn, which is achieved by adjusting iteratively the weights to minimize the error between the network predictions and the measured toxicity values at the endpoints under study. Neural networks have several advantages over other methodologies: They can handle higher-order interactions between variables and non-linearities and have no need of input-data classification. In the study by Moore et al. (2003), Neural net methods had better performance than other methodologies, especially probabilistic neural nets.

ECOWIN 2000

Developer:

João Gomes Ferreira, Geochemical and Ecological Modeling group (GEM), Faculty of Sciences and Technology, New University of Lisbon.

ECOWIN Model Description:

The system has been developed over the last 10 years, and runs on WindowsNT and Windows 95 or 98 (Server of Ecological Models). The first version was published in 1995 by Ferreira (Ferreira, 1995). It seems that Ecowin2000 is the second edition and there is no other release between and beyond them. This model does not have a good technical support. However it has been used as part of EASA²'s package.

Purpose:

EcoWin2000 is an ecological modeling system which is used to simulate changes in the water quality and ecology of rivers, lakes, estuaries and coastal waters. The architecture of the system was described in detail in a paper published in the journal of Ecological Modeling; Ferreira, 1995 (Server of Ecological Models).

Basic (Server of Ecological Models):

EcoWin2000 consists in a shell, which manages the input and output, and a set of "objects" which perform the calculations. The software is written in C++, and the model objects encapsulate different forcing functions and state variables, which may be turned on and off for a particular simulation. MS-Excel is used as a platform between the model and the user, both for building the necessary input files to run a model and for generating output of results. User files are stored in native Excel 97 format.

EcoWin2000 is used to build dynamic models, which may vary only with time (zero-D), or may vary also in space: longitudinally (one-D), in two dimensions (two-D), or in layers (three-D). It is also easy to changing the system morphology and bathymetry, and making alterations to pollutant loads, or other system boundary conditions, and deciding what objects your model will use for its calculations.

² Ecosystem Approach to Sustainable Aquaculture (EASA) is an EU funded Framework 6 RTD project with 16 research partners from 13 member states. It is the successor to several 4th and 5th Framework Programme projects which have helped to push forward our understanding of the effects of aquaculture on the environment especially in the Mediterranean (Ecosystem Approach for Sustainable Aquaculture).

However, it is necessary to be fluent in C++ in order to extend the functionality of a particular object - for instance you may be using a phytoplankton object in your model and decide to extend its properties to allow it to grow only when silica is present - i.e. to become a diatom. For that, you need to write a few lines of code (Server of Ecological Models).

A simplified scheme based on the Carlingford Lough model which is used in EcoWin2000 is illustrated in the following figure.

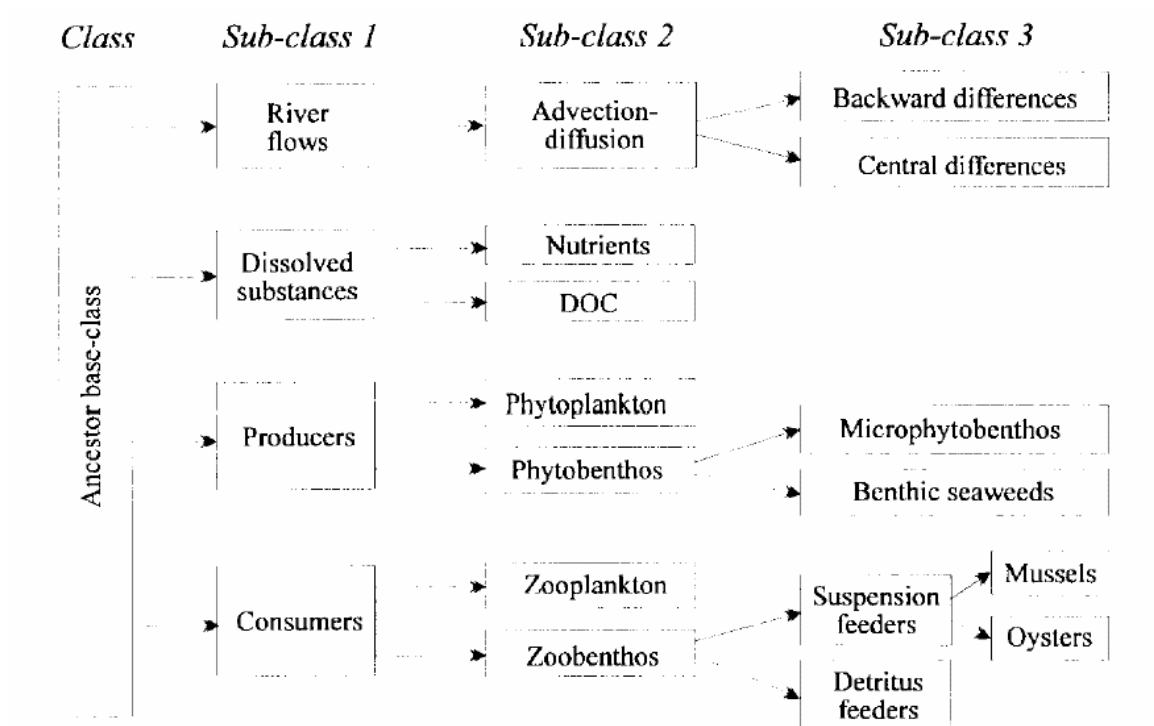


Figure 5: Simplified scheme of a typical object hierarchy, showing taxonomic relation in EcoWin (Ferreira, J.G., 1995).

Several target organisms have been considered in this model including; mussels, oysters, scallops and shrimp, under different culture conditions (monoculture and polyculture). This modeling approach considers key processes at the ecosystem scale that condition individual scope for growth, and simulates individual growth and population dynamics of cultivated species (Ecosystem Approach for Sustainable Aquaculture).

Typical outputs include:

- Effects of overstocking on exploitation carrying capacity;
- Yield response to changes in culture practice;

- Impacts on target species of changes in anthropogenic inputs;
- Environmental modifications due to changes in aquaculture pressures (e.g. phytoplankton depletion).

Application and Examples:

The EcoWin2000 ecological model has been used in systems in the EU and China, and is currently being applied in southern Africa (Ecosystem Approach for Sustainable Aquaculture). It is mostly used for the estuarine ecological modeling. In the following publications some application examples of EcoWin200 are reported;

A.M.Nobre, J.G.Ferreira, A.Newton, T.Simas, J.D.Icely, R.Neves, 2005. Management of coastal eutrophication: Integration of field data, ecosystem-scale simulations and screening models. *Journal of Marine Systems*, 56 (3/4), 375-390.

Alvera-Azcarate, A., Ferreira, J.G., & Nunes, J.P., 2003. Modelling eutrophication in mesotidal and macrotidal estuaries. The role of intertidal seaweeds. *Estuarine, Coastal and Shelf Science*, 57(4), 715-724.

Nunes, J.P, Ferreira, J.G., Gazeau, F., Lencart-Silva, J., Zhang, X.L, Zhu M.Y. & Fang J.G., 2003. A model for sustainable management of shellfish polyculture in coastal bays. *Aquaculture*, 219/1-4, 257-277.

Risk Analysis and Management Alternatives Software **(RAMAS®)**

Developer: Applied Biomathematics®

RAMAS Model Description:

RAMAS® is a software package widely used in ecological model construction (Akçakaya,2000a Brook et al., 2000,Ginzburg et al., 1990, Godbout et al., 2004) . RAMAS® contains specific data to predict the future changes in the population due to alteration of one or several parameters that can affect the endpoints under study. Risk assessments for species extinction, explosion or recovery are also available with RAMAS® software. There are nine different RAMAS® modules available. Each one of these modules can model different parameters affecting endpoints under study. Some modules included in RAMAS® useful for watershed ecological modeling are the following:

- **RAMAS Red List:** Version 2.0 classifies the species under study assigning a level of threat following the guidelines set by the International Union for the Conservation of Nature (IUCN). The inputs in the model are related to species individual number. The input can be a number, a range or a range plus an estimated number. Depending on the input level of uncertainty, the output can be a single category or a range between different categories. The way RAMAS Red List incorporates uncertainty is based on fuzzy logic approach and it's defined in Akçakaya et al. (2000b). The categories in which RAMAS Red List can classify the species are: extinct, extinct in the wild, critically endangered, vulnerable, near threatened, least concern or data deficient.
- **RAMAS Metapop:** most species are structured in fragmented habitats due to environmental or anthropogenic barriers. The input for the model is species-specific information of the dynamics of each population, the spatial structure and the interaction among populations. Some of the outputs obtained from RAMAS Metapop are risk of species extinction; risk of metapopulation decline to a range of abundances, probability of population growth to a range of abundances etc. The model is probabilistic but stochasticity from environmental and demographic variables can be incorporated. (Pastorok et al., 2002) RAMAS Metapop have high regulatory acceptance and is currently used by several regulatory agencies (Pastorok et al., 2002).

- **RAMAS GIS:** this module of the program is exactly the same as RAMAS Metapop but introduces a GIS system that is very useful to assess habitat suitability. RAMAS GIS uses a patch-recognition algorithm and identifies suitable areas as patches where some population can survive. RAMAS GIS is linked to the population model (demographic input) and both are used to perform the Population Risk Analysis. RAMAS GIS introduces stochastic methods in risk analysis using a method called matrix selection (Akçakaya, 2000c).
- **RAMAS Landscape** this module includes RAMAS GIS (and therefore RAMAS Metapop) and a landscape model, LANDIS. Under such a model, the ecological endpoints in the species under study can be measured based on the predicted changes in the landscape in where they live. LANDIS is a well known model with a high number of publications and is supported by agencies like the U.S. Forest Service, Department of Agriculture and funded by others like NASA. It's based on stochastic simulations of parameters such as wind or fire and it's available on-line . The last version of LANDIS is LANDIS-II . A successful application of RAMAS Metapop and LANDIS was tested by Akçakaya (2001).
- **RAMAS Multispecies Assessment:** this module is built with RAMAS GIS (therefore, habitat suitability maps) and introduces a metapopulation model. The overlaying of the maps resulting from the two models (habitat and population) result in a Multi Species Conservation value (MCV) which is obtained by the sum of different extinction risks and contribution of each species to that extinction risk. The MCV is a useful figure used for landscape conservation, planning, and management.
- **RAMAS Ecotoxicology and RAMAS Ecosystem:** these two models carry out ecological risk assessments based on two concepts, food chain (RAMAS Ecosystem) or structured single populations (RAMAS Ecotoxicology). RAMAS Ecotoxicology is used to perform population-level ecological risk assessments for environmental contaminants. It imports data from standard laboratory bioassays, incorporates these data into the parameters of a population model, and performs a risk assessment by analyzing population-level differences between control and impacted samples. RAMAS Ecosystem is used to trace the path followed by the contaminants through the food chain, taking into account factors such as bioaccumulation, dose-response and predator-prey functions to simulate dynamics and estimate risk or adverse events. Both models use probabilistic approaches to estimate the effects of toxic substances on the endpoints and also use Monte-Carlo simulations to account for environmental and demographic stochasticity and treatment of error (Pastorok et al., 2002).

- **RAMAS CAST:** this module is used to identify clusters within the data available. CAST uses several statistical methods to identify possible clusters present in the data such as Knox, Mantel, Ederer-Meyer-Mantel, nearest neighbor etc. Identification of clusters may be useful for planning or management.
- **RAMAS STAGE:** analyzes discrete-time models for species with virtually any life history. It is useful for modeling species with complex life histories or other biologies in which stage membership (rather than age) determines the demographic characteristics of an individual. RAMAS STAGE can perform a risk assessment based on general life histories and environmental fluctuations. RAMAS Stage is a novel implementation of a Lefkovitch matrix (an evolution of the Leslie matrix). Leslie matrix is explained in more detail in another section of this report. RAMAS Stage was originally developed for the United States electric power industry under the sponsorship of the Electric Power Research Institute (EPRI).

CompMech

Developer: Electric Power Research Institute (EPRI).

CompMech Model Description:

CompMech is a program which its final goal is to assess ecological and economic consequences for different scenarios implemented by utilities companies. CompMech can predict fish population response to increased mortality, loss of habitat and release of toxicants. CompMech is based on the idea that the most abundant species have compensatory mechanisms to offset decreased growth, reproduction or survival of some individuals by increasing these same rates in the rest of individuals within the same population (Pastorok et al., 2002, Jager et al., 1999).

The CompMech approach over the past decade has been to represent in simulation models the processes underlying the growth, reproduction, and survival of individual fish and then to aggregate over individuals to the population level. The models can be used to make short-term predictions of survival, growth, habitat utilization, and consumption for critical life stages. For the long term, the models can be used to project population abundance through time to assess the risk that the abundance will fall below some threshold requiring mitigation. If mitigation is required, alternative measures can be evaluated using the model. For both short and long-term predictions, the model is used to compare the consequences and economics of alternative operational scenarios and to provide a perspective on the incremental effects attributable to plant operation as compared to natural mortality and other impacts such as fishing. (EPRI, 2006) Models have been developed and applied to key species representing a cross-section of life-history strategies. These particular species are known to experience mortalities and/or habitat alterations because of the operation of steam and hydroelectric generation facilities. Models for additional species are developed by modifying modules from these existing models. The models can be used to make short-term predictions of survival, growth, habitat utilization, and consumption for critical life stages. For the long term, the models can be used to project population abundance through time to assess the risk that the abundance will fall below some threshold requiring mitigation. If mitigation is required, alternative measures can be evaluated using the model. For both short- and long-term predictions, the models are used to compare the consequences and economics of alternative operational scenarios and to provide a perspective on the incremental effects attributable to plant operation as compared to natural mortality and other impacts such as fishing. Some of the applications that have been carried out with CompMech (CompMech, 2006).

CompMech is designed to use as much or as little site-specific data as is available. The need for site-specific data is determined primarily by the assessment issues and the costs of regulatory alternatives (i.e., more-costly decisions might warrant more-extensive site-specific data collection). The abiotic environment is characterized spatially and temporally in terms of the dominant physical and chemical variables thought to influence the dynamics of the population(s) of concern. The types of fisheries information typically collected during monitoring programs, such as density, size, and age composition, are used to characterize the fish populations. Data on prey availability and predation intensity can be useful but are not essential. Data on fecundity, bioenergetic parameters relating to consumption and respiration, and acute and chronic responses to toxicants are usually obtained from the literature (EPRI, 2006).

CompMech Model Application:

CompMech has been applied by utilities and resource management agencies in assessments involving direct mortality due to entrainment, impingement, or fishing; instream flow; habitat alteration (e.g., thermal discharges, water-level fluctuations, water diversions, exotic species, impoundments etc.) and ecotoxicity. Jager et al. (1999) used CompMech to model the effect of changes in hydrologic conditions, population fragmentation (impoundments) and habitat alteration on white sturgeon.

CompMech has a probabilistic basis but incorporates stochasticity by specifying the probability of survival of each individual and then randomly determining if the individual survives at each time-step (Pastorok et al., 2002). CompMech uses Monte-Carlo simulations to introduce stochasticity in the model (Regan et al., 2003). Spatial and temporal variability can be modeled explicitly depending on data availability and purpose of the model.

Decision Support System for Evaluating River Basin Strategies (DESERT)

Developer: International Institute for Applied Systems Analysis (IIASA) in Laxenburg, Austria

DESERT Model Description:

The DESERT 1.1 software was developed in cooperation between the International Institute for Applied System Analysis, Laxenburg, Austria and the Institute for Water and Environmental Problems, Barnaul, Russia. DESERT is provided to the public domain for research and academic purposes and is a decision support system (DSS) for river water quality modeling and policy analysis. The purpose of this software is to supply a flexible and easy-to-use Microsoft® Windows based tool for decision support of water quality management on a river basin scale. The driving principle (Somlyody, 1997) of the development was to utilize the state-of-the-art knowledge on water quality control (hydraulics, water quality, uncertainty and parameter estimation, economic instruments, optimization methods, etc.) and to integrate them using present day computers to achieve an interdisciplinary tool for policy development. DESERT integrates in a single package data management, model calibration, simulation, optimization and presentation of results (De Marchi et al., 1999). The software incorporates a number of useful tools like a dBase style database engine for managing input data, simulation and calibration of hydraulics and water quality models, graphical representation of computed data and optimization based on programming a dynamic algorithm. DESERT facilitates calibration of water quality models by supplying a stochastic method for parameter estimation. It accomplishes optimal wasteload allocation by using dynamic programming, and allows the use of non-linear objective and transition functions. The DESERT package provides a useful and powerful instrument for water quality assessment and decision making in emission control, including selection of wastewater treatment alternatives, standard setting and enforcement.

DESERT 1.1 is designed to run on MS-DOS based Personal Computers. To run the optimization of wasteload allocation in large basin systems, a larger amount of both hard disk and RAM memory is required. Operating without an 80x87 math coprocessor is possible, but practically not feasible for any meaningful river network.

DESERT has been written completely in C⁺⁺ language to facilitate object oriented programming with improved capability for code management. It also extensively uses the Object Linking and Embedding (OLE) libraries of Microsoft Windows to exchange data with external spreadsheets for plotting and post-processing simulation results (Ivanov, et al., 1996). The linking of the

different units is a characteristic feature of DESERT and shown in Figure 6. The Data Management Unit uses a dBase compatible relational database engine to handle input data, which allows the user to treat the large amount of heterogeneous data (e.g., data on the river network, effluents, treatment plants, monitoring network, etc.) necessary for a watershed scale assessment. The Display Unit draws the spatial distribution of the river basin, with options of scaling and selection.

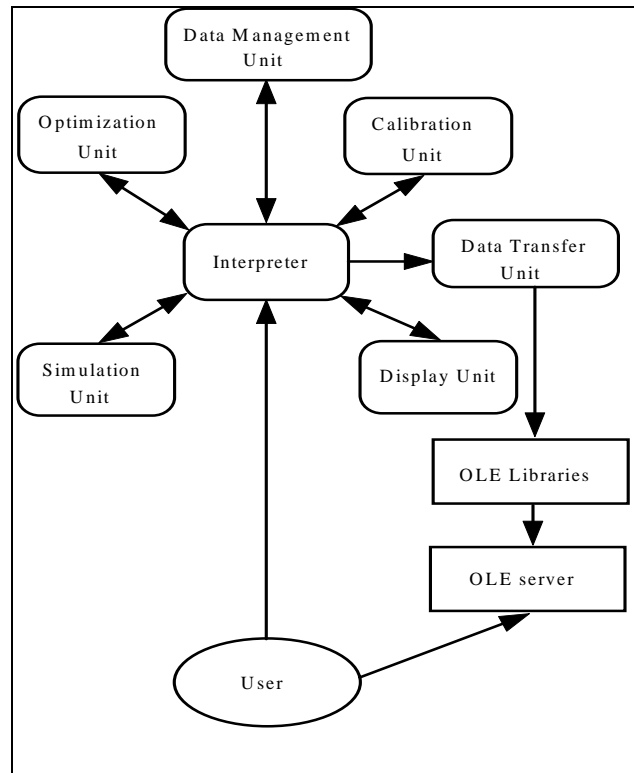


Figure 6. Schematic of the DESERT software.

The hydraulic models used in the Hydraulic Unit of DESERT for rivers and open channels are based on mass continuity and momentum equations of fluid mechanics. DESERT represents an alternative to both these approaches. The Water Quality Simulation Unit supplies five different ways to simulate mass balance equations (Ivanov et al., 1996). These mass balance equations may be combined and applied in different reaches of the same river basin. Also, and more importantly, for three of these approaches the description of reaction processes can be given through an interpreted language similar to BASIC. This fact has two advantages. First, it liberates the user from the necessity of using only predefined functions. The model formulation can be set up by the user with much freedom. That is, the user can specify as many variables as desired and define whatever reaction may be needed. Second, the user can write the model directly in a window supplied by DESERT. The Data Transfer Unit facilitates the transfer of

simulation data to Microsoft Excel, where data can be independently processed, stored, and plotted. The Calibration Unit has tools that use a stochastic method for parameter estimation using the Hornberger-Spear-Young Generalized Sensitivity Analysis (GSA) Method (De Marchi, et al., 1999). This technique generates a set of parameter vectors based on specified random distribution of each parameter. Model performance is judged on knowledge of the system, or on the “behavior definition” (e.g., lower and upper bounds of state variables, distance of model trajectory from the observed values, etc.). In the Optimization Unit DESERT uses dynamic programming, DP, which decomposes a problem into a sequence of decisions or subproblems, each having one or a reduced number of decisions. These sub-problems are resolved recursively, by considering the sub-optimal solution(s) of one sub-problem as input(s) to the subsequent sub-problem. The selection of optimal wastewater treatment alternatives in a river basin is a temporally and spatially sequential decision problem. Spatially, decisions are made at a series of locations in a river basin. Due to the downstream propagation of river pollutants, the water quality at a particular location along a river is entirely determined by the water quality at the immediate upstream discharge/control point.

DESERT Model Application:

The application of DESERT for three medium size river basins (the Nitra Basin in Slovakia and the Morava Basin in the Czech Republic, both in the Danube basin, while the Narew Basin in Poland in the Vistula basin, in the range of 5000 – 28000 km² catchment area) suggests an initial strategy to focus on low-cost/high-gain measures, with the ability to blend in policy for tackling long-term issues (Somlyody, 1997). Results obtained reveal that significant improvement of dissolved oxygen can be attained with low investment levels (measured in investment cost as a percentage of the best available technology cost which would be required by the most stringent EU requirements). The aspiration-led decision support (ALDS), which was an extension of goal programming, was tested for the Nitra River Basin in Slovakia while developing DESERT (Somlyody, 1997). For this basin, some of the six criteria used were DO, BOD₅, NH₄-N, TAC, and IC. About sixty solutions were derived and analyzed during two sessions. One optimization run with 100 variables took 2-4 minutes. Conclusions by running the DESERT model on the Nitra basin were summarized as follows: (i) The ALDS method is very efficient and its interactive usage does not cause any difficulties; (ii) due to the presence of discrete variables refined solutions can be found much easier than the Single Criterion Decision Analysis.

The re-aeration rate was quite uncertain in the Nitra River DO problem (Somlyody, 1997). By using the DESERT model, the first step was the development of a least cost DO policy under “nominal” re-aeration coefficient. A second parameter value was assumed and the simulation was performed. Finally, optimization was made for the second value, and violation/over-performance and over-expenditure/saving were assessed. The evaluation showed that for e.g.,

under a $DO > 0.3$ mg/L criteria, +/- 25% change in the re-aeration rate leads to a 20% increase in DO.

DESERT can easily deal with large amounts of data and perform reliable hydraulic and water quality simulations (De Marchi et al., 1999). It also offers tools for facilitating model calibration. DESERT's DP optimization tools are powerful and more than adequate for classical wasteload allocation. However, the optimization tools are not flexible for determining costs and water quality not resulting from least cost strategies. It is also not possible to track how costs are distributed among the different players in the watershed.

Spreadsheet Tool for River Environment Assessment Management and Planning (STREAMPLAN)

Developer: International Institute for Applied Systems Analysis (IIASA) in Laxenburg, Austria

STREAMPLAN Model Description:

STREAMPLAN (a Spreadsheet Tool for River Environmental Assessment Management and PLANning) is a decision support system designed to assist in the evaluation of alternative strategies for water quality management at the river basin level. STREAMPLAN is provided to the public domain for research and academic purposes and the purpose of this integrated easy-to-use software is to allow decision makers to evaluate the implications of policy related water quality management measures related to performance standards, economic instruments and financial resources. STREAMPLAN was developed at the International Institute for Applied Systems Analysis (IIASA) in Laxenburg, Austria. IIASA's project on Degraded River Basins in Central and Eastern Europe, where severe water quality problems coupled with limited financial resources made identifying cost-effective approaches to improving environmental quality a top priority. This provided the background of development of STREAMPLAN and it has been proved that this software can be applied to any river basin in developed or developing countries, where effective water quality management strategies need to be identified (De Marchi et al., 1996).

STREAMPLAN is a spreadsheet (Excel 5.0) based computer software, which integrates the Excel computing environment with water quality management policy and water quality modeling. STREAMPLAN is based on simple mathematical descriptions of processes of water quality modeling and management policy in a steady-state (De Marchi et al., 1996) formulation. The spreadsheet computing environment of STREAMPLAN provides the user with greater flexibility and comprehensiveness in designing and analyzing water quality management policy issues in degraded river basins than with the conventional software. A distinctive feature of STREAMPLAN is the integration of a detailed model of municipal wastewater generation (March et al., 1999) with the water quality model and policy analysis tools. Cost and removal rates of different wastewater treatment plant (WWTP) upgrade schemes, based on projected wasteloads and the description of existing facilities can be determined by using optional subroutines in STREAMPLAN. Evaluation of a wide range of policy options (March et al., 1999) including uniform emission reduction and effluent standard based strategies, ambient water quality and least cost strategies and strategies with economic instruments are some of the analytical options available with STREAMPLAN.

The four basic components (De Marchi et al., 1996) of STREAMPLAN are (1) a conceptual framework for water quality management in river basins; (2) a database related to the conceptual framework; (3) a management model capable of simulating various flow, load and policy conditions and generating optimal solutions for user specified problems; and (4) an interface which is rich, functional and flexible to provide operations in water quality management. In the conceptual framework, a watershed is modeled as a river network consisting of a network of interlinked reaches and a set of point sources along it. Nonpoint sources in sub-watersheds are modeled as point sources at locations where the discharge from the sub-watershed is released to the river basin. Background load and discharge inputs to the network are considered as uncontrollable point sources. Point sources in STREAMPLAN are municipal, industrial or agricultural controllable sources of pollution. STREAMPLAN uses three different data bases: the static, the designs and the scenario data bases (De Marchi et al., 1996). The management model is a mathematical description of the processes related to water quality management in river basins and consists of three major models: (a) a water quantity and quality simulation model; (b) a socio-economic model; and (c) an optimization model. STREAMPLAN has a rich, functional and flexible interface consisting of both tabular and graphical interfaces.

- (a) *Water quantity and quality simulation model:* A simple hydraulic model is used to calculate mean velocity and mean depth in each river reach for the water quality model. Mean velocity and hydraulic depth are calculated for each reach by using the Chezy or Manning's formulae (De Marchi et al., 1999) for trapezoidal and semicircular channels. The water quality model simulates the fate of up to six specified pollutants, the default of which include BOD, NH₄-N, NO₃-N, DO, and total phosphorous (TP). The additional sixth component can be specified by users to customize the model to their particular needs. The implemented water quality model is one-dimensional, linear and steady-state. Among the many processes considered in the model are decay of BOD, natural-re-aeration and oxidation of ammonium.
- (b) *Socio-economic model:* Some of the tasks of the socioeconomic model (De Marchi et al., 1999) include modeling the effect of cot changes on municipal residential water demand, modeling the flow of revenues in the system, and modeling the use of economic instruments. Thus with the ability to model the effect of price on water use, it is possible to observe the effect that increasing the water tariff, either by an increase in the cost of wastewater treatment or an increase in effluent charges, will have on the quantity of wastewater produced.

The socio-economic model uses two components of cost- fixed cost and variable cost. Fixed costs are defined as investment cost (IC) and sewerage upgrade cost. Variable cost include operations, maintenance and replacement (OMR) cost and effluent charges. The revenue side includes water tariffs, monthly fees and fees for the connection to the system. Cost recovery,

i.e. the difference between costs and revenues can be examined at a source, group or river basin level. STREAMPLAN handles four types of economic instruments: effluent charges on specific pollutants, effluent fines, subsidies and water tariffs.

- (c) *Optimization Model*: The optimization model generates the optimum solution for treatment alternatives at the treatment plants included in the objective function. The objective function is formulated as cost minimization subject to one or more constraints such as ambient water quality, effluents, total emissions and/or minimum treatment levels. In the objective function, cost can be specified as the sum of IC, OMR costs and effluent charges, or any combination of these costs.

The software structure of STREAMPLAN has six major workbooks, two software algorithms, a tools library and a help workbook. The software algorithms are used for linear programming optimization. The major workbooks are *Main.xls*, *Static.xls*, *Designs.xls*, *Scenario.xls*, *Model.xls* and *Lp.xls*. There is an optional workbook called WWTP workbook, which can be linked with STREAMPLAN to generate the cost information and effluent water quality for different treatment alternatives for municipal treatment plants. The *Main* workbook sets up the computing environment for STREAMPLAN. The *Static* workbook stores all data which do not change from scenario to scenario. The *Designs* workbook is usually used as an interface. The *Scenario* workbook contains information on different scenarios analyzed in the *Model* workbook. The *Model* workbook is the engine where the water quality simulation is performed. It extracts data from the *Static*, *Designs* and *Scenario* workbooks, and computes the water quality in the river reaches. The *Lp* workbook sets out the optimization problem, which is solved by the algorithms, and also produces the optimized treatment alternatives in tabular form.

STREAMPLAN Model Application:

STREAMPLAN has been successfully applied to the Nitra River in Slovakia, the Morava River in Czech Republic, the Sio and Sajó Rivers in Hungary, and the Narew and Oder Rivers in Poland (Marachi et al., 1999). In the Nitra Basin STREAMPLAN was used to estimate (Somlyódy, 1997) the incremental cost of nitrogen and phosphorous emission reductions (over and above of meeting a local DO goal of 5 mg/L), which was a critical issue in efforts to restore the Black Sea. The costs estimated from STREAMPLAN were rather high and consequently could only be implemented in the long term. “Cost surfaces” vary from sub-basin to sub-basin. Regional least-cost nutrient reduction policies need to be developed on the Danube River basin scale. The STREAMPLAN type of methodology can also be used in this basin by aggregating sub-basins and larger regions into point sources and their emission reduction “table” including effluent loads and costs for different alternatives (Somlyódy, 1997).

STREAMPLAN shows the impact of alternative cost recovery-schemes on the different subjects (i.e., central government, regional authorities, residential customers, etc.) involved in water quality policies. STREAMPLAN was used in the Narew River basin to assess the impact on residential customers to adopting best available technology (BAT) and improving the sewerage system to meet the EU effluent standards. Using STREAMPLAN, half of the Investment Costs of upgrading WWTP and extending sewerage systems were recovered by increasing the monthly water tariffs (fixed costs). This caused significant initial impact on households and residential customers reduced their water consumption by almost 10%.

Among some of the limitations (De Marchi et al., 1996) of STREAMPLAN are: (i) steady and uniform flow hydraulics are considered in each reach, which might not be the actual case; (ii) distributed lateral flows are not explicitly modeled for either hydraulics or water quality; and (iii) parameters related to hydraulics (e.g., roughness coefficients) and water quality (e.g., coefficients of water quality constituents and temperature correction factors) are taken as input and cannot be calibrated by STREAMPLAN. However, STREAMPLAN makes it simpler to assess the effects of changes in population, sewer conditions, household water consumption, and pretreatment of industrial discharges on the water quality in the river system (De Marchi et al., 1999). It also features a wide array of water quality policies and tracks the cost of implementing them at different levels.

Deterministic and Stochastic Matrix Models

Deterministic and Stochastic Matrix Model Description:

1. **Deterministic Matrix Models:** these matrices have been used in population modeling, especially fish populations, since 1950. These models assume that survival and fecundity are functions of the age or stage to which an organism belongs (Pastorok et al. 2002). The simplest model of this type is Leslie's population projection matrix (Sharov, 1996, Pastorok, 2002):

$$N(t) = L * N(t-1)$$

Where $N(t)$ and $N(t-1)$ are vectors of the numbers of organisms in each age class (N_0, N_1, \dots, N_K)

$$L = \begin{matrix} & s_0 f_1 & s_1 f_2 & s_2 f_3 & \dots & s_{(k-1)} f_k & 0 \\ \begin{matrix} s_0 \\ 0 \\ 0 \\ 0 \end{matrix} & 0 & s_1 & 0 & \dots & 0 & 0 \\ & 0 & 0 & s_2 & \dots & 0 & 0 \\ & 0 & 0 & 0 & \dots & s_k & 0 \end{matrix}$$

Where

S_K = age-specific survivorship probability

f_K = average fecundity at age K

In this kind of models it is assumed that individuals within the same age or stage have the same survival probabilities or fecundity rates. This kind of models assume that vital rates do not suffer variations due to environmental fluctuations (such as habitat or hydrologic changes) or individual variability. Since parameters such as survivorship or average fecundity are fixed and external effects on these parameters are not taken into account, stochasticity is not included; therefore the model is totally deterministic, based on fixed survivorship probabilities. Some software packages such as RAMAS Stage include deterministic matrix models concepts such as Leslie or Lefkovich formulations. However, RAMAS STAGE is able to introduce variability and account for stochasticity introducing environmental parameters that can affect population (RAMAS, 2006). This model can be used to estimate the effect of different factors such as chemical pollutants or habitat impairment on the endpoints by changing the survivorship probability or fecundity for each scenario based on laboratory tests or field observations. Deterministic

matrix models have high credibility if the parameters introduced are accurate and are used by several regulatory agencies (Pastorok et al., 2002)

2. Stochastic Matrix Models: these models assume like the deterministic matrix models that the survival rate and fecundity are functions of the age class or stage in which an organism resides. However, stochastic matrix models are able to incorporate environmental and/or demographic variability in the survival probabilities and fecundities (Pastorok et al., 2002, Caswell, H., 2000). These models, like the deterministic models, have high credibility and are also implemented by several regulatory agencies.

VORTEX (version 9.58 7)

Developed by:

Bob Lacy (Department of Conservation Biology, Chicago Zoological Society, Brookfield, Illinois, USA).

VORTEX Model Description:

VORTEX's first version was developed in 1992 by Lacy, R.C. and T. Kreeger but they have published upgrades with the new version in February 2006. VORTEX simulates a population by stepping through a series of events that describe the typical life cycle of sexually reproducing, diploid organisms. The program was written originally to model mammalian and avian populations, but its capabilities have improved so that it can now be used for modeling some reptiles and amphibians and perhaps could be used for fish, invertebrates, or even plants—if they have relatively low fecundity or could be modeled as if they do.

The Vortex computer program is a simulation of the effects of deterministic forces as well as demographic, environmental and genetic stochastic events on wildlife populations. It is an attempt to model many of the extinction vortices that can threaten persistence of small populations (hence, its name). Vortex models population dynamics as discrete, sequential events that occur according to probabilities that are random variables following user-specified distributions. Vortex simulates a population by stepping through a series of events that describe an annual cycle of a typical sexually reproducing, diploid organism: mate selection, reproduction, mortality, increment of age by one year, migration among populations, removals, supplementation, and then truncation (if necessary) to the carrying capacity. Although Vortex simulates life events on an annual cycle, a user could model "years" that are other than 12 months duration. The simulation of the population is iterated many times to generate the distribution of fates that the population might experience.

Vortex is an individual-based model. That is, it creates a representation of each animal in its memory and follows the fate of the animal through each year of its lifetime. Vortex keeps track of the sex, age, and parentage of each animal. Demographic events (birth, sex determination, mating, dispersal, and death) are modeled by determining for each animal in each year of the simulation whether any of the events occur. (See Figure 8 below.)

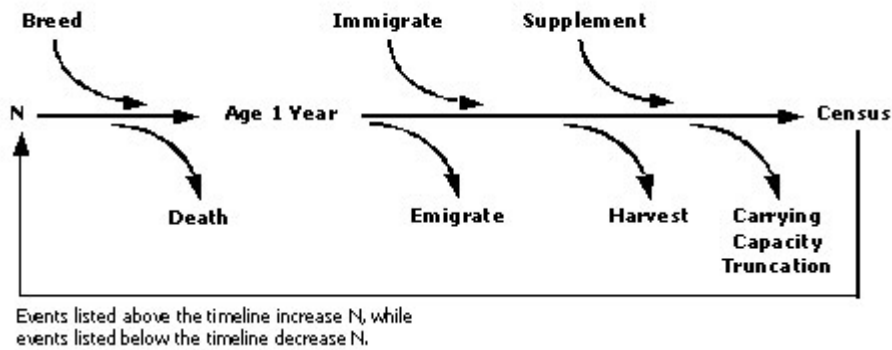


Figure 7. Vortex Simulation Model Timeline

Vortex requires a lot of population-specific data. For example, the user must specify the amount of annual variation in each demographic rate caused by fluctuations in the environment. In addition, the frequency of each type of catastrophe (drought, flood, epidemic disease) and the effects of the catastrophes on survival and reproduction must be specified. Rates of migration (dispersal) between each pair of local populations must be specified. Because Vortex requires specification of many biological parameters, it is not necessarily a good model for the examination of population dynamics that would result from some generalized life history. It is most usefully applied to the analysis of a specific population in a specific environment.

In the program explanation that follows, demographic rates are described as constants specified by the user. Although this is the way the program is most commonly and easily used, Vortex does provide the capability to specify most demographic rates as functions of time, density, and other parameters.

VORTEX Model Applications:

Some projects which used this model are:

- An analysis of the impacts of harvest of dugongs in the Torres Strait between Papua New Guinea and Australia and along the Queensland coast. Submitted by Rob Heinsohn, Australian National University,
- Analyses of Orangutan populations in Sumatra and Borneo. Submitted by IUCN/SSC Conservation Breeding Specialist Group,
- Population viability analysis of giant pandas in the Yele Nature Reserve,
- Evaluating recovery strategies for an ocelot (*Leopardus pardalis*) population in the united states,
- Long-term trends in great bustard (*Otis tarda*) populations in Portugal,

- A population viability analysis for the Island Fox on Santa Catalina Island, California,
- Minimum viable population and conservation status of the Atlantic Forest spiny rat *Trinomys eliasi*,
- The sustainability of the common crane (*Grus grus*) flock breeding in Norfolk,
- Estimation and management of genetic diversity in small populations of plains zebra (*Equus quagga*) in KwaZulu-Natal, South Africa,

and more which can be found in scientific literatures.

Stream REach Management, An Expert System (STREAMES)

Developers: Spain: University of Barcelona, CSIC-CEAC, University of Girona, Catalan Water Agency (ACA), Austria: University of Vienna, France: CNRS-CESAC, Agence de l'Eau, Germany: IGB-FVB, Greece: University of Crete, OANAK, Italy: University Tor Vergata, Provincia di Roma, and Portugal: University of Evora, DRA-A.

STREAMES Model Description:

STREAMES is a project sponsored by several European countries that seeks to develop an Environmental Decision Support System (EDSS) based on artificial intelligence to support and advice water managers in the management of human-altered streams. The project has its focus on studying the increase of nutrient loads in streams from point sources and non point sources (due to changes in land-use or stream modification, which reduces the ability to respond to increased loads). The nutrient and pollution load is one of the main handicaps to overcome for water managers to comply with the 2000/60/EEC Water Framework Directive which main objective is to achieve a good ecological state for the river (Comas et al., 2002a). The project is mainly focused on Mediterranean streams because in such locations the scarcity of water makes the problem even worse (Comas et al. 2002b). The EDSS of the model is integrated by a rule-based reasoning component (RBS) with a Geographic Information System (GIS) and linked to a numerical model (MONERIS model modified for Mediterranean regions) to estimate point and non-point sources. The STREAMES project and the EDSS development model has to deal with problems such as missing data or the dilemma of using a single model for all the streams or different models for different streams (Vicente et al., 2004).

In order to develop the Model (still under construction), different teams are working on different areas of expertise. These areas of expertise are (from STREAMES web-page, 2006):

1. Analyses at the catchment scale. Terrestrial nutrient sources to stream ecosystem: point sources versus non-point sources.
 - a. **Estimate** point and non-point sources of nitrogen and phosphorus for each of the study catchment areas.
 - b. **Relate** non-point sources to catchments features (land use, topography, landscape configuration, hydrogeomorphic units distribution).
 - c. **Analyse** seasonal variability in point and non-point sources in relation to measured in-stream loads and hydrology.

The results obtained from this group are integrated using a Geographic Information System (GIS) in order to evaluate the relationships between point and non-point sources with land-use/land cover

2. Analyses at the reach scale: effects of high nutrient loads on stream nutrient transport, transformation and retention. In this section, the ability of the stream for self-recovery and nutrient retention is studied. Biological, physical and chemical parameters that can affect nutrient concentrations in the streams are taken into account in order to be included in the final model. Hydrologic and morphologic conditions of the streams and their changes as well as sediment retention are some of the focus in this area of expertise.

3. Analyses at the sub-reach scale: the role of the stream biota on the control of nutrient retention. The objective of this section is to examine the influence of in-stream biological processes on nutrient retention in streams affected by high nutrient loads.

The hypothesis used is that, under similar stream discharge conditions, nutrient retention in streams with high nutrient loads will be lower than in less polluted streams if biota mostly controls nutrient retention. Enhanced primary production due to high nutrient loads represents an important source of energy and carbon to heterotrophic bacteria. Along with high nitrification rates, the processing of this organic pool can ultimately induce severe oxygen depletion and stimulate anaerobic processes. This fact leads to heterogeneity in biological responses and physicochemical variability in the streambed. Hence, depending on the "quality" of the nutrient loads, either autotrophic or heterotrophic processes will control the removal of dissolved nutrients from the water column. Overall, these metabolic changes at the sub-reach scale may affect stream nutrient retention at the reach scale. These changes are being quantified in order to be able to predict the direction of change in nutrient retention in front of a particular disturbance (e.g., nutrient load increases).

4. Expert System development: this is the last step after the acquisition of knowledge is done. The decision making interface is programmed after obtaining what is called the Knowledge Base (KB), which is a manual of operation on stream management. The KB is obtained with three different mechanisms: an extensive literature review, interviews to scientists and water managers and obtaining data from experimental campaigns (Comas et al., 2002a). The EDSS will be integrated with a GIS in order to make most effective management decisions.

The Expert System will be able to provide three different outputs for each different scenario:

1. Diagnosis, which is the % of self-purification capacity of the stream reach
2. Solutions: list of management strategies at reach scale to maximize self-purification
3. Prognosis: simulation of scenarios and % of success according to the adopted solution.

Gestion Intégrée des Bassins versants à l'aide d'un Système Informatisé (GIBSI)

Developer: University of Quebec. National Institute for Scientific Research (INRS)

GIBSI Model Description:

GIBSI is a watershed-based, user-friendly software system for integrated management of surface water quality. The effects of agricultural, industrial and municipal management scenarios can be analyzed under GIBSI framework (Rousseau et al., 2000). The GIBSI model has been designed for two types of users: the water resources manager and the technical expert. GIBSI is composed of a Microsoft Access™ based Relational Data-Base Management System (RDBMS), physically-based simulation models (hydrology, soil erosion, agricultural-chemical transport and water quality), and a Geographic Information System (GIS). The GIS used is GRASSLAND. Typical data stored in the database include spatial and attribute data (digital elevation model, soil characteristics, meteorological data, gauge locations, crop management, livestock production etc.). GIBSI is a modular model, which means that the system allows, if necessary, the integration of new system components or replacement of existing ones (Rousseau et al., 2000). The simulation models and their description are described in Table 1.

GIBSI can model different scenarios depending on the anthropogenic activities in the area under study (Rousseau et al., 2000). The different scenarios can be modeled changing parameters in any of the following elements:

1. Point sources management model: waste water treatment plants and industrial discharge points
2. Agricultural production systems: number and type of livestock, crop management practices and crop rotation systems, application of fertilizers, pesticides and manure etc.
3. Land use classes: uses given to the land.
4. Hydraulics: addition or removal of reservoirs, hydraulic characteristics of dams etc.

GIBSI provides a means to identify the river segments which may be suitable for specific water uses. Additionally, if an in-situ assessment of ecological integrity of several river segments is known, the simulated parameters from GIBSI may be used to complement the ecological assessment of a watercourse. If more data regarding physical characteristics of the stream segment (riparian vegetation, land-use, sinuosity etc.) are available, the model can be used to

study the impact of human-induced stresses and their consequences on stream habitat (Rousseau et al., 2000).

GIBSI Model Application:

In the Chaudière River Basin (Canada) basin, GIBSI was used to model two different scenarios. The first was a timber harvest scenario and the second an implementation of a municipal clean water program scenario. The basin had a total area of 6680 Km² and about 180,000 citizens lived in the area. The first scenario resulted in a clear increase of run-off peaks and shorter times-to-peak and recession times were also predicted by the model. In the second scenario, a comparison between the conditions in 1978 (2% of wastewater treated) and 1997 (98% of wastewater treated) was made.

In both cases, coliform and phosphorus concentrations were modeled. These simulations did not consider contaminant loads from agricultural run-off and combined sewer overflows. GIBSI successfully detected the decreases in coliform and phosphorus concentrations between the two scenarios but quality problems were still present in both cases, which suggested that current quality problems may be due to agricultural runoff, combined sewer overflows, septic systems in rural housings or inadequately treated discharges from industries not connected to a sewer system.

Table 1. Models and features included in GIBSI (from Mailhot et al., 1997 and Villeneuve et al., 1998)

MODEL	Simulated processes	Simulated variables	Required input data	Time Step
Hydrology Model (HYDROTEL)	Snowmelt	Runoff height	Meteorological	Day or less
	Evapotranspiration	River flow rate	Land use	
	Saturated and non saturated soil water flow	Soil water content in three soil layers	Elevation model	
Soil erosion model (RUSLE)	Runoff and river flow	Snow cover	Soil characteristics	Event-based
	Detachment of soil particles	Sediment load	Meteorological	
	Transport of eroded soil particles		Elevation model	
	Sedimentation of eroded soil particles		Hydrological	
Pollutant transport (SWAT/EPIC)			Crop management	Day
	Nitrogen cycle	Nitrate and organic nitrogen	Soil characteristics	
	Ammonium adsorption-desorption	Mineral and organic phosphorus	Meteorological	
	Phosphorus cycle	Dissolved and particulate pesticides	Hydrological	
	Desorption of soluble phosphorus at soil surface		Crop management	
Water Quality (QUAL2E)			Soil erosion	Steady state or transient simulation
			Simulated concentrations of water contaminants (point and nonpoint sources)	
	Nitrogen cycle	Nitrite and nitrate		
	Phosphorus cycle	Ammonia		
	Algal growth	BOD		
	BOD	Dissolved Oxygen		
	Atmospheric reaeration	Dissolved and organic Phosphorus		

Contaminants in Aquatic and Terrestrial Ecosystems Model **(CATS)**

Developer:

National Institute of Public Health and Environmental Protection (RIVM), Bilthoven, The Netherlands.

CATS Model Description:

Contaminants in Aquatic and Terrestrial ecosystems (CATS) model was designed as a family of dynamic multicompartiment models to study bioaccumulation and the combined effects of nutrients and micropollutants. The model was developed by the National Institute of Public Health and Environmental Protection (RIVM), Bilthoven, The Netherlands. Persistent chemicals and heavy metals were found in Dutch rivers, sediment and soils. The local differences (Traas and Aldenberg, 1996) in emission history, sorption characteristics of soils and sediments led to different degrees of contamination between the locations. Both the abiotic characteristics of the exposure medium and the properties of organisms affect the availability of toxicants to organisms (bio-availability). Hence the concept that the characteristics of both the biotic and abiotic components of the ecosystem be considered for a regional risk assessment of toxicants to ecosystems provided the background for the development of the CATS models.

In CATS models the fate of the toxicant in the abiotic compartments of the ecosystem is integrated to the uptake of the toxicant in the biotic components of the ecosystem (Traas and Aldenberg, 1996). Thus the relations between toxicant load, partitioning of the toxicant over water, soil or sediment and the uptake of toxicant by organisms can be studied. The actual bioavailability of the toxicant is determined by the degree of contamination and loading, sorption characteristics of water, soil or sediment and the characteristics of the organisms itself (Traas and Aldenberg, 1996). The CATS model requires the specification of the uncertainty (Traas et al., 1996) in contaminant load, initial conditions of variables, and model coefficients. It is then run many times with Monte Carlo sampling from model parameters and the yields model output distributions. The term model parameter is used to indicate any constant such as input terms (toxicant load), initial conditions (biomass and concentrations), and model coefficients for relevant processes.

CATS is an integrated aquatic ecosystem model, which combines a eutrophication module (Janse et al., 1998), a fate module, an existing food web model of micropollutants, and an effects module. In CATS models an intermediate level of complexity is introduced based on physico-geographical regions or main water-body structure. These main model structures can be made specific for locations or regions by feeding the model with parameters from ecosystem units, soil maps, databases or other geographical data sources. The ecosystem structure of the CATS model is illustrated in Figure 9 below.

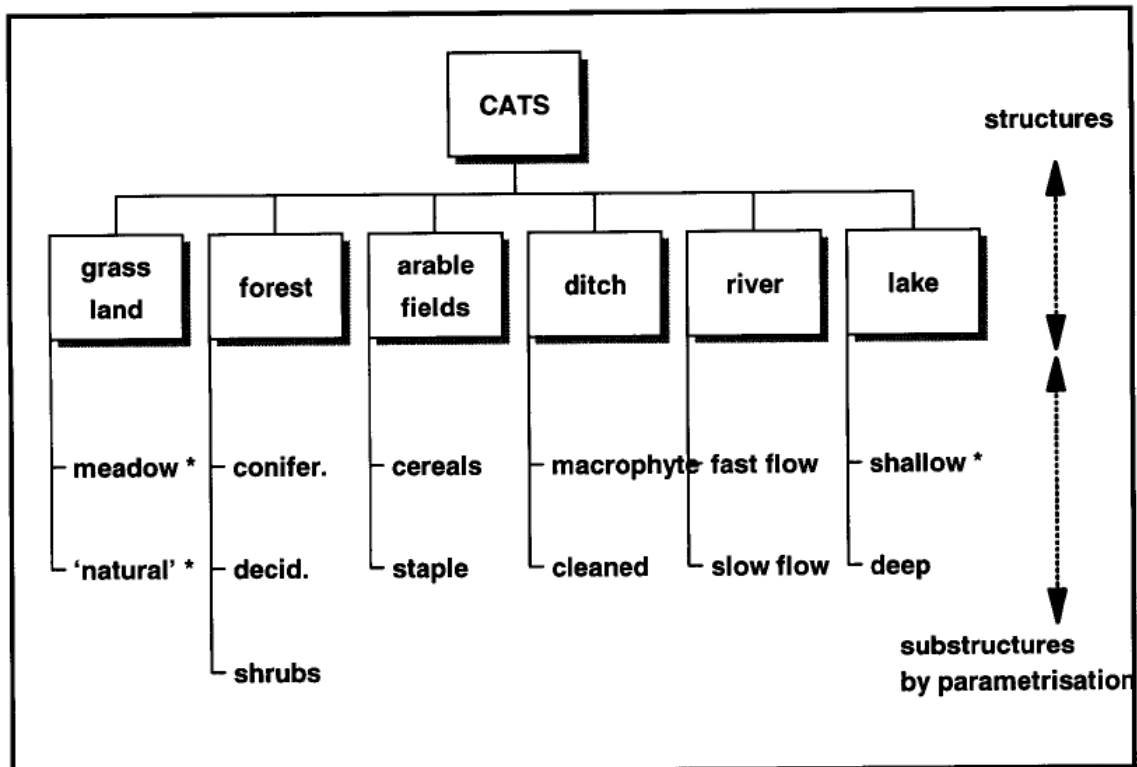


Figure 8. Model structure and Parameterization of CATS model

Since CATS model considers both the abiotic and biotic components of the ecosystem, along with the effects of the toxicants, the following properties are considered in the model:

- (1) *Abiotic properties*: These include hydrological properties (Traas et al., 1996) like inflow of water including suspended matter and associated toxicant, and the outflow of suspended matter and dissolved and sorbed toxicants.
- (2) *Biotic properties*: In CATS models, the food web consists of functional groups (Traas et al., 1996). Processes relevant to bioaccumulation are merged with classic logistic growth, which yielded a new growth model. Functional groups are formed combining species with similar food preferences and with similar roles in nutrient cycling.
- (3) *Toxicant properties*: These include properties like the toxicant concentrations in the water, sediments and the food web, the toxicant sorption to organic carbon, and degradation of the toxicant in the water phase, consisting of biodegradation, hydrolysis and photolysis.

In CATS model, the aquatic system is assumed well mixed (point model) and average daily conditions are modeled. The abiotic fate of nutrients (Koelmans et al., 2001) in model ecosystems is described as a closed loop. Biodegradation of pollutants is modeled as a function of temperature and light. Temperature dependence is incorporated in the eutrophication module (Janse et al., 1998). The food web consists of two types of algae, periphyton, macrophytes and different groups of zooplankton, zoobenthos, snails and insects. Change in biomass is modeled as a function of consumption, excretion, defecation, mortality, respiration, predation, direct and indirect toxic effects (Koelmans et al., 2001). CATS includes the effects of the contaminants on

different organisms by incorporating a logistic concentration-effect function for mortality. For each 'functional group' this allows the prediction of effects of time-varying concentrations.

CATS Model Application:

Application of CATS models for regional assessment of bioaccumulation risks proved feasible (Traas and Aldenberg, 1996). As an example of aquatic regional risk assessment the fate and bioaccumulation of Tributyltin (TBT) in Lake Westeinder, the Netherlands, was modeled. The Dutch ban on antifouling agents containing TBT was simulated with a load reduction scenario (Traas and Aldenberg, 1996, Traas et al., 1996). By integrating Monte Carlo sampling with a calibration procedure, probability distributions of TBT concentrations in the food web are matched to the measured variation in TBT concentrations. Subsequently, these distributions are used for the dynamic risk analysis of TBT accumulation in water, sediment and the food web in the whole lake and a typical marina (Traas et al., 1996). Model predictions indicate a fast decrease of the concentrations of TBT in water, suspended sediments and the zebra mussel (*Dreissena polymorpha*). TBT concentrations in sediment, chironomid, amphipods, and benthivorous fish are predicted to decrease at a much slower rate (Traas et al., 1996). The relative proportion of sediment uptake increases for (partly) benthivorous fish after TBT load reduction. Substantial risks of TBT are calculated for fish and zooplankton in marinas (Traas and Aldenberg, 1996), both before and during load reduction.

Green Bay Mass Balance Study (GBMS)

Developer:

United States, Environmental Protection Agency (USEPA).

GBMS Model Description:

The Green Bay Mass Balance Study (GBMBS) was conducted in 1989-90 by the USEPA to pilot the technique of mass balance analysis in understanding the sources and effects of toxic pollutants in the Great Lakes food chain. The objective of the study (www.epa.gov) was to evaluate the feasibility of mass balance modeling for toxic substances (mainly PCBs at the congeners level) as a basic planning and management tool in restoring Great Lakes water quality. Successful application of the methodologies employed in the Study offer an accurate basis for pollution control and a foundation for setting objectives for Lakewide Management Plans and Remedial Action Plans. The Study was headed by EPA's Great Lakes National Program Office (GLNPO) and the Wisconsin Department of Natural Resources, and had many participants from the Federal, state, interagency, and academic communities. The study focused on four representative chemicals or chemical classes: PCBs, dieldrin, cadmium, and lead.

Some of the specific objectives (www.epa.gov) of the GBMS included: (i) Assessing the technical and economic feasibility of the mass balance approach for use in the management of pollutant loadings and impacts on Great Lakes ecosystems; (ii) Assessing the technical and economic feasibility of the mass balance approach for use in the management of pollutant loadings and impacts on Great Lakes ecosystems; (iii) Calibrating the mass balance model for sources, transport routes, and fates of pollutants in the Great Lakes ecosystem; and (iv) Demonstrating methods and priorities for further studies of toxic pollutants in the Great Lakes.

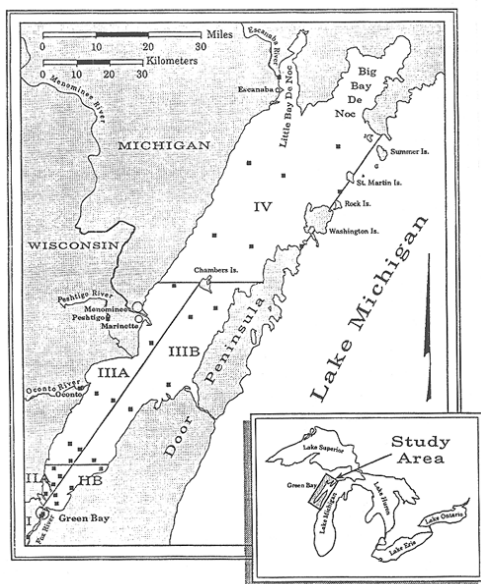


Figure 9. Map showing the location of Green Bay

The Green Bay Model was built on the basic model framework that had been previously developed for Saginaw Bay and for the Great Lakes (www.epa.gov). This would involve an integrated modeling framework consisted of a suite of individual models to simulate hydraulics, sorbent dynamics and toxic chemicals a time variable model, as shown in Figure 11 below. A water transport model (Green Bay Chloride mass balance model; GBCL) was coupled to a conventional chlorophyll-based nutrient driven eutrophication model (GBEUTRO). The eutrophication model generates organic carbon-related solids (biotic solids) which in turn are input to a long term solids model (GBTS) and a sorbent dynamics model (Green Bay Organic Carbon Sorbent model, GBOCS). The output of GBOCS forms an input to the contaminant exposure model (GBTOX) the output of which forms the input to the food chain model. Combination of the separate computer programs thus formed a modeling framework which makes a quantitative link between nutrient loading, carbon cycling, contaminant cycling and food chain accumulation.

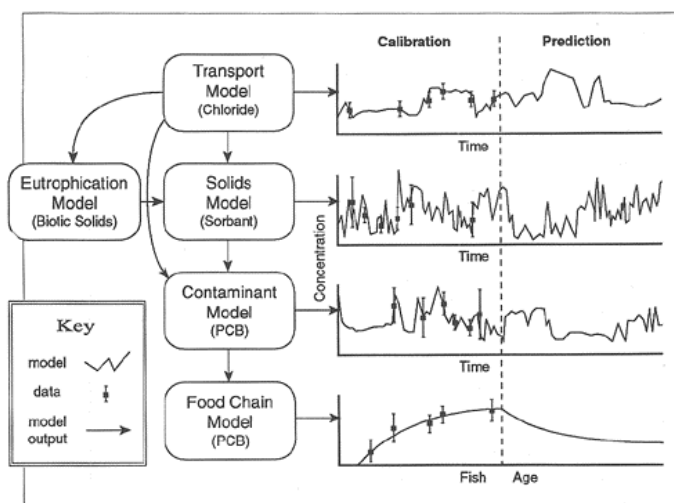


Figure 10. Green Bay Modeling Process

Each model produces output in the form of concentrations computed at different locations in the Bay and at future times. The model is calibrated by changing model process coefficients so that the computed concentrations match the measured concentrations. The more specific model framework (www.epa.gov) includes the interactions occurring between air and water, water and sediment, and the food chain. The model links the sources of the contaminant to the mass in water, sediment, and biota in space and time. Therefore the model once calibrated and deemed valid, can be used to compute future concentrations under any altered load condition.

PCBs enter the Green Bay system from the atmosphere, and from tributaries, primarily the Fox River. The computer model program, which keeps track of the mass of PCBs in space and time is called a "mass balance model" because the principal thermodynamic law of conservation of mass is maintained at all times. Thus, if mass is lost from one physical, chemical, or biological component of the model it must be gained in another. A "mass balance model" can be defined simply as "an equation where matter and energy entering a system, minus matter and energy leaving the system, equal matter and energy stored, transformed, or degraded within the system"

(USEPA). More precisely, a mass balance model is an accounting device to ensure that differences between inputs and outputs during any particular interval of time, within any particular volume in space, are equal to the net sum of the production, retention, and decay processes within the volume (USEPA). Mass balance models can be run at any of several levels, or tiers. A screening model (a preliminary approach utilizing existing data) can be run at very minimal cost to give very rough ideas of the magnitude of a lake's toxicants problem. A loadings model (an intermediate approach) can be used to identify whole lake total maximum daily loadings (TMDL's). However, a full mass balance study is needed to set specific wasteload allocations for individual sources. GBMB being a mass balance model has the following four strengths (USEPA): (i) it establishes a framework for the organization and synthesis of data; (ii) it provides a basis for managers to minimize costs and enhance information flow; (iii) it is a useful tools for understanding processes that lie behind the data; and (iv) it demonstrate linkages between inputs and system responses.

GBMS Model Application:

Results of the sub-model component GBTOX were successfully compared (www.epa.ie) with particulate phase and dissolved PCB concentrations that were collected for the GBMB study. The GBMBS modelling framework was successfully applied to a major follow up project, the Lake Michigan Mass Balance Study (LMMBS) in the Great Lakes. The model design for the Lake Michigan Mass Balance Project (USEPA, 1997) is based upon the linked sub-model approach used in the Green Bay Mass Balance Study, and retains the same basic models: hydrodynamics, sediment transport, sediment bed dynamics, eutrophication/sorbent dynamics, contaminant transport and fate, and food web bioaccumulation. A mass budget and mass balance model (USEPA, 1997) was constructed for a limited group of hazardous air pollutants (HAPs)/contaminants which are present in Lake Michigan at concentrations which pose a risk to aquatic and terrestrial organisms (including humans). The chemicals selected were PCB congeners, *Trans*-nonachlor, Atrazine and major breakdown products (de-ethyl atrazine, de-isopropylatrazine), and Total Mercury.

Some of the limitations (www.epa.gov) associated with GBMB being a mass balance model are: (i) oversimplification of natural processes; (ii) extensive data requirements; and (iii) no rigorous methods for quantifying model prediction uncertainty. However, when toxicity is not expected and the emphasis is on the spatial distribution of the chemicals, the GBMB model framework is the most accurate (Koelmans et al., 2001).

ATLSS

Developer:

University of Tennessee, supported by Cooperative Agreement with the U.S. Geological Survey and awards from the National Science Foundation, software assistance from Ardent Software, Inc. and the O2 Database Management System, and ParaSoft Corporation and the Insure++ System (ATLSS, 2006).

The overall ATLSS project is coordinated by Donald DeAngelis of the U.S. Geological Survey (BRD). The model components are constructed at the Institute for Environmental Modeling of the University of Tennessee at Knoxville (UTK). Other key organization and parties who have been involved in the modeling components of the project include: Florida International University, University of Florida, USGS, University of Washington, ORNL, Netherlands Institute of Ecology, Chesapeake Biological Laboratory at University of Maryland; and Forschungszentrum Julich, Germany. Financial support for the project is provided by several agencies, all coordinated through the USGS.

ATLSS Model Description:

ATLSS is mainly developed for ecological modeling of the Freshwater Wetlands of the Everglades and Big Cypress Swamp. It is reported that the first version of the model was run in 1997. Detailed information about history of ATLSS model run is provided at ATLSS home page at <http://atlss.org/> (ATLSS, 2006).

The ATLSS (Across Trophic Level System Simulation) program addresses CERP³'s need for quantitative projections of effects of scenarios on biota of the Greater Everglades and can provide guidance to monitoring in an adaptive assessment framework (USGS, 2003). A key objective is to compare the future effects of alternative hydrologic scenarios on the biotic components of the systems (ATLSS, 2006).

The immediate objective of ATLSS was to provide a rational, scientific basis for ranking the water management scenarios as part of to the planning process for Everglades restoration. The longer term goals of ATLSS were demonstrated to help achieve a better understanding of components of the Everglades ecosystem, to provide an integrative tool for empirical studies, to provide a framework monitoring and adaptive management schemes and, to promote the coordination and integration of modelers and empirical ecologists at different universities and research centers (USGS, 2003).

ATLSS Model Application:

ATLSS is a set of models for selected Everglades biota, which can translate the hydrologic scenarios into effects on habitat and demographic variables of populations (USGS, 2003). Due to the varying scales at which trophic interactions occur, and the importance of population structure

³ Comprehensive Everglades Restoration Plan

and individual behavior for population prediction in higher trophic level organisms, it was found that use of a single modeling approach is not appropriate.

Therefore, ATLSS is developed as a set of models designed to integrate three approaches for different trophic levels of the system (Across Trophic Level System Simulation (ATLSS) homepage): process models for lower trophic levels (including benthic insects, periphyton and zooplankton), structured population models for five functional groups of fish and macroinvertebrates, and individual-based models for large consumers (wood storks, great blue herons, white ibis, American alligators, white-tailed deer, and Florida panther).

These are integrated across the freshwater landscape of the Everglades and Big Cypress Swamp and coupled to GIS maps for cover type. Spatial scales of resolution for the models are as small as 100 m, with the capability to vary this based upon the scale of available input data. The system is then coupled to a hydrology model, and used to assess the effects of alternative proposed restoration scenarios on trophic structure (ATLSS, 2006).

ATLSS is constructed as a multimodel, meaning that it includes a collection of linked models for various physical and biotic systems components. The ATLSS models are all linked through a common framework of vegetative, topographic, and land use maps that allow for the necessary interaction between spatially explicit information on physical processes and the dynamics of organism response across the landscape (USGS, 2003). The general structure of ATLSS model is presented in the following figure.

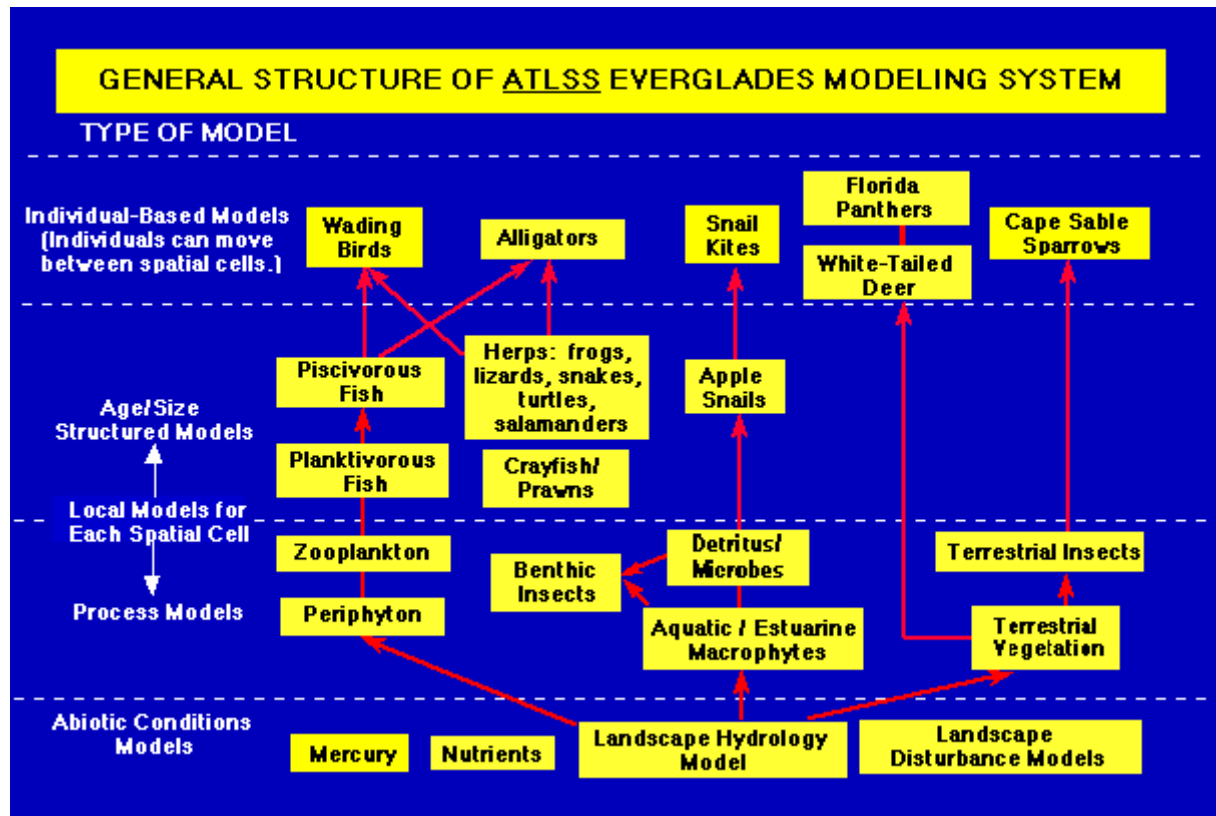


Figure 11. General structure of ATLSS model (ATLSS, 2006).

An essential component of restoration planning in South Florida has been the development and use of computer simulation models for the major physical processes driving the system, notably models of hydrology incorporating effects of alternative human control systems and non controlled inputs such as rainfall. The USGS's ATLSS Program utilizes the outputs of such physical system models as inputs to a variety of ecological models that compare the relative impacts of alternative hydrologic scenarios on the biotic components of South Florida (USGS, 2003).

ATLSS submodels are able to simulate population or condition of (ATLSS, 2006):

Alligators / Cape Sable Seaside Sparrows / Crayfish / Deer / Fish / Florida Panthers /
Hydrology / Snail Kite / Landscape/Vegetation / Wading Birds.

Hydrology, Fish and Crayfish submodels are explained in brief in the following:

One of the key features of the ATLSS models is the use of a high resolution hydrology model based on vegetation maps to convert the low resolution hydrologic output of the South Florida Water Management Model (1 water value per 2 x 2 mile cell) to the higher resolution needed to model ecological processes and the distribution of wildlife species. The ATLSS High Resolution Hydrology Model post-processes the output of the South Florida Water Management Model (WMM) using an algorithm based on conservation of water volume, and redistributes the water volume over a surface of high resolution topography (ATLSS "pseudotopography") to produce a high resolution map of water depth. This process is repeated on daily timesteps (corresponding to the daily output of the WMM) to create a map of water depth across the wetlands of South Florida with over 3000 separate values within each 2 x 2 mile cell (using topography based on the 28.5 meter resolution of a LandSat image).

The ATLSS Landscape Fish model (ALFISH) has as its main objective the ability to compare in a spatially-explicit manner the relative effects of alternative hydrologic scenarios on fresh-water fish densities across South Florida. Another objective is to provide a measure of the dynamic, spatially-explicit food resources available to wading birds.

The purpose of crayfish model is to examine how crayfish species respond to proposed hydrologic management in the Florida Everglades. This project will construct a spatially explicit, stage-structured population model for two species of procambarid crayfishes, the Everglades crayfish (*Procambarus alleni*) and the slough crayfish (*P. fallax*), building on up to 18 years of crayfish population data available from Drs. Joel Trexler and William Loftus. This model will provide a mechanism to estimate pre-drainage distributions of crayfish by coupling it to the natural systems model. Moreover, alternative hydrologic management scenarios may be compared to each other and with pre-drainage crayfish model outputs to evaluate the efficacy of proposed hydromanagement scenarios. Because white ibises (*Eudocimus albus*) forage primarily on crayfish while nesting, the availability of crayfish has obvious implications for recovering populations of this species. The crayfish model will allow managers to evaluate restoration alternatives, and examine how these alternatives may be compared to pre-drainage estimates of crayfish community composition.

Patuxent Landscape Model (PLM)

Developer:

The Patuxent Landscape Model (PLM) was developed by the University of Maryland in 1998 with funding for the project provided by the U.S. EPA (in conjunction with the National Science Foundation), Office of Research and Development, National Center for Environmental Research and Quality Assurance and the U.S. EPA Office of Policy, Planning and Evaluation. The Patuxent Landscape Model was designed to serve as a tool for systemic analysis of the interactions among physical and biological dynamics of the Patuxent watershed (Maryland, USA), conditioned on socioeconomic behavior in the region. A companion socioeconomic model of the region's land use dynamics was developed and linked with the PLM. This coupling provided more dynamic feedbacks, adjusting the socioeconomic change of the region in response to the ecological perturbations (Voinov et al. 1999). The PLM is an outgrowth of the Coastal Ecosystem Landscape Spatial Simulation model, which was later applied to a series of wetland areas like the Everglades. The sophisticated structure of PLM is supported by several general-purpose software packages, which have been developed and refined to meet the needs of PLM. The unit model is developed using the application STELLA. The model equations generated from STELLA are exported to a Spatial Modeling Environment (SME) through a program which translates the STELLA file into the Modular Modeling Language (Voinov et al., 1999). The SME links icon-based modeling environment with distributed computing resources. The users run the front end package, which is the SME user interface. This interface allows the user to define projects, simulation models, input/output configurations, and simulation runs with different calibration data. All of these objects are stored in the database (Voinov et al., 1999) for sharing by individuals or groups.

Patuxent Landscape Model Description:

In the PLM an ecological model is coupled to an economic model for exchange of data between them, and also to incorporate the socioeconomic and ecological dynamics. The relationships and the linkages between the economic and ecological subsystems are shown in Figure X below. To run the ecological and economic modules in harmony with each other, the spatial representation of both should be matched such that land use or land cover transformations in one module can be communicated to the other directly to the other one inside the same model.

(1) *Ecological Model:* The modeled landscape is partitioned into a spatial grid of square unit cells. The model is hierarchical in structure, and the ecosystem-level unit model is replicated in each of the unit cells representing the landscape. A raster-based geographic information system (GIS) is used to store all the spatially referenced data included in the model. Although the same unit model runs in each cell, individual models are parametrized according to habitat type and georeferenced information for a particular cell. There is a parameter database (Voinov et al., 1999), which stores habitat-dependent information like is stored in a parameter database like initial conditions, rate parameters, stoichiometric ratios, etc. The habitat type and other spatial characteristics are referenced through links to GIS files.

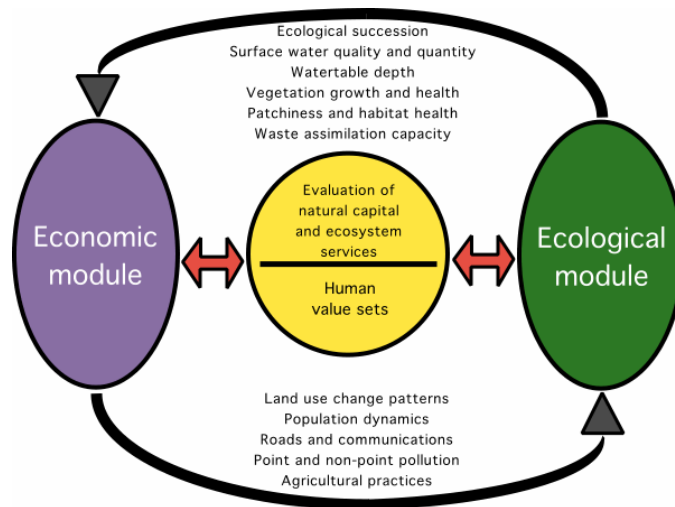


Figure 12. Relationships and linkages between the two modules of the PLM

The unit ecological model of PLM is based on the General Ecosystem Model (GEM). In the unit model (Voinov et al., 1999), the rainfall is assumed to infiltrate immediately to the unsaturated layer and only accumulates as surface water if the unsaturated layer becomes saturated or if the daily infiltration rate is exceeded. Surface water may be present in cells as rivers, creeks and ponds. Within the day time step, surface water flux will also account for the shallow subsurface fluxes that rapidly bring the water distributed over the landscape into the micro channels and eventually to the river. The nutrients considered in the PLM are nitrogen and phosphorous. However, the conceptualization of the nutrients on the surface differs from that in the GEM. In the PLM unit model the macrophytes are represented by two state variables for photosynthetic and non-photosynthetic plant matter. The carbon to nutrient ratios (C:N:P ratios) for both state variables link to different steps in the nutrient cycle.

The unit models in each cell exchange matter and information across space. The horizontal fluxes that join the unit models together are defined by surface and subsurface hydrology. The spatial hydrology module calculates the amount of water fluxed over the surface and in the saturated sediment. The fluxes are driven by cell-to-cell head differences of surface water and saturated sediment water, respectively. Water fluxes between cells carry dissolved and suspended material. At each time step, first the unit model updates the stocks within each cell due to vertical fluxing and then cells communicate to flux matter horizontally, simulating flows and determining ecological conditions across the landscape (Voinov et al., 1999).

The PLM employs a time step of 1 day, so that most of the ecological variables are updated daily. However, certain processes like some hydrologic functions can be run at shorter time steps whereas certain external forcing functions are updated on a monthly or yearly basis.

(2) *Economic model*: The spatial and temporal design of the PLM ecological module helps in providing a linkage with the companion economic module. The economic model predicts the probability of land use change within the seven counties of the Patuxent watershed. The first step in the economic modeling process is to estimate, statistically, models that explain the value of land parcels in different uses. An extensive GIS data base that includes geo-coded records of all parcels in the tax assessment databases of the seven counties was used. Some of the spatial

features, which were used to explain the value of land in residential use were (www.uvm.edu, a): distance to employment centers, access to public infrastructure (roads, recreational facilities, shopping centers, sewer and water services), and proximity to desirable (e.g. waterfront) and undesirable (e.g. waste dumps). Next, qualitative- dependent variable models of historical land use conversion decisions are estimated. This determines which factors affect land use conversion and parameters of those conversion functions are estimated. Once these parameters have been estimated, the model is used to generate the relative likelihoods of conversion of different parcels in the landscape. Thus, a spatial pattern of relative development pressure is obtained as a function of characteristics of the parcels and their locations (www.uvm.edu, a). Since the explanatory variables used to predict the values in residential and alternative uses and the costs of conversion are all functions of ecological features, human infrastructure, and government policies, the effects of changes in any of these variables can be simulated.

The calibration of the PLM was done in a multi-tier approach. The calibration and testing was performed at several space and time scales. The modular nature of the model facilitated the tests to be carried for various parts of the model as well as the whole model (Voinov et al, 1999). Initial unit model calibrations were handled in STELLA, and the fine tuning was performed using the Model Performance Index (MPI) (Voinov et al., 1999). At the same time certain modules were put into the spatial context and calibration of the spatial model was carried out.

Patuxent Landscape Model Application:

The Patuxent Landscape Model was applied to the Gwynns Falls watershed in urban Baltimore as part of the NSF funded Baltimore Urban LTER project. These models and their associated data bases provide a unique capability to test various policy scenarios and ecosystem restoration options at the whole watershed scale, for both a largely rural/suburban watershed (the Patuxent) and a largely urban/commercial watershed (Gwynns Falls). The Patuxent Landscape Model (PLM) was used as a tool for whole watershed analysis and restoration, specifically : develop and test the socioeconomic sectors and their dynamic links to the ecological sectors, apply the approach to the Gwynns Falls watershed and intercompare with the Patuxent.

The approach used in this application had the following objectives (www.uvm.edu, b): (i) Define and test ecosystem health indicators for watersheds; (ii) Explore alternative scenarios using the integrated Patuxent Landscape Model (PLM) and the Gwynns Falls Landscape Model (GFLM). A Multi-criteria decision analysis (MCDA) approach was used to formally analyze the scenarios and their trade-offs.

Among the results (www.uvm.edu, b) of this research were the development of increased capabilities in critical areas of watershed management and ecological restoring. The results also included development of useful and workable indicators and the ability to assess the ecological health of whole watersheds. The proposed research also increased capabilities critical to watershed-based management and ecological restoration (www.uvm.edu, b), like the development of the ability to assess the relative effects of various spatially explicit policy and management options on ecosystem health at the whole watershed scale, and the development of the ability to design effective whole watershed restoration strategies. This was critical to developing the ability to address non-point sources of nutrients and other pollutants.

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Appendix: CLEAR LAKE SIMULATION

Clear Lake is the water body under study using the AQUATOX 2.1 model. A description of the model is attached to this report.

Watershed description: Clear Lake is located in California, approximately 80 miles north of San Francisco and is within the borders of the Sacramento River Basin. The lake surface is around 70 square miles with 100 miles of shoreline. Its average and maximum depths are 27 and 60 feet respectively. Clear Lake has several tributaries which drain a total area of 441 square miles. Some of these tributaries are Adobe Creek, Burns Valley Creek, Clover Creek, Cole Creek, Forbes Creek, Kelsey Creek, Kelsey Creek, Manning Creek, Middle Creek, Molesworth Creek, Morrison Creek, Schindler Creek and Scotts Creek. Clear lake is impounded by the Clear Lake dam in the southeastern part of the lake. The land-use in the area is mainly forest, shrubs and grassland. The urban area represent only a 2.5 percent approximately. The lake is in an active, volcanic area. Several monitoring stations are located in the watershed. For the present study, two stations belonging to the California’s Department of Water Resources (DWR) were used for the inflow calculations. Another gage located in Clear Lake Dam and belonging to the USGS was used to compile outflow data. Figure 1 shows graphically Clear Lake’s watershed, main tributaries and flow gages.

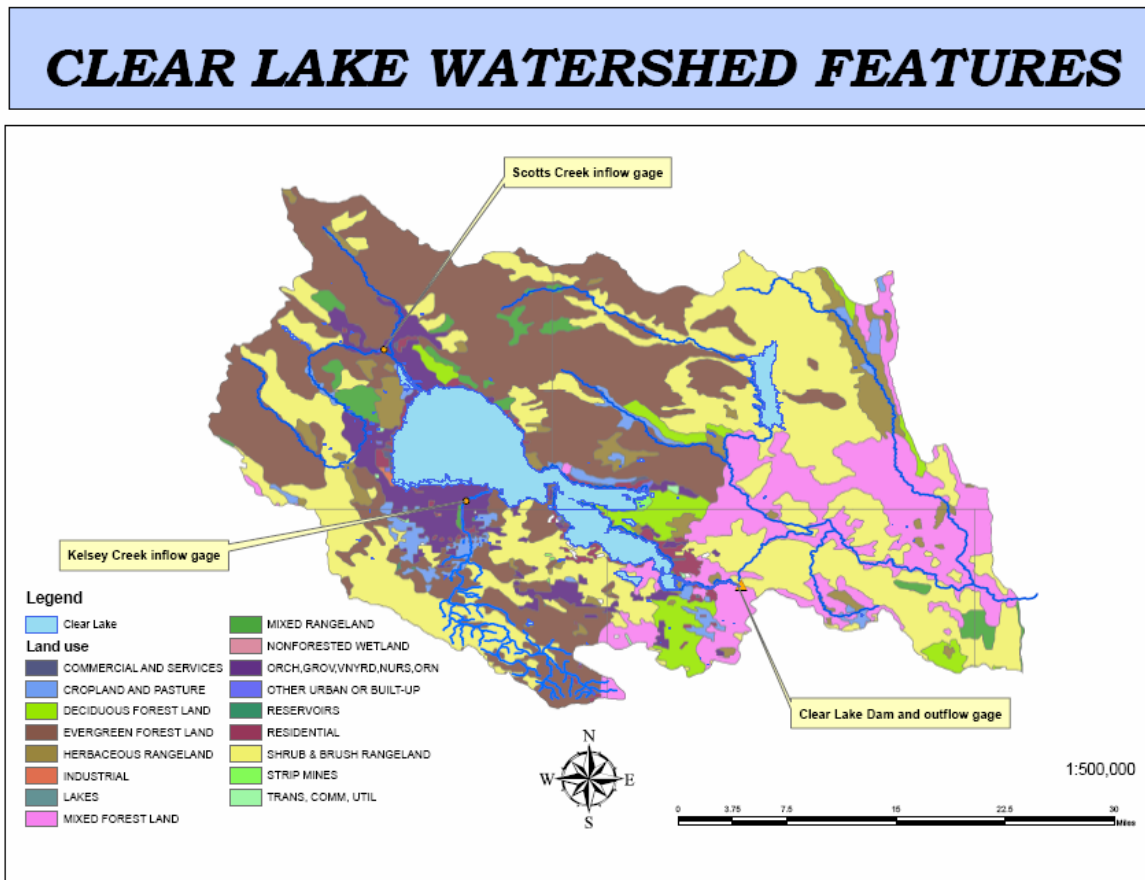


Figure 1. Clear Lake Watershed Features

Waterbody uses. Clear lake was included in the 1998 and 2002 303(d) list, primarily for nutrient impairment and causing blue-green algal blooms episodes such as those experienced in years 1990 and 1991. Clear Lake is the only waterbody included in the 303(d) list in the watershed. The beneficial uses declared in the *Sacramento River Basin and San Joaquin River Basin Water Control Plan (Basin Plan) for the California Water Quality Control Board Central Valley region (SSJ Basin Plan)* are municipal water supply, agriculture (irrigation and stock watering), recreation (contact and non-contact), warm freshwater habitat, warm spawning and wildlife habitat. The Basin Plan also identifies cold freshwater habitat as a potential future beneficial use of the waterbody.

Water Quality Goals: narrative Water Quality Objectives (WQO) for nutrient-related parameters were identified when the TMDL process was carried out in Clear Lake . The nutrient-related WQOs was the following: ‘*Water shall not contain biostimulatory substances which promote aquatic growths in concentrations that cause nuisance or adversely affect beneficial uses*’. Since the TMDL load allocation process needs numeric targets, an accurate study based on historic data was carried out detecting the factors affecting blue-green algae blooms in previous years. Data from compliant years (years in which blue-green algae were not present) were compiled and studied. The conclusion after this analysis was that the maximum possible concentration of chlchlorophyl-a was 73µg/l, which represents the highest level of this compound in summer peaks for compliant years.

Factors affecting Algal Blooms: Clear Lake is a naturally eutrophic waterbody, with high levels of phosphorus coming from the volcanic soils and sediments in the watershed and entering the lake. Two ways of phosphorus loadings exist in the waterbody. The first one is streamflow loading carrying load from soils dragged by the tributaries. The second one is known as *internal loading* and consists of dissolved orthophosphorus delivered by lakebed sediments in an environment of low dissolved oxygen caused, in most cases, by biomass decay on the lakebed. Internal phosphorus loading is considered the most important source of phosphorus in the waterbody. The fact that a weak relationship between watershed loading and in-lake water quality was found support this theory. Besides phosphorus, nitrogen is another important element in blue-green algae growth. Nitrogen is thought to be a limiting nutrient for algae-blooming. The value for the dissolved nitrogen-phosphorus ratio is situated between 15:1 and 7:1 from January to June. A ratio value greater than 15 means that the environment is phosphorus limited and a value smaller than 7 means that it is nitrogen limited. In the months ranging from July to December, the ratio value is smaller than 7, which means that nitrogen is a limiting factor for algae growth. The fact that compliant years such as 1983 showed extraordinarily great loads of phosphorus empower the idea that nitrogen may be a limiting factor in blue-green algae regardless of the total phosphorus load.

The fact that in summer months nitrogen is a limiting nutrient led the experts to think that a major source of nitrogen in Clear Lake is provided by nitrogen-fixing species of phytoplankton, which may produce an environment saturated in both, nitrogen and phosphorus. Under these conditions, the uptake of these nutrients is not limited by the availability of either of these nutrients, and the traditional nitrogen-phosphorus ratio becomes less useful. This theory would

explain the fact that dry periods are more likely to experience algal blooms. Decaying water levels enhance internal production of phosphorus (orthophosphorus) due to biomass decay, which produces low oxygen concentrations which enhance sediment delivery of phosphorus. The low water volume in the lake produces an increase in nutrient concentration (less dilution), which combined with high temperatures usually associated with drought periods foster blue-green algae blooms. Other chemicals such as iron are considered to play an important role in nitrogen fixation, but the importance of the role played by this element in blue-green algae blooms is challenging due sparse data available. However, a weak positive relationship between iron and blue-green algae concentration in dry periods was observed by experts. Iron is present in the watershed soils and introduced in the waterbody via erosion. Anthropogenic sources of iron (other than amplified erosion due to mining or construction) are unknown.

In conclusion:

- Clear Lake is naturally eutrophic. There's evidence that the lake is nitrogen-limited in Summer and Fall seasons when blue-green algae blooms occur.
- A potential source of nitrogen could be provided by nitrogen/fixing phytoplankton, which means that nitrogen is not a limiting nutrient anymore.
- Internal loads of P from sediments are more important than external loads
- Drought conditions experience higher than normal TP concentrations due to reduced dilution effects. Besides, internal P loading is triggered by biomass decay which create a low oxygen environment.

Model Scenarios:

AQUATOX was used to simulate different scenarios for Clear Lake. The main scope of the model was to reproduce the response of blue-green algae with (i) nutrient loads variations, and (ii) water inflow and outflow changes and, therefore, reservoir volume changes. Seven different situations were modeled. The input conditions and the results obtained for each of them are described.

Scenario 1: The input data entered for this scenario represent the conditions existing during predevelopment conditions within the watershed. The length of the simulation corresponds to one year (1970), which was considered in the TMDL waterbody assessment as an average year because it was not included in a dry period and blue-green algae blooms were not observed. The initial conditions for this scenario are described as follows:

a. Nutrient initial conditions: the initial conditions (in mg/l) were 0.08 for ammonia, 0.55 for nitrate and 0.1 for phosphorus. These values were the default values existing in the model for the Clear Lake tutorial in AQUATOX and were kept the same.

b. Oxygen and CO₂: the values weren't changed from the default conditions and their values were 6.5 and 0.7 mg/l respectively. Since no data was found for these parameters and the different period in which the model was tested, these values were kept the same for all the scenarios run.

c. Plants simulated: the plants that were simulated in the model were diatoms, green algae and blue-green algae (only in phytoplankton form). The initial conditions of each of them were 0.1,

1.0, and 0.21 mg/l respectively. The initial values in the reservoir were kept the same for all the seven scenarios since the main goal of the modeling process was to observe the effects of nutrient and flow changes in algae population. A change in initial conditions would make the different simulations not comparable because we wouldn't be able to know if the output is due to changes in variable or initial conditions.

d. Invertebrates: some invertebrates were included in the simulation. Amphipod, , Chironamid and Daphnia. However, invertebrates dynamics weren't the main scope of the modeling process.

e. Fish: Silverside, Bluegill, Catfish and Largemouth were modeled. The same thing happens with fish. They were not considered the main scope of the modeling process and therefore, all the values were kept the same as default values.

f. Water flow and reservoir volume: the water inflow was introduced in the model for each day in 1970. The outflow was kept constant for that year (default value) and set to $1.3 \cdot 10^5$ m³/d. The initial reservoir volume was considered to be $1.4 \cdot 10^9$ m³ (default initial conditions). For further scenarios, dynamic inflow and outflow daily data was obtained from different agencies and introduced in AQUATOX. The inflow and outflow gaging stations can be seen in Figure 1.

g. Water temperature: an annual mean temperature and a temperature range in both, the epilimnion and the hypolimnion. The temperatures used in the scenarios were the following:

For epilimnion: average temperature: 18°C, range of temperature: 16°C.

For hypolimnion: average temperature: 17°C, range of temperatures: 14°C.

AQUATOX is able to generate temperature changes for the different seasons based on the given temperatures averages and ranges. The figures showing the outputs from the different model runs show the seasonal temperature variation.

h. pH: the pH value was set to 8 and kept constant in the different scenarios

i. Inflow loadings: all the inflow loadings in the different scenarios were assumed to be entering the waterbody through its main tributaries. Non point sources or direct atmospheric deposition were not considered in the different runs. The nutrients that were considered to be entering Clear Lake were ammonia, nitrates and phosphorus. In the first scenario, ammonia inflow loading was considered 0mg/l, nitrates 1 mg/l and phosphorus 0.4963 mg/l. Ammonia and nitrates were left in this scenario equal to the default value. Phosphorus value corresponds to a total inflow loading of 370 Kg/d, that was estimated to be the predevelopment phosphorus inflow loading or natural loading for Clear Lake.

After setting the initial parameters, the program was run. The results are plotted in the next figures.

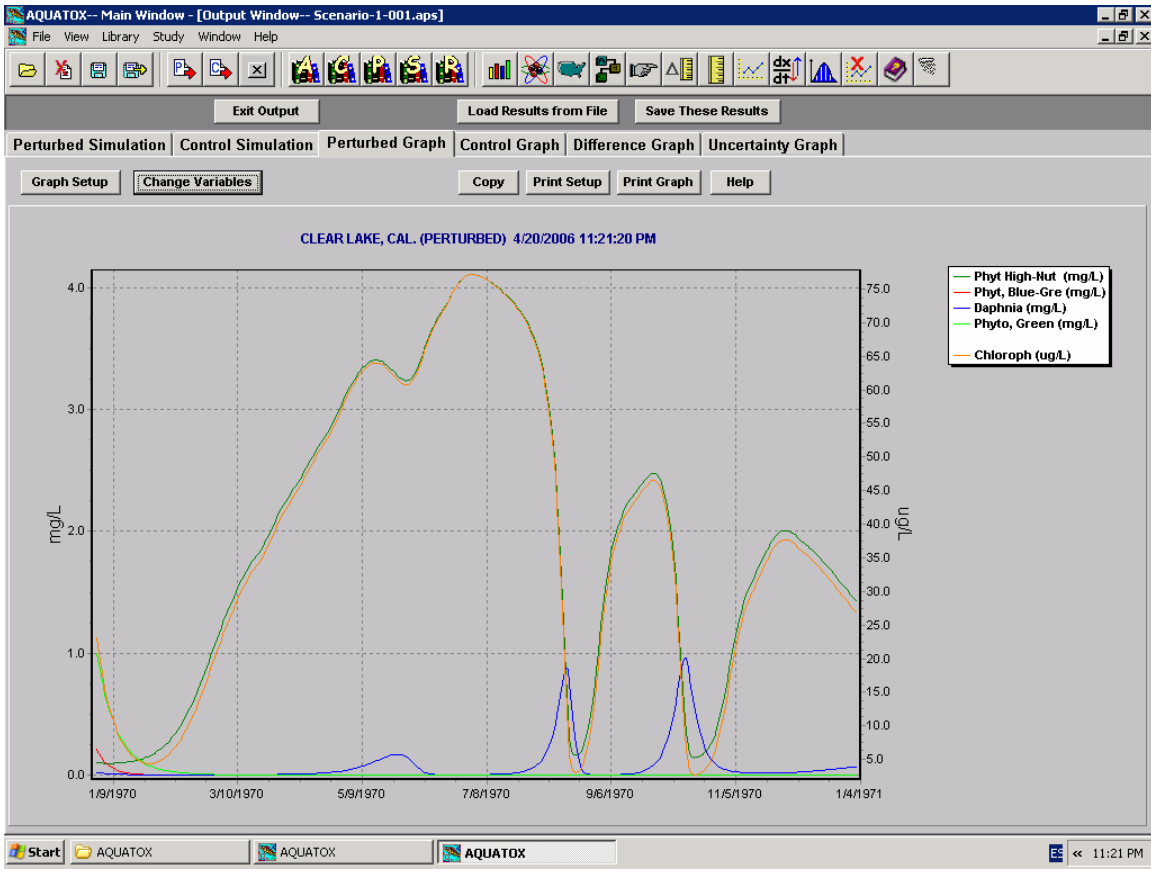


Figure 2. Algae growth and chlorophyll concentration for year 1970

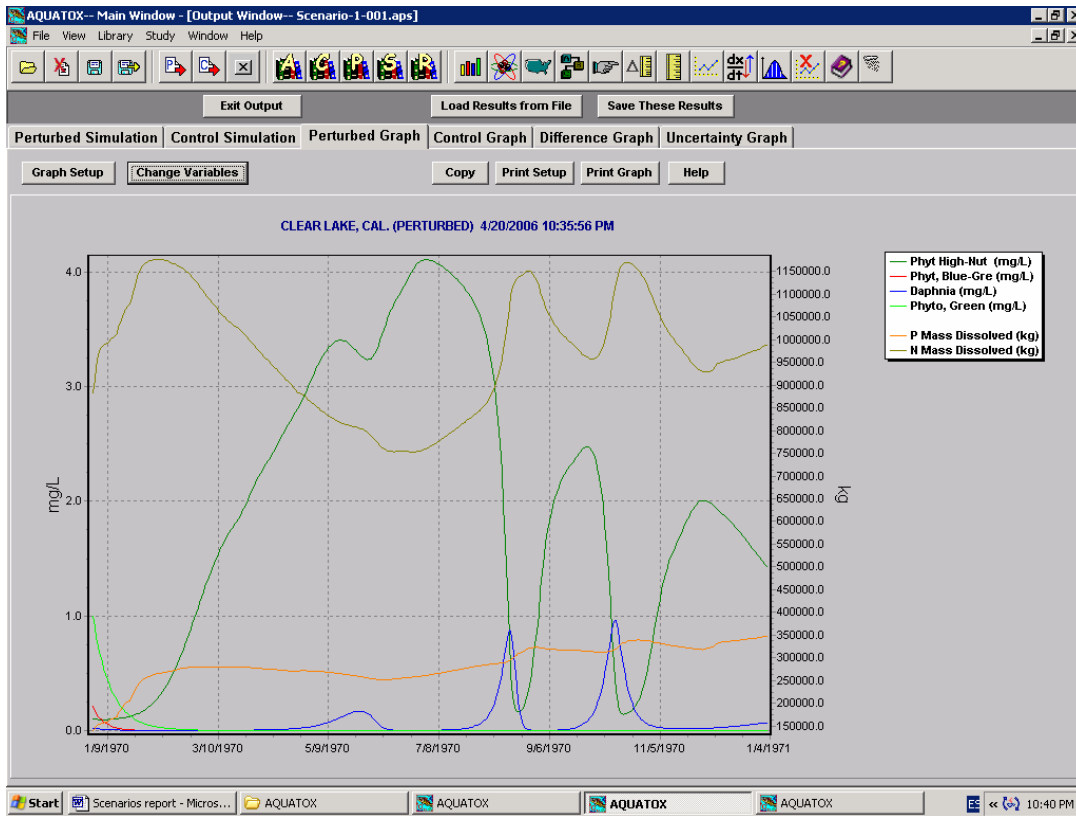


Figure 3. Algae growth and dissolved nutrients fluctuations

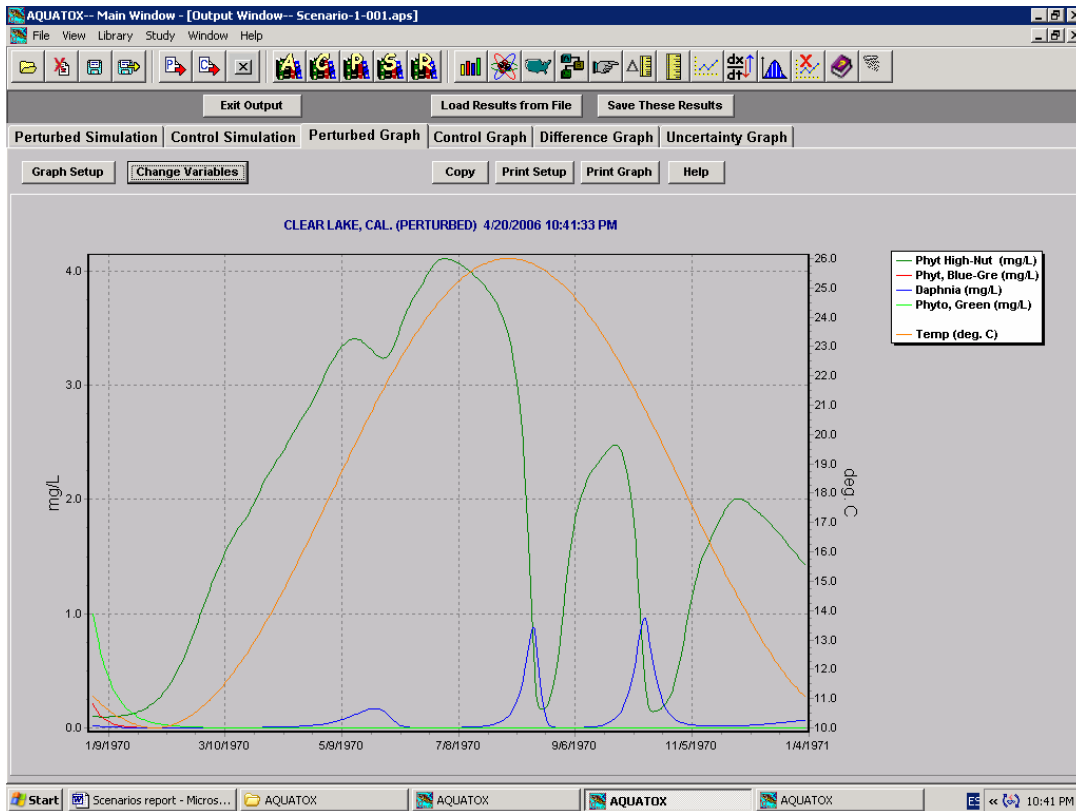


Figure 4. Algae growth and temperature changes in year 1970

As expected, no growth of blue-green algae was observed under these conditions. However, some conclusions can be drawn after this simulation. High temperatures periods foster algae growth and nitrogen could be a limiting factor for algae growth (see nitrogen decrease during green algae blooming period). This results agree very well with the TMDL report carried out in Clear Lake. Three different peaks for algae growth are observed, which match almost perfectly the increases of a certain threshold (1,150,000 kg) of dissolved nitrogen in the lake. The observed nitrogen-phosphorus ratio for green algae bloom from the model roughly 4. It should be noticed that the standard set after the TMDL process for chlorophyll-a ($73\mu\text{g/l}$) would be violated during the peak of the greatest green algae bloom under these conditions.

Scenario 2: The main goal of this scenario was to see if drought periods have a significant effect on blue-green algae growth. Since the TMDL process in Clear Lake stated that years in dry periods were more prone to have blue-green algae blooms, inflow data for one dry year was inputted in the model. The year chosen was 1987 (included in a drought period). Data for inflow from the main tributaries and outflow in the dam were retrieved and entered in the model. The results obtained in this case are shown in the following figures.

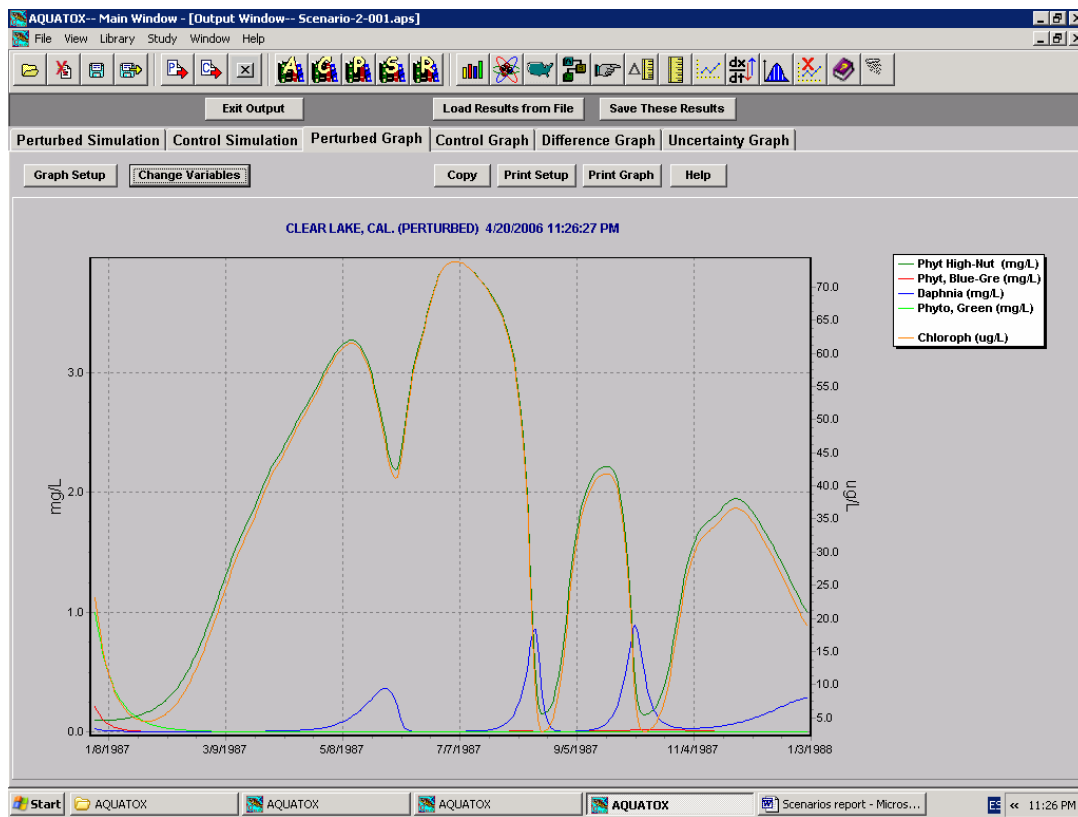


Figure 5. Algae growth and chlorophyll-a concentration in year 1987

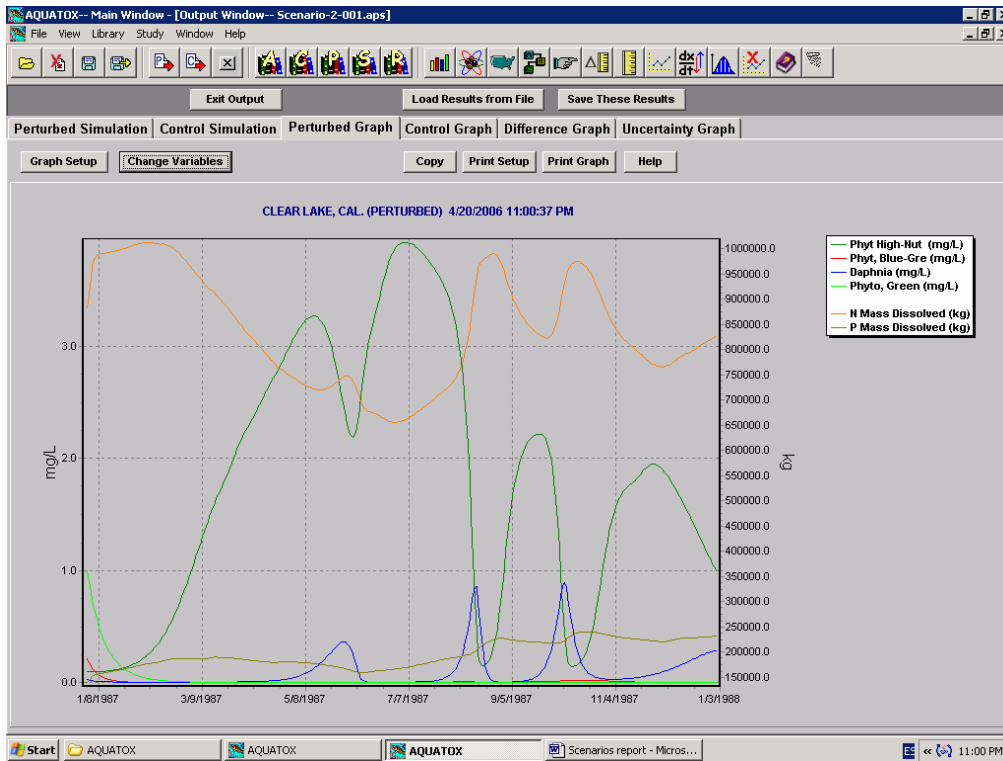


Figure 6. Algae growth and nutrient fluctuations in 1987

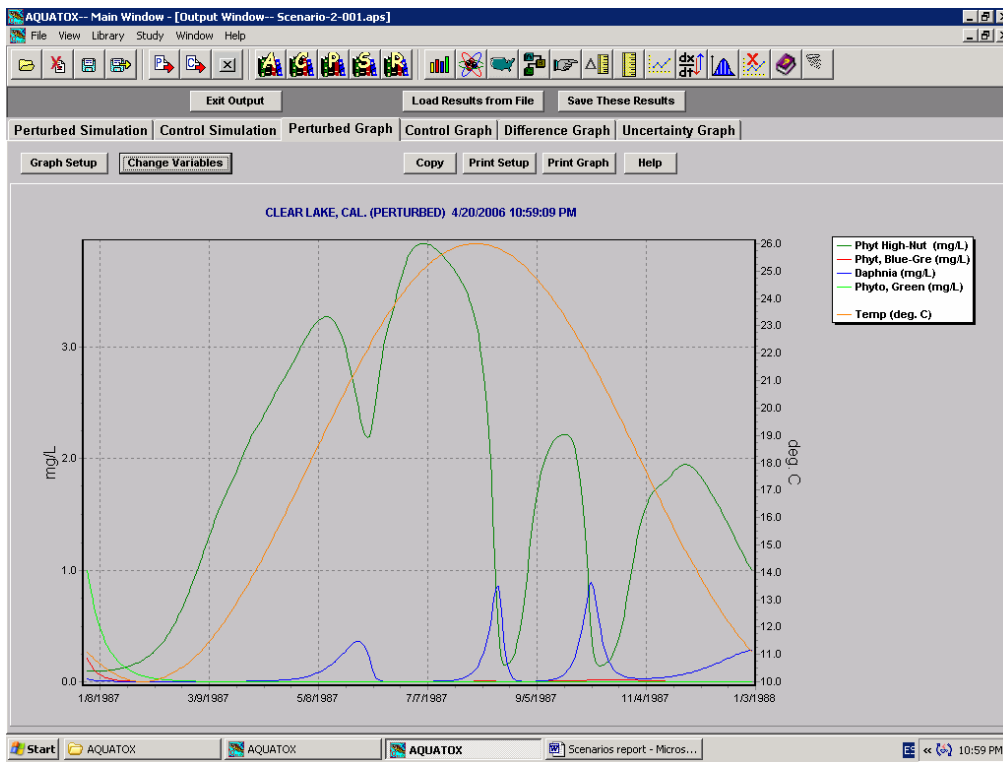


Figure 7. Algae growth and temperature variations in 1987

In this case, the results are exactly the same as in the previous scenario, which seems to enhance the fact that the lake is nitrogen limited. However, the fact that green algae bloom starts at N-P ratios of 4 (usually a value of 7 is considered optimum for algae growth), may enhance the idea that in the lake some atmospheric nitrogen fixing organisms may exist as stated in the introduction of the present report. Temperature seems also to play a role since the biggest blooms are when higher temperatures are observed. However, accurate data for temperature variations were not available and this parameter was kept the same for all the simulations. In this scenario, the maximum chlorophyll-a concentration during the big bloom is slightly greater than the standard set in the TMDL process.

Scenario 3: The main goal of this scenario was to see if an increase of the initial concentration of total soluble phosphorous in the lake as well as an increase of total soluble phosphorous in the inflow loading have a significant effect on blue-green algae growth. Since the lake is nitrogen-limited in the summer months, in this scenario the phosphorous concentrations were increased. The initial concentration of total soluble phosphorous was increased five times from 0.1 mg/L in the previous two scenarios to 0.5 mg/L in this scenario. Also, the inflow loading of phosphorous was increased by 10% from 0.4963 mg/l in the previous two scenarios to 0.5359 mg/L in this scenario. The simulation year was kept as 1987 as the previous scenario since this was a drought period. In all successive scenarios the simulation period was kept as 1987 to simulate the worst case condition and determine the effect that the initial concentrations and inflow loadings of the nutrients have on algal blooms. The results obtained in this case are shown in the Figures 8 through 10.

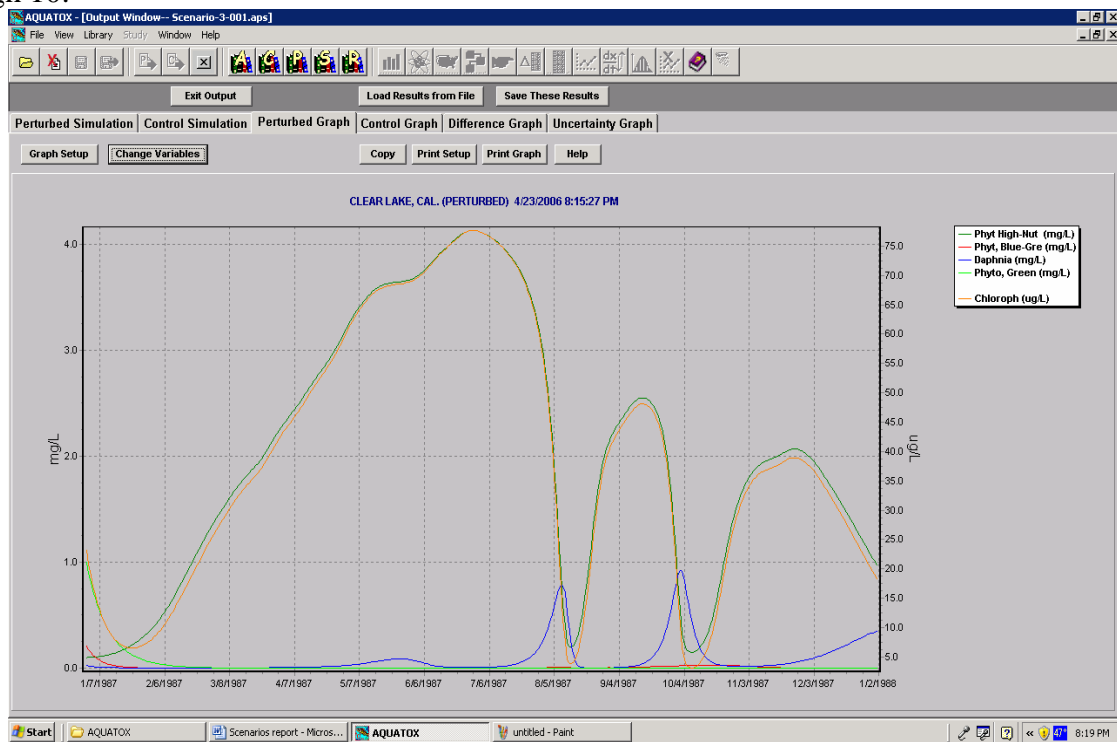


Figure 8. Algae growth and chlorophyll-a concentration for Scenario 3

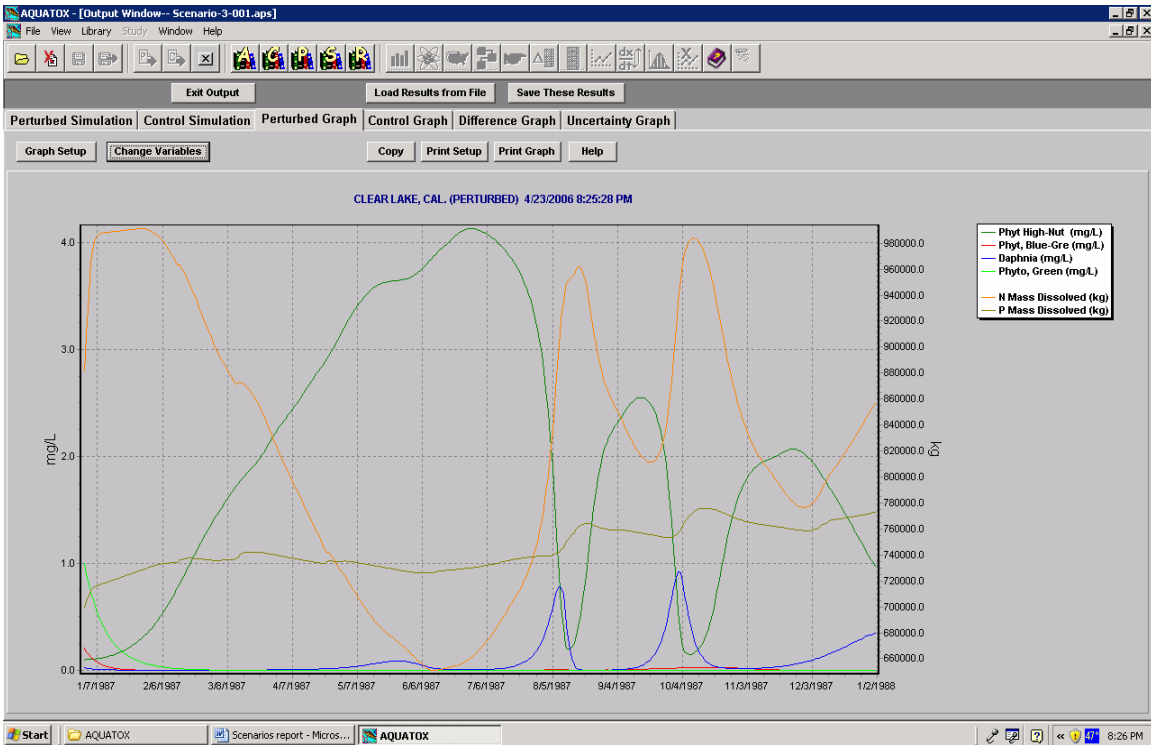


Figure 9. Algae growth and nutrient fluctuations for Scenario 3

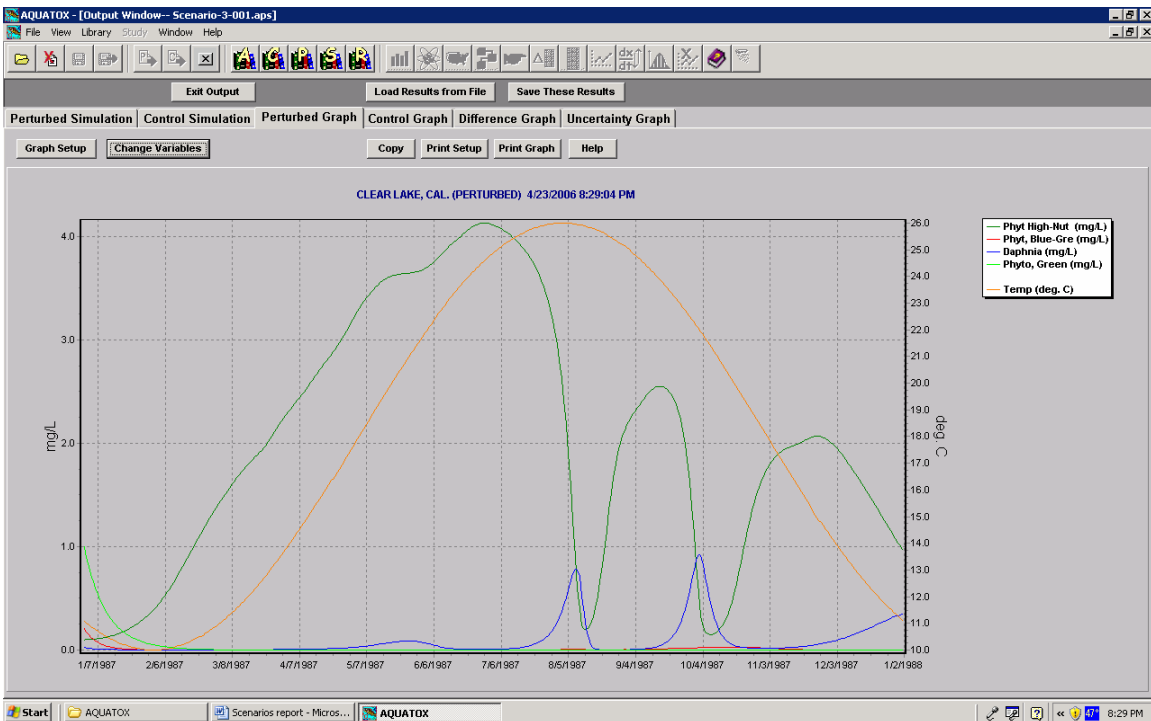


Figure 10. Algae growth and temperature variations for Scenario 3

By comparing the results of Scenarios 2 and 3 in the plots for chlorophyll-a, it can be observed that in the summer months a decrease of chlorophyll-a corresponding to a decrease of phytoplankton observed in case of scenario 2 was no longer present in scenario 3 with elevated

phosphorous concentrations. By comparing the results of Scenarios 2 and 3 in the plots for nutrient fluctuations, it was observed that the total dissolved phosphorous was at a much higher concentration throughout the simulation period in Scenario 3 as compared to Scenario 2. This is only obvious since Scenario 3 was run with a much higher phosphorous concentration both in the initial conditions and in the inflow loading. It was also observed by comparing the same plots that the total dissolved nitrogen in Scenario 3 showed a significant decrease in the summer months as compared to that in Scenario 2. This is not very well understood, but could possibly imply that the atmospheric nitrogen fixing organisms, referred earlier in the report, are not able to perform as good as that in the previous scenario especially during the summer months in presence of elevated phosphorous concentrations. It is to be noted that in this scenario there were no signs of blue-green algal bloom.

Scenario 4: The main goal of this scenario was to see if an increase of nitrogen, both as ammonia and nitrogen, in the inflow loadings to the lake has a significant effect on blue-green algae growth. The phosphorous concentrations both in the initial conditions and in the inflow loadings were kept the same as in Scenario 3. Since the lake is nitrogen-limited, in this scenario the initial concentrations of nitrogen both as ammonia and nitrate were not changed and kept the same as in the previous scenarios. The inflow loading of ammonia (both NH_3 and NH_4^+) was increased from 0 before to 0.1 mg/L as N and the inflow loading of nitrate was doubled from 1.0 mg/L in the previous scenarios to 2.0 mg/L in this scenario. The results obtained in this case are shown in the Figures 11 through 13.

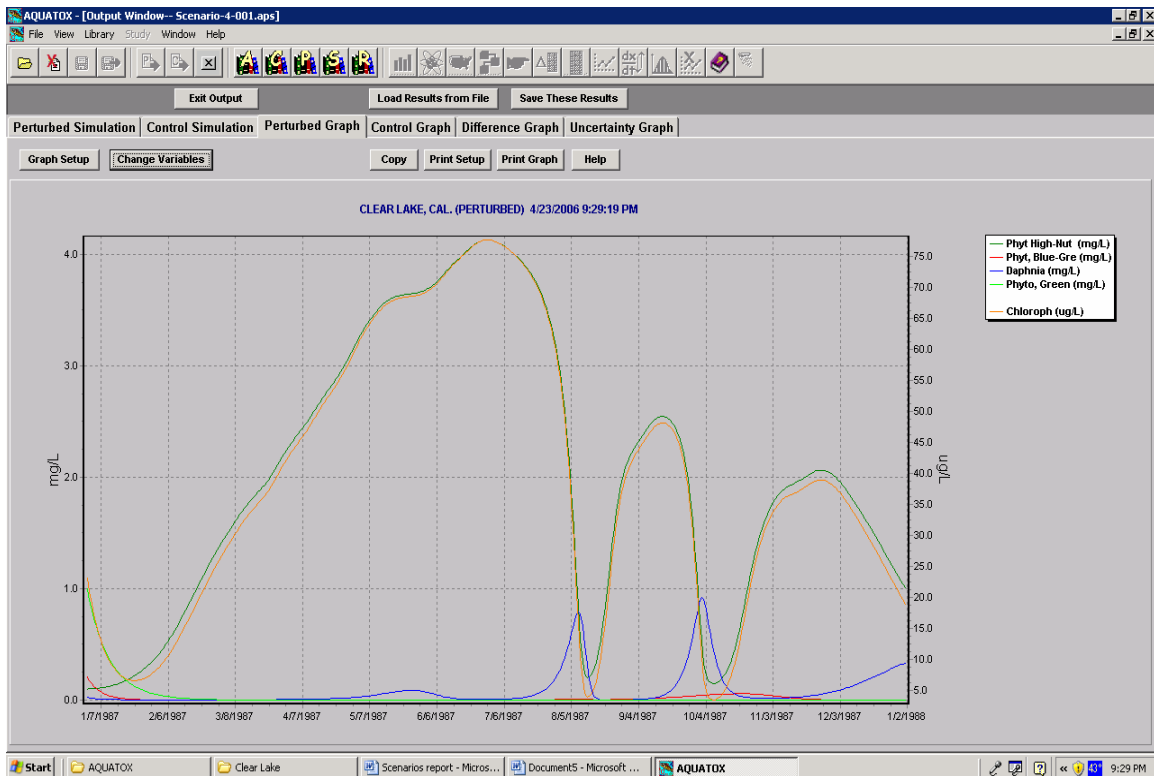


Figure 11. Algae growth and chlorophyll-a concentration for Scenario 4

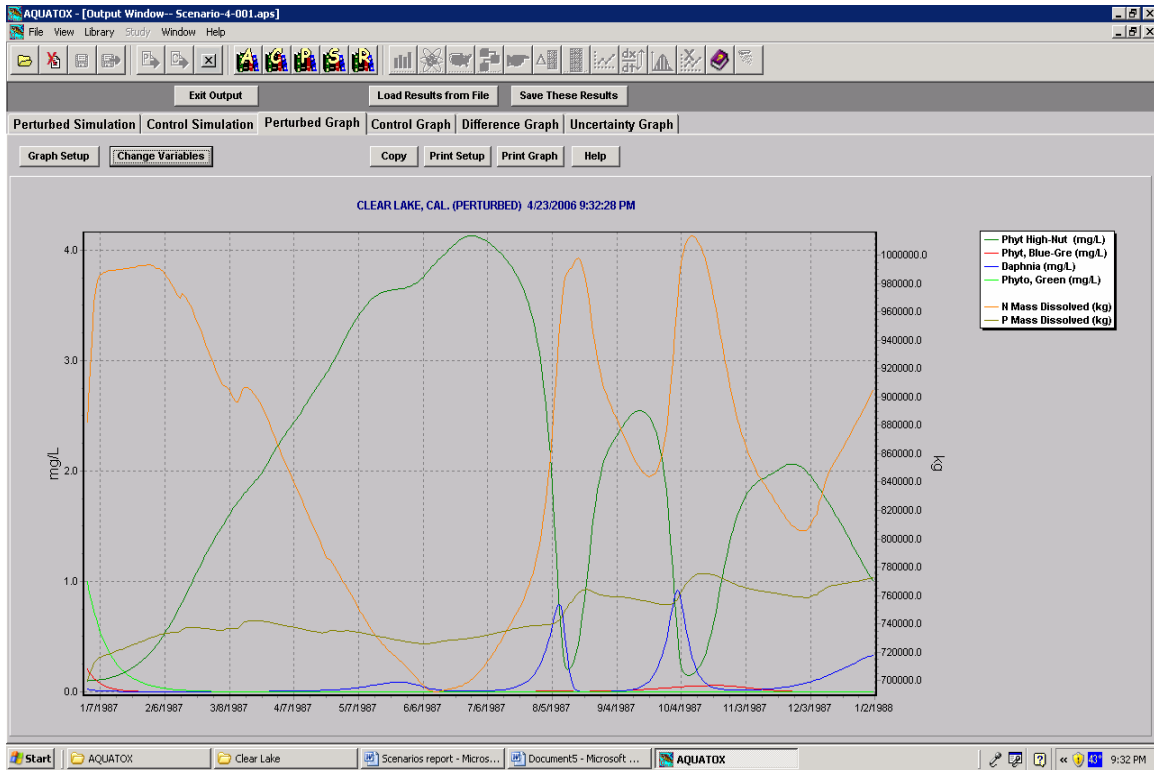


Figure 12. Algae growth and nutrient fluctuations for Scenario 4

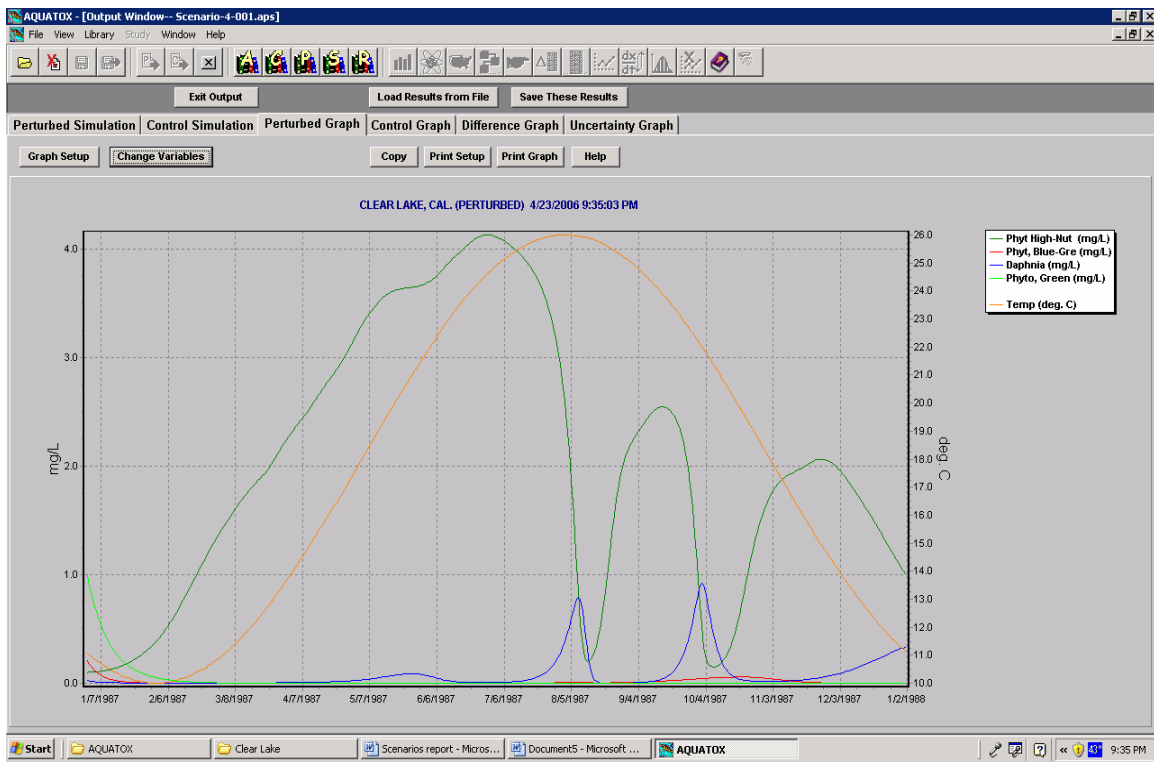


Figure 13. Algae growth and temperature variations for Scenario 4

By comparing the results of Scenarios 3 and 4 in the plots for chlorophyll-a, no significant differences can be observed. This means that increasing the nitrogen in the inflow loading by the amount specified in this scenario had no effect on the phytoplankton and chlorophyll-a concentrations in the lake. By comparing the results of Scenarios 3 and 4 in the plots for nutrient fluctuations, no significant differences can be observed in the total dissolved nitrogen between the two plots. This could imply that the increase in the nitrogen inflow loadings specified in this scenario was not sufficient to show any appreciable increase in the total dissolved nitrogen in the lake. However, by comparing the total dissolved phosphorous between the two plots it was observed that the total dissolved phosphorous was at a higher level throughout the simulation period in Scenario 3 as compared to Scenario 4. This was not expected since the phosphorous load was not changed from Scenario 3. The possible explanation for this could be that in presence of higher nitrogen in the lake some of the plants and microorganisms might have a higher uptake of phosphorous, thus reducing the soluble phosphorous concentration in the lake from the previous scenario. It is to be noted that in this scenario, there was not observable signs of blue-green algal bloom.

Scenario 5: The main goal of this scenario was to see if an increase of nitrogen, both as ammonia and nitrogen, in the inflow loadings to the lake has a significant effect on blue-green algae growth. The phosphorous concentrations both in the initial conditions and in the inflow loadings were kept the same as previous scenarios. Since the lake is nitrogen-limited, in this scenario the initial concentrations of nitrogen both as ammonia and nitrate were not changed and kept the same as before. The inflow loading of ammonia (both NH₃ and NH₄⁺) was increased from 0.1 to 2.0 mg/L as N and the inflow loading of nitrate was doubled from 2.0 mg/L in the Scenario 4 to 4.0 mg/L in this scenario. The results obtained in this case are shown in the Figures 14 through 16. All other variables are kept as before.

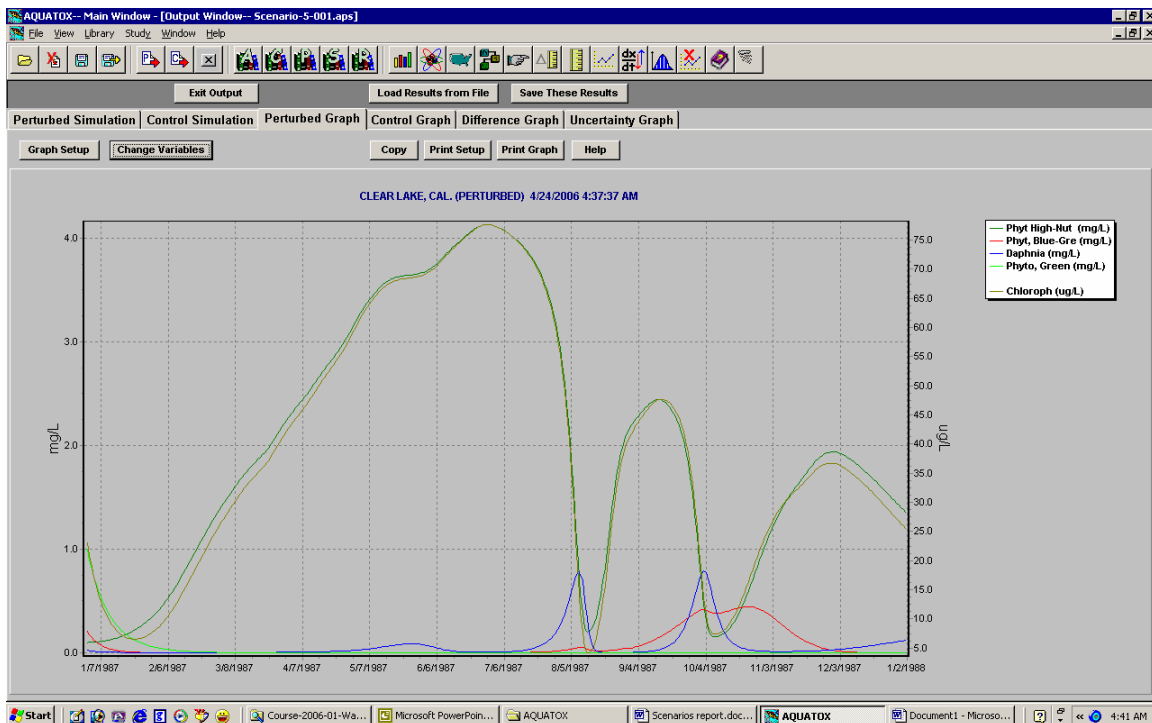


Figure 14. Algae growth and chlorophyll-a concentration for Scenario 5

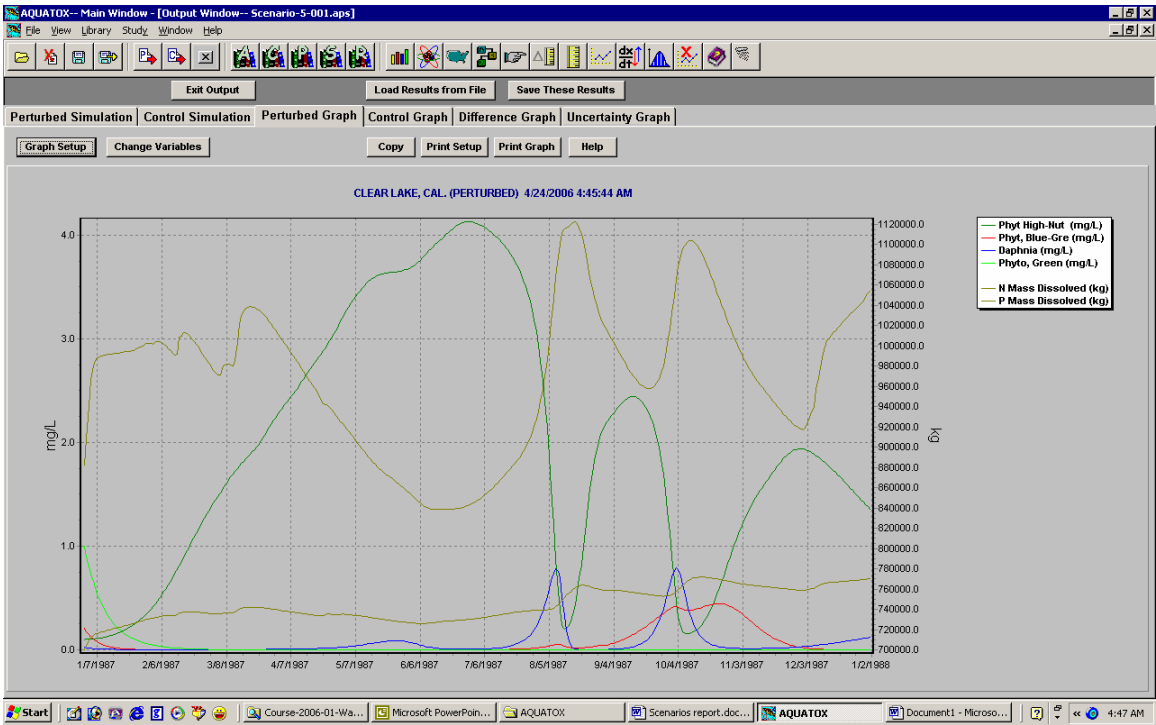


Figure 15. Algae growth and nutrient fluctuations for Scenario 5

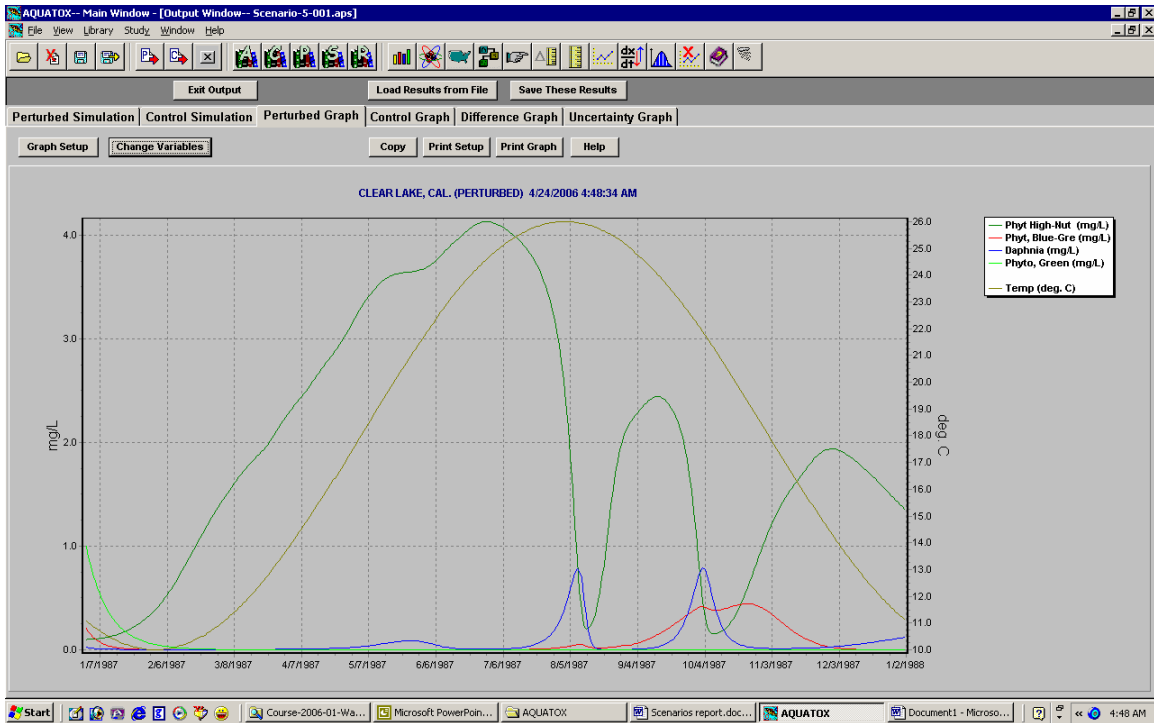


Figure 16. Algae growth and temperature variations for Scenario 5

The first recognizable population of Blue-Green Algae can be recognized in the results of this scenario. The growth of Blue-Green Algae is started in July during the maximum temperature of the year. The maximum concentration of this kind of algae is observed in the end of October with concentration of less than 0.5 mg/L.

By comparing the results of Scenarios 4 and 5 in the plots for chlorophyll-a, no significant differences can be observed in two first peak, but the maximum concentration of chlorophyll-a in the third peak is about 10% less than the Scenario 4. This means that increasing the nitrogen in the inflow loading by the amount specified in this scenario had no effect on the phytoplankton and chlorophyll-a concentration in the lake.

By comparing the results of Scenarios 4 and 5 in the plots for nutrient fluctuations, up to 30% increase in the total dissolved nitrogen can be observed. This occurred because of the increase in the nitrogen inflow loadings specified in this scenario. No recognizable difference between the total dissolved phosphorous in two plots can be observed.

Scenario 6: The main goal of this scenario was to see the effects of a larger increase in inflow loadings of nitrogen, both as ammonia and nitrogen, on blue-green algae growth pattern. In this scenario the initial concentrations of nitrogen both as ammonia and nitrate were not changed and kept the same as before. The inflow loading of ammonia (both NH_3 and NH_4^+) was increased from 2.0 to 4.0 mg/L as N and the inflow loading of nitrate was doubled from 4.0 mg/L in the Scenario 5 to 8.0 mg/L in this scenario. The results obtained in this case are shown in the Figures 17 through 19. All other variables are kept as Scenario 5.

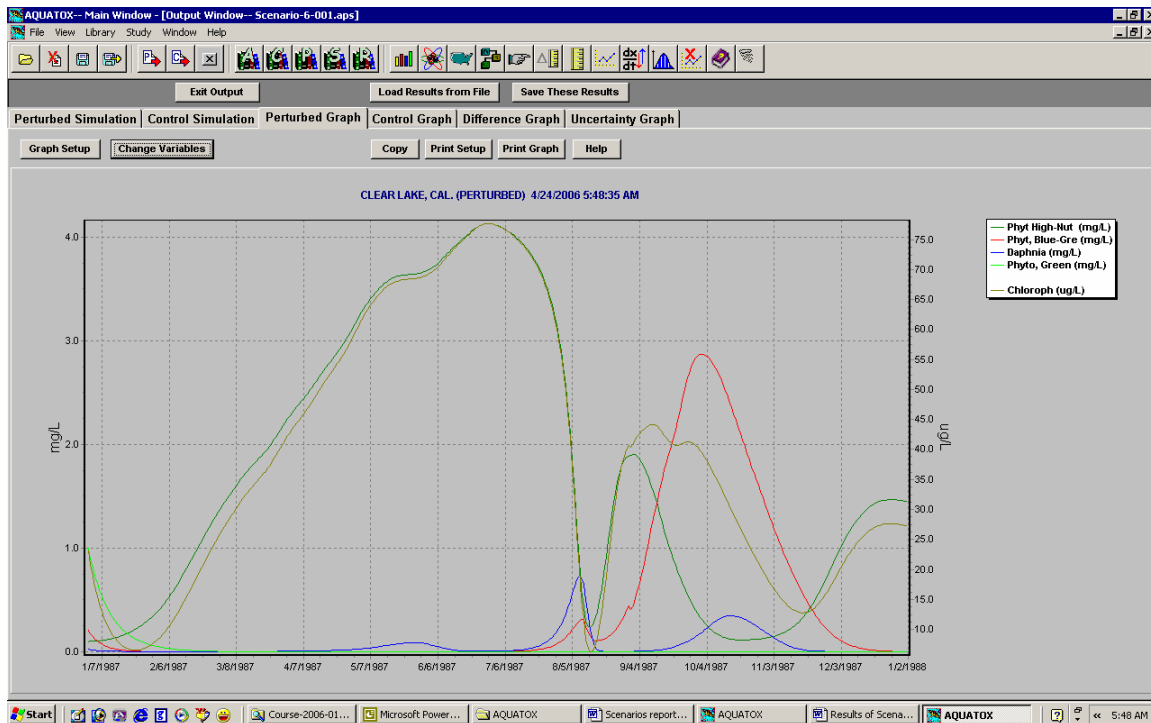


Figure 17. Algae growth and chlorophyll-a concentration for Scenario 6

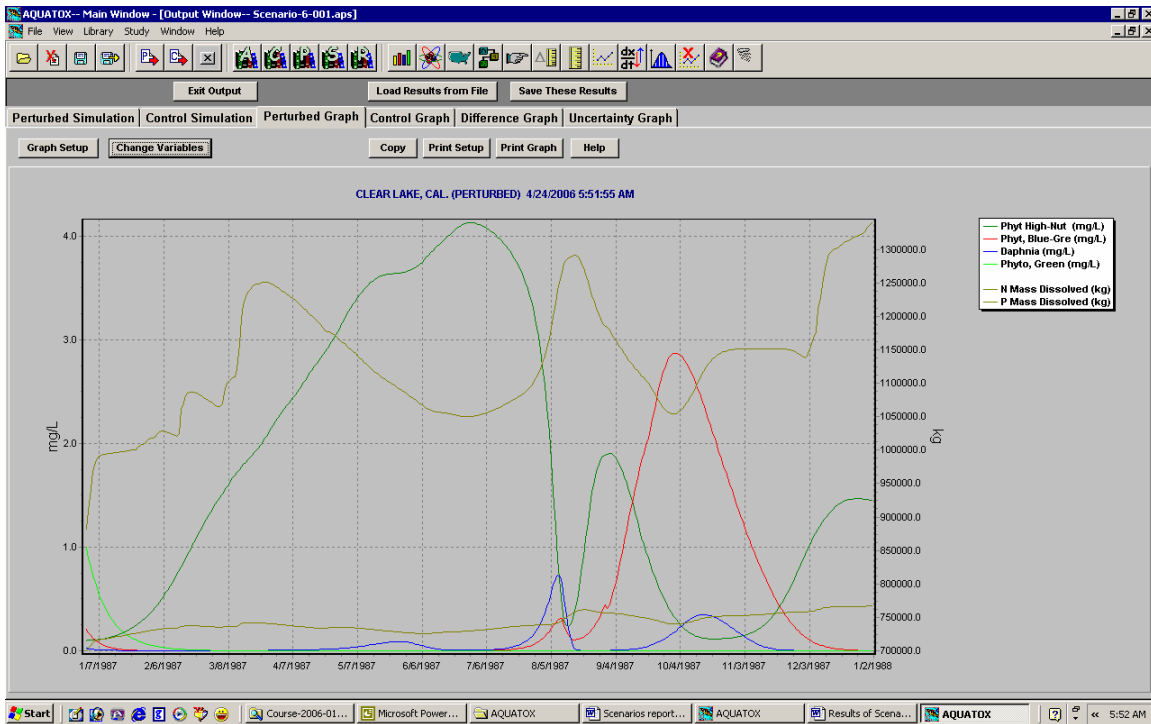


Figure 18. Algae growth and nutrient fluctuations for Scenario 6

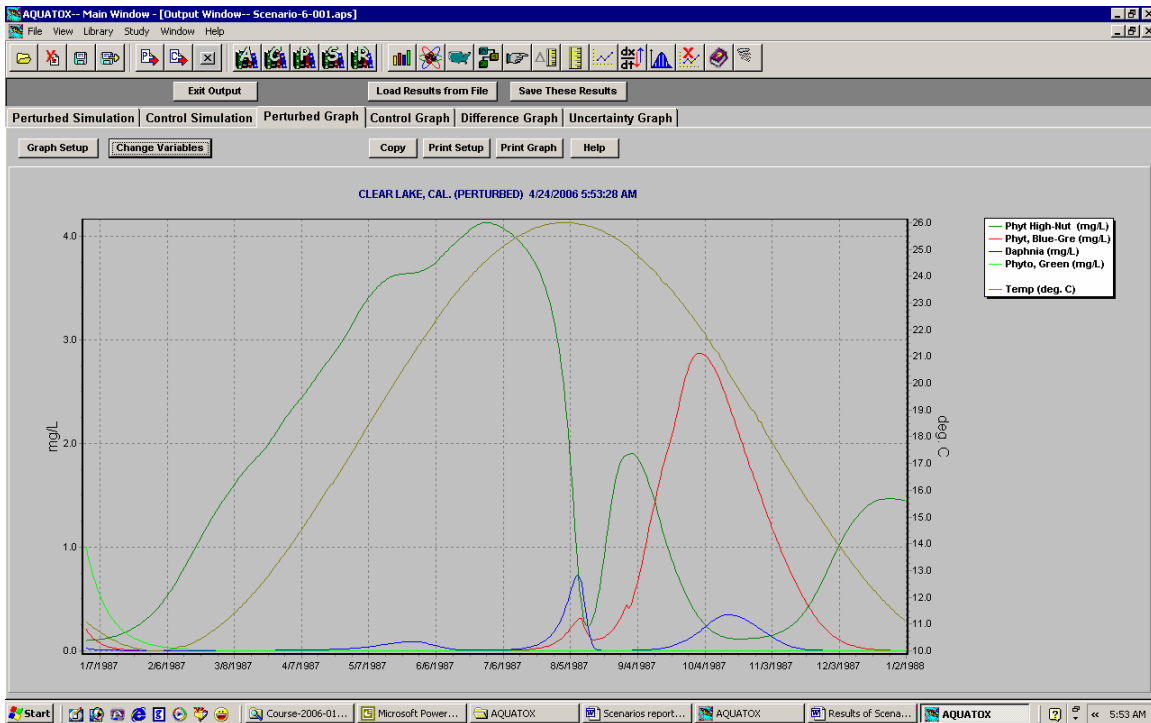


Figure 19. Algae growth and temperature variations for Scenario 6

A significant increase in population of Blue-Green Algae can be recognized in the results of this scenario. The occurrence of Blue-Green Algae occurs in the same month but the growth rate is clearly faster than growth rate in the scenario 5. The maximum concentration is observed in the

beginning of October with the concentration of about 3 mg/L which is 600% more than observed maximum concentration in scenario 5.

By comparing the results of Scenarios 5 and 6 in the plots for chlorophyll-a, no significant differences can be observed before appearance of Blue-Green algae, but after that the chlorophyll-a shows another pattern. This means that increasing in Blue-Green algae has some effects on the phytoplankton and chlorophyll-a concentration in the lake. However it has no effects on violation of standard. Also it shows that phytoplankton and chlorophyll-a concentration are affected due to more complex biological processes than only existence of nutrients.

By comparing the results of Scenarios 4 and 5 in the plots for nutrient fluctuations, up to 15% increase in the total dissolved nitrogen can be observed. The increase in the nitrogen inflow loadings is the primary reason. A decrease in total dissolved phosphorous concentrations during occurrence of Blue-Green algae can be observed.

Scenario 7: The main goal of this scenario was to see and compare the difference between effects of increase in inflow loadings of nitrogen and effects of accumulated nutrient in the lake. All variables are kept as Scenario 5 otherwise mentioned. The initial concentration of ammonia (both NH_3 and NH_4^+) was increased twice from 0.08 mg/L in the previous scenario (from scenario 2 to scenario 6) to 0.16 mg/L in this scenario. The initial concentration of Nitrate is also increased from 0.55 mg/L to 1.1 mg/L. In this scenario the inflow loading of ammonia and nitrate were kept unchanged from scenario 5. The results obtained in this case are shown in the Figures 20 through 22.

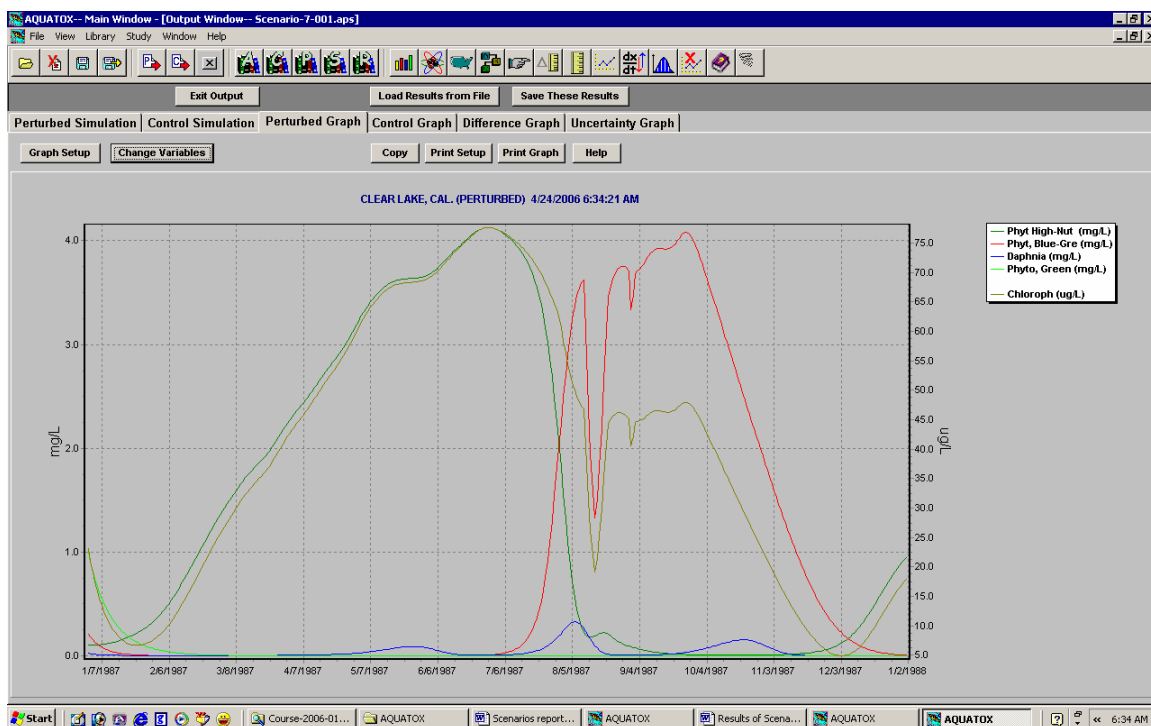


Figure 20. Algae growth and chlorophyll-a concentration for Scenario 7.

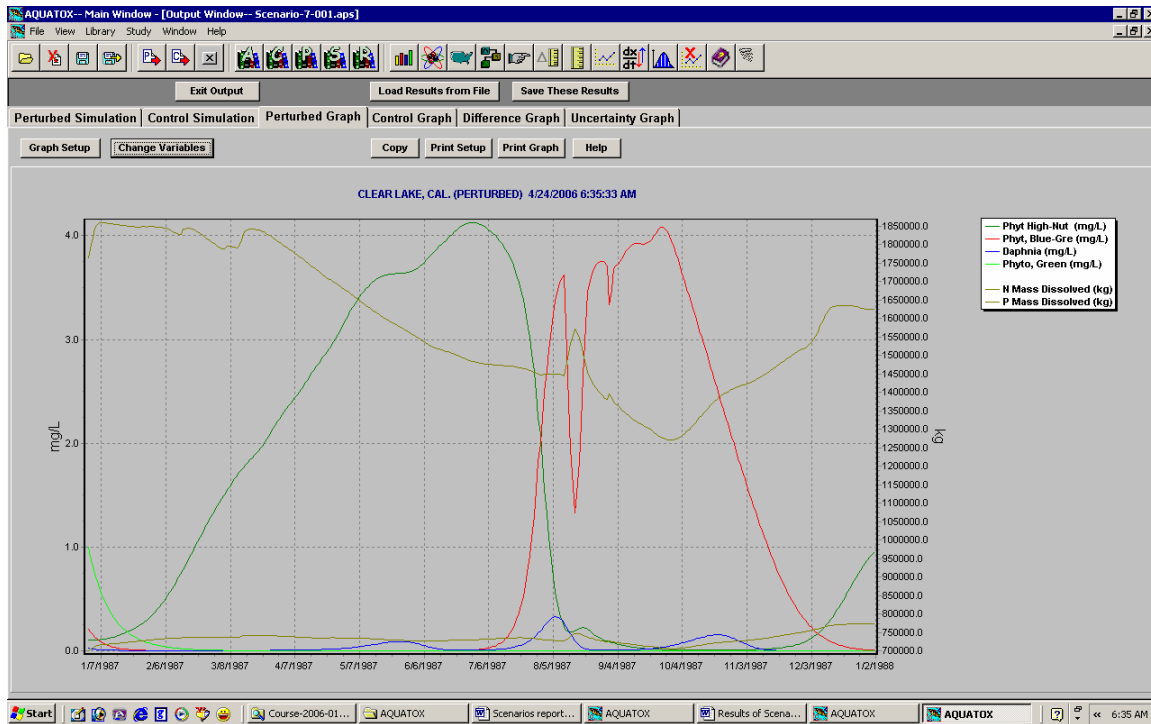


Figure 21. Algae growth and nutrient fluctuations for Scenario 7

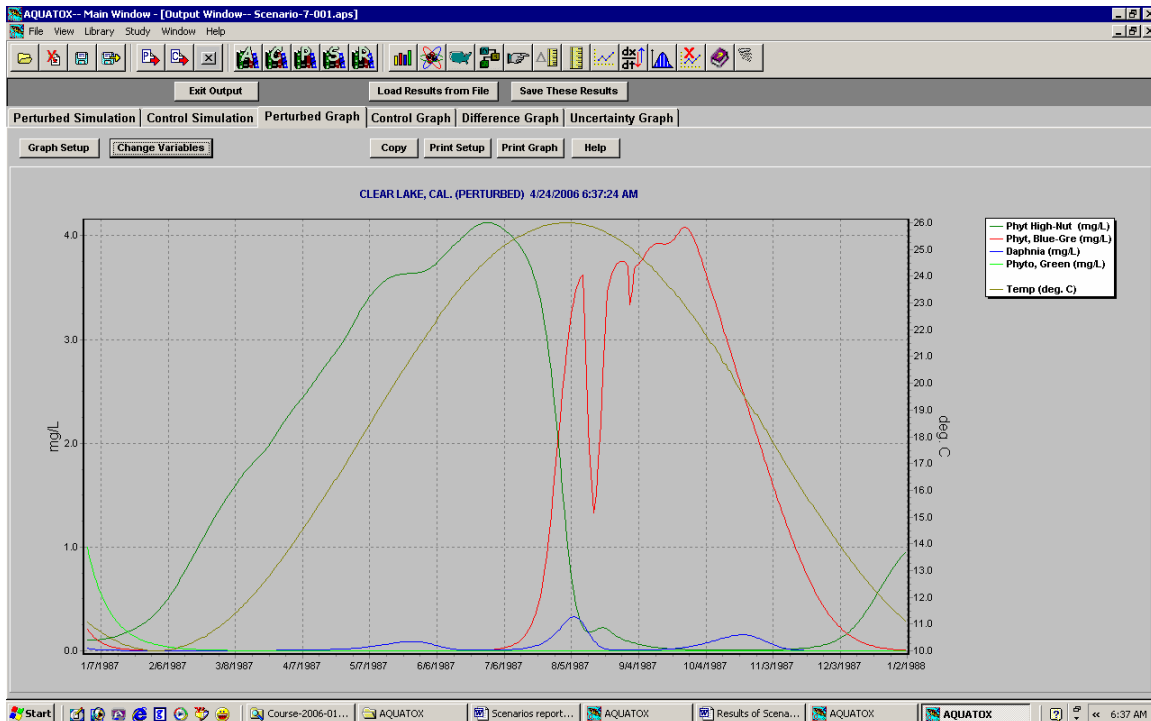


Figure 22. Algae growth and temperature variations for Scenario 7

A significant increase in concentration and duration of Blue-Green Algal bloom can be recognized in the results of this scenario. The occurrence of Blue-Green Algae occurs in July, a few months earlier than what observed in scenario 5 and 6. The maximum concentration is

around 4 mg/L which is 800% and 33% more than observed maximum concentration in scenario 5 and 6 respectively. By comparing the results of Scenarios 5 and 7 in the plots for chlorophyll-a, no significant differences can be observed before appearance of Blue-Green algae, but after that the chlorophyll-a shows another pattern which is also different from the results of scenario 6. However it still has no effects on violation of standard. It seems that both chlorophyll-a and blue-green algae follow the same pattern in this period. By comparing the results of Scenarios 5 and 7 in the plots for nutrient fluctuations, less fluctuation in total dissolved nitrogen can be observed. The high initial concentration of Nitrogen is the main responsible reason. Clear drop in total dissolved nitrogen during occurrence of Blue-Green algae can also be observed.

A summary of the different scenario runs, as described above are given in Table 1 below.

Table 1. Summary Variable Changed in the Different Scenarios

Scenarios	Initial Conditions			Average Daily Flow		Inflow Loadings		
	NH ₃ & NH ₄ ⁺ as N	NO ₃ As N	Total Sol. P	Inflow	Outflow	NH ₃ & NH ₄ ⁺ as N	NO ₃ as N	Total Sol. P
	mg/L	mg/L	Mg/L	m ³ /d	m ³ /d	Mg/L	mg/L	mg/L
<i>Scenario 1</i>	0.08	0.55	0.1	7.45x10 ⁵	1.3x10 ⁵	0	1.0	0.4963
<i>Scenario 2</i>	0.08	0.55	0.1	1.18x10 ⁵	1.36x10 ⁵	0	1.0	0.4963
<i>Scenario 3</i>	0.08	0.55	0.5	1.18x10 ⁵	1.36x10 ⁵	0	1.0	0.5459
<i>Scenario 4</i>	0.08	0.55	0.5	1.18x10 ⁵	1.36x10 ⁵	0.1	2.0	0.5459
<i>Scenario 5</i>	0.08	0.55	0.5	1.18x10 ⁵	1.36x10 ⁵	2.0	4.0	0.5459
<i>Scenario 6</i>	0.08	0.55	0.5	1.18x10 ⁵	1.36x10 ⁵	4.0	8.0	0.5459
<i>Scenario 7</i>	0.16	1.0	0.5	1.18x10 ⁵	1.36x10 ⁵	2.0	4.0	0.5459

Main conclusions from the modeling process:

The modeling process after the seven scenarios, led to several basic conclusions listed below.

1. The standard was most likely set observing green-algae growth patterns because the chlorophyll-a concentrations are higher with green algae than with blue-green algae bloomings. Besides, the highest values reached in green algae bloomings are very similar to the standard set in the TMDL process (73µg/l), which made us think that this was the way experts set the standard.

2. The theory of presence of nitrogen-fixing phytoplankton organisms is backed by the AQUATOX 2.1 model, since algae growth is observed with N/P ratios lower than 7, which is considered to be the threshold for nitrogen limited environments.

3. One year period is too short for a simulation period. The waterbody nutrient loading can take more than one year. In order to see the effects of long-term nutrient loading in Clear Lake, the nutrients initial conditions or nutrient loadings were artificially increased to account for this factor.

4. The time of blue-green algae blooming peaks do not correspond to the highest temperatures, possibly because in the hottest months (summer), the nitrogen and phosphorous loads are not high enough yet. The reasons why this is so have been explained in point 3.

5. Nitrogen is the controlling factor for blue-green algae, only when the dissolved nitrogen concentration increases to a certain level, a blue-green algae blooming occurs.

However, and due to time and data availability restrictions some hypothesis couldn't be tested and some limitations of the model are explained. These are as follows.

1. The effects of dry periods over blue-green algae blooms. Even though all except one of the model runs are under a dry year flow regime, the effects of a drought period are most likely observed in a period longer than one year. Changes in reservoir volume and other factors associated with these periods such as oxygen depletion, may play an important role that was not observed in shorter simulations.

2. The data for inflowing water into the reservoir is limited. The flow data coming from two combined gaging stations named previously in this report do not represent the total flow entering the reservoir. However, the flow taken into account for the different runs is believed to be the most part of the incoming flow. Greater inflows in the reservoir area mean a greater amount of nutrient entering the reservoir, especially nitrogen. A greater amount of nitrogen could mean that the green and blue-green algae blooms might occur earlier in the year if the temperature is not a limiting factor.

3. Lack of information of the real initial conditions. Initial nutrient concentrations as well as algae presence at the beginning of the modeling process, are very important parameters needed to get a realistic simulation. The different scenarios tested were done only for a period of time of one year. Increasing initial concentrations of nutrients had a very significant impact on algae blooms, which shows the importance of initial conditions, especially in longer runs. Concentration of nutrients may occur especially in colder months in which algae growth is limited by temperature and, therefore, there's no consumption of these.

Despite of the limitations just cited, the model shows its power when it comes to predict the effect of external parameter change with time. More time would be needed and more data should be collected in order to carry on a sound study for the situation of Clear Lake, CA. However, AQUATOX 2.1 proved to be a highly efficient and very robust tool for environmental modeling. Not only that, but AQUATOX 2.1 is probably one of the most versatile models in ecology. The model is able to simulate a large amount of parameters (chemical and physical parameters, plants and animals dynamics etc.) using a very user-friendly interface that makes the modeling process (data input, data output, importing and exporting results etc.) much easier than one would expect with such a complete model. Besides, the manual available for the model, the tutorials available

when downloading the software from the EPA web-site, as well as a step-wise wizard for data input make this model surprisingly user-friendly. It was not the scope of the present project to evaluate whether the algorithms used for each of the parameter calculations (i.e. algae growth, oxygen depletion, nutrient concentration etc) were accurate or reliable enough to trust the results obtained. Such a task would require much more time than the authors of the present report had. However, the fact that AQUATOX 2.1 is supported and distributed by EPA, a public U.S. agency, make us think that is a very reliable model. Probably, nowadays the AQUATOX 2.1 is the most advanced environmental model worldwide.