ANNOTATED BIBLIOGRAPHY FOR AQUATOX

EPA- 820-B-13-002

Review

Abt Associates Inc. 2005. Linking Ecological Risk Assessment and Economic Benefits Bethesda MD.

The authors conducted an extensive search of the environmental and economic literature; they identified 173 articles on AQUATOX—more than we found 8 years later. Abt Associates concluded that, of the models they investigated, AQUATOX holds the most potential for generalized risk assessment use, and also has potential for use in regulatory scenarios including development of water quality criteria, total maximum daily loads (TMDL's), and analysis of management alternatives. They present several case studies with various models, including a very informative, detailed AQUATOX case study on economic valuation of the effects of a pesticide on largemouth bass in an Iowa reservoir.

Bartell, S. M., R.A. Pastorok, H. R. Akcakaya, H. Regan, S. Ferson, and C. Mackay. 2003. Realism and relevance of ecological models used in chemical risk assessment. Human and Ecological Risk Assessment 9:907-938.

See Pastorok et al. 2001 below

Bontje, D. M. 2010. Analysis of toxic effects and nutrient stress in aquatic ecosystems. PhD Thesis, Vrije Universiteit, Amsterdam, The Netherlands.

As is customary in Europe, this thesis includes several published papers co-authored by the doctoral candidate. AQUATOX formulations were reviewed, and AQUATOX biotc parameters were used for invertebrates in one of his models.

Booty, W. 2001. Options for Modelling of Transboundary Water Quality. Environment Programme, Mekong River Commission Secretariat.

A consultant assessed available water quality models for use in representing the transport and effects of nutrients and contaminants (mainly pesticides) in the Mekong River. He recommended using a general water quality risk assessment model such as AQUATOX, which is written in an object-oriented language and can be modified to match the level of required complexity.

Borah, D., G. Yagow, A. Saleh, P. Barnes, W. Rosenthal, E. Krug, and L. Hauck. 2006. Sediment and nutrient modeling for TMDL development and implementation. Transactions of the ASAE 49:967-986.

This paper reviews numerous models that have the potential to be used for TMDL applications; most are watershed models. AQUATOX is described briefly and is deemed suitable for analyzing receiving water qualities in nutrient TMDLs. The authors observe that "Simple models are easy to use but have limitations; comprehensive models are labor and data intensive but offer extensive analysis tools." The implication is that AQUATOX falls in the latter category.

Brils, J. and B. Harris. 2009. Towards Risk-Based Management of European River Basins: Key-findings and Recommendations of the RISKBASE Project. RTD Framework Programme (FP6), Utrecht, The Netherlands.

This booklet by the European RISKBASE group states that AQUATOX is one of the most promising models developed for higher tier, site-specific risk assessments at the ecosystem level.

Galic, N., U. Hommen, J. M. Baveco, and P. J. van den Brink. 2010. Potential application of population models in the European ecological risk assessment of chemicals II: Review of models and their potential to address environmental protection aims. Integrated Environmental Assessment and Management 6:338-360.

This paper presents an extensive review of models with the potential for use in risk assessment of chemicals. AQUATOX is given as an example of modeling the indirect effects in food webs. The case study is based on Sourisseau et al. (2008); the review describes in detail the calibration and application to an artificial stream including sensitivity analysis and validation. Both direct and indirect effects were predicted.

Hawkins, T. 2005. Critical Evaluation of the Aquatox Model. Carnegie Mellon University, Pittsburgh PA.

This graduate student project involved a detailed evaluation of AQUATOX Release 2. The conclusion was that AQUATOX is a powerful tool for the simulation of aquatic ecosystems. Numerous suggestions for improving the model, such as sensitivity analysis, comprehensive context-sensitive Help, and log scales for plots, have been implemented in later releases.

Imhoff, J. C., J. S. Clough, R. A. Park, and A. Stoddard. 2004. Evaluation of Chemical Bioaccumulation Models of Aquatic Ecosystems: Final Report. U.S. Environmental Protection Agency, Athens GA.

See next paper.

Imhoff, J. C., J. S. Clough, R. A. Park, A. Stoddard, and E. Hayter. 2005. Comparison of Chemical Bioaccumulation Models to Assist in Model Selection for Ecological Assessments and TMDL Development *in* Watershed Williamsburg, Virginia.

The above two papers compare bioaccumulation models on the basis of a number of characteristics. AQUATOX is more complex than the other models reviewed in this study, but the incorporation of a eutrophication model in AQUATOX simplifies the definition of toxicant partition calculations among organic carbon compartments. It also accounts for a complete mass balance of inorganic solids and organic matter, including exchange of these materials between the water column and sediment bed.

Kianirad, E., D. Bedoya, I. Ghosh, K. McGarvey, and V. Novotny. 2006. Technical Report No. 7, Review of Watershed Ecological Models. Technical Report No. 7, Center for Urban Environmental Studies, Northeastern University, Boston MA.

This review was undertaken as a class project at Northeastern University. The authors concluded that it is "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." They cited the user-friendly interface, including the wizard for data input, as making the modeling process easy for such a complete model. The documentation and tutorials were also found to facilitate model application.

Kinerson, R. S., J. L. Kittle, and P. B. Duda. 2009. BASINS: better assessment science integrating point and nonpoint sources. Pages 1-24 Decision Support Systems for Risk-Based Management of Contaminated Sites. Springer.

AQUATOX is mentioned briefly as an example of a model that, although distributed independently, utilizes the extension architecture of BASINS so that one can proceed directly from BASINS into AQUATOX. In this way the GIS and results from component models, such as HSPF, can be used to drive AQUATOX simulations.

Koelmans, A. A., A. Van der Heidje, L. M. Knijff, and R. H. Aalderink. 2001. Integrated Modelling of Eutrophication and Organic Contaminant Fate & Effects in Aquatic Ecosystems. A Review. Water Research 35:3517-3536.

At the time of the review the authors considered AQUATOX to be one of two models that integrated contaminant fate and effects with eutrophication, with AQUATOX being "the most complete and versatile model described in the literature."

Limno-Tech Inc. 2002. Descriptive Inventory of Models with Prospective Relevance to Ecological Impacts of Water Withdrawals. The Great Lakes Commission, Ann Arbor, Michigan.

AQUATOX is described in detail in a one-page fact sheet and can be easily compared with other models in this extensive inventory. They state: "AQUATOX is one of the few general ecological risk models that represents the combined fate and effects of toxic chemicals." They list potential applications including water quality criteria and standards, Total Maximum Daily Loads, ecological risk assessments, analysis of proposed management alternatives, and identification of the most important among multiple stressors.

Liu, Y., H. Guo, Y. Fan, and L. Wang. 2005. [Research advance on lake ecosystem dynamic models]. Ying Yong Sheng Tai Xue Bao [The journal of applied ecology] 16:1169-1175.

AQUATOX is described along with several other simulation models that can be used to represent the dynamics of lake ecosystems. Article is in Chinese and indexed in Science Direct.

Long, W. 2010. Ecological Modelling as a Tool for Coastal Ecosystem Management. *in* A. Ramanathan, P. Bhattacharya, T. Dittmar, M. Bala Krishna Prasad, and B. R. Neupane, editors. Management and Sustainable Development of Coastal Zone Environments. Springer Heidelberg, Germany.

AQUATOX is characterized as the most comprehensive chemical model available. It is described as being a public-domain, mechanistic model that integrates aquatic ecosystem, chemical fate, and ecotoxicological constructs and that can be used to evaluate the effects of numerous stressors in a variety of environments.

Pastorok, R. A., S. M. Bartell, S. Ferson, and L. R. Ginzburg, editors. 2002. Ecological Modeling in Risk Assessment. Lewis, Boca Raton, Florida.

The authors concluded that AQUATOX is suitable for detailed ecological assessments. AQUATOX, Release 1.0, was judged to have *high* realism, relevance, degree of development and consistency, credibility, and resource efficiency; *medium* treatment of uncertainty and regulatory acceptance; and *low* ease of estimating parameters.

Pastorok, R. A., D. Preziosi, and D. Rudnick. 2008. Ecotoxicological Model of Populations, Ecosystems, and Landscapes. Pages 1165-1186 *in* S. E. Jørgensen and B. D. Fath, editors. Ecotoxicology. Vol. [2] of Encyclopedia of Ecology, 5 vols. Elsevier, Oxford.

This article reviews the rationale for using ecotoxicological models in chemical risk assessments, compares models on the basis of numerous factors, and gives examples of applications. A detailed example is presented of using AQUATOX in risk assessment of permethrin for mosquito control on Long Island, New York. AQUATOX predicted an absence of longer-term community-level impacts for aquatic invertebrates, which was judged to be consistent with the findings previously reported in the open literature for wetlands exposed to vector control pesticides.

Preziosi, D. V. and R. A. Pastorok. 2008. Ecological food web analysis for chemical risk assessment. Science of the Total Environment 406:491-502.

Ecological food web analysis has generally received little attention from risk assessors. Simple models that include bioaccumulation have been used for years; complex models, especially ones that represent effects as well, have only recently gained regulatory acceptance. One such model is AQUATOX, which consists of bioenergetics, nutrient responses, and environmental fate and ecotoxicity of chemicals in an integrated package.

Russell, C. S., and D. D. Baumann. 2009. The evolution of water resource planning and decision making. Edward Elgar Publishing.

AQUATOX is mentioned in this general review as being an U.S. EPA-sponsored model that extends water quality modeling to representing the fate and effects of organic chemicals over time and space. Reference is made to the proposed linkage with HSPF to model PCB contamination in the Housatonic River in Massachusetts (an application that was later dropped).

Sharma, D., and A. Kansal. 2013. Assessment of river quality models: a review. Reviews in Environmental Science and Biotechnology 12:285-311.

This review provides detailed descriptions and comparisons of concepts, assumptions, strengths, limitations, water quality parameters being simulated, dimensions, hydraulic characteristics, pollutant state, process description, method of solution and pollutant transport processes in six river-quality models, including AQUATOX.

Van den Brink, P. J., D. J. Baird, H. J. Baveco, and A. Focks. 2013. The use of traits-based approaches and eco (toxico) logical models to advance the ecological risk assessment framework for chemicals. Integrated Environmental Assessment and Management.

AQUATOX is given as an example of a complex model requiring substantial effort for calibration and analysis. Such models are needed for ecological research assessment, but effort is required to reduce uncertainty in extrapolations.

Wickwire, T., M. S. Johnson, B. K. Hope, and M. S. Greenberg. 2011. Spatially Explicit Ecological Exposure Models: A Rationale for and Path Toward Their Increased Acceptance and Use. Integrated Environmental Assessment and Management 7:158-168.

AQUATOX is compared, in tabular form, with an extensive list of spatially explicit exposure models. However, the emphasis is on wildlife models, and few of the other models are aquatic.

Yagow, G., B. Wilson, P. Srivastava, and C. Obropta. 2006. Use of biological indicators in TMDL assessment and implementation. Transactions of the ASAE 49:1023-1032.

Various biological indicators are used by states to assess water quality as part of U.S. EPA's Total Maximum Daily Load (TMDL) program. These indicators are based on varying combinations of algal, macroinvertebrate, and fish data. The use of biological indicators can be improved through modeling procedures that better define cause-and-effect relationships. AQUATOX is cited as a model having the potential to provide a better conceptual understanding and to represent these relationships in a TMDL applcation.

Applications

Ahmadi-Mamaqani, Y., N. Khorasani, K. Talebi, S. H. Hashemi, G. Rafiee, and F. Bahadori-Khosroshahi. 2011. Diazinon fate and toxicity in the Tajan River (Iran) ecosystem. Environmental Engineering Science 28:1-10.

It is not clear from the paper as to how much data were available to calibrate AQUATOX for this project. The application involved the fate and possible effects of the pesticide diazinon in the Tajan River, Iran. Simulated loss of the pesticide from a particular reach was primarily through discharge, with burial and three degradation processes (microbial, hydrolysis, and photolysis) only being of minor importance. Field data confirmed the importance of washout. However, the model did indicate that diazinon could exist in the water column long enough to have severe effects on the river fauna. Of particular concern is the possible contamination of sturgeon, which use the river as spawning grounds.

Bilaletdin, Ä., T. Frisk, V. Podsechin, H. Kaipainen, and N. Filatov. 2011. A general water protection plan of Lake Onega in Russia. Water resources management 25:2919-2930.

A joint Finnish-Russian project combined the steady-state Vollenweider model with the dynamic Danish Phophorus P2 and AQUATOX models to assess the impacts of various phosphorus loading scenarios on the second largest lake in Europe. The models predicted that reducing the total phosphorus loading of the largest wastewater treatment plant from 103.6 tons per year to 61 tons would decrease the peak phytoplankton biomass by almost 40%.

Blancher, E. C. 2010. Modeling Nutrients and Multiple Algal Groups Using AQUATOX: Watershed Management Implications for the Braden River Reservoir, Bradenton Florida. Proceedings of the Water Environment Federation 2010:6393-6410.

AQUATOX was used in conjunction with nutrient loading models to determine the possible impacts to water quality due to changes in the watershed of a small reservoir in southern Florida over the past 30 years. Reasonable predictions were obtained for chlorophyll *a* and green and blue-green algal (cyanobacteria) dynamics in response to loading scenarios and chemical controls with the algaecides copper sulphate and calcium peroxide. The model also provided indirect evidence of the more recent impact of the invasive cyanobacterium *Cylindrospermopsis* because when it was included in the latter years of the simulation a better fit to observed chlorophyll *a* was obtained.

Blancher, E.C., S. Sklenar, R Park and J.L. Wood. 2002. Determining the Linkages for a Nutrient TMDL in a Stream Listed as Use-Impaired for Endangered Species. National Total Maximum Daily Load Conference. Proceeding of Water Environment Federation Conference held in Phoenix, Arizona November 2002.

The Cahaba River in a rapidly urbanizing area south of Birmingham, Alabama, was placed on the 303(d) list as use-impaired from nutrients. Analysis of data shows a weak empirical relationship between total phosphorus and periphytic chlorophyll a in the Cahaba River, confounded by various in-stream limiting factors such as light, turbidity, scour, herbivory and possibly herbicide toxicity. This complex system was represented by U.S. EPA's AQUATOX model, which accounts for additional in-stream processes not available in other water quality models. It resulted in a verifiable linkage between total phosphorus and algal biomass and provided the linkages to ecosystem trophic levels that can determine the target level of total phosphorus that is protective of endangered species' habitats.

See also Park et al. 2002

Borg, G. M. 2009. EPA's COUNCIL FOR REGULATORY ENVIRONMENTAL MODELING: A CASE STUDY OF SCIENCE POLICY IMPLEMENTATION. Michigan Technological University.

This paper is interesting in that it is a thesis submitted for a degree of master of science in environmental policy in a Social Sciences Department. It is based in part on insights obtained by the author while a summer intern in the CREM (U.S. EPA's Council for Regulatory Environmental Modeling) office. She presents AQUATOX in a detailed case study. The author found that the model met various objective criteria for regulatory use such as having thoroughly evaluated equations and code. She states that "The AQUATOX model is an example of a transparent model with good evaluation, validation, and thorough documentation. It makes clear the possible insufficiency of outside information that can be used to fully validate all of the outputs that the model creates…[This] helps in avoidance of future legal trouble over lack of transparency or full disclosure of the model's limitations."

Carleton, J. N., R. A. Park, and J. S. Clough. 2009. Ecosystem Modeling Applied to Nutrient Criteria Development in Rivers. Environmental Management 44:485-492.

The AQUATOX ecosystem model was used to analyze impairment thresholds keyed to biological indices, including percentage cyanobacterial biomass of sestonic algae, and benthic chlorophyll *a*. The calibrated model was used to simulate responses of these indices to concurrent reductions in phosphorus, nitrogen, and suspended sediment in the enriched Blue Earth River in southern Minnesota. Results suggest that the indices would respond strongly to changes in phosphorus and suspended sediment, and less strongly to changes in nitrogen concentration. With concurrent reductions in all three constituents, a total phosphorus concentration of 0.1 mg/L was identified as a threshold concentration for prevention of both excessive periphyton growth and sestonic cyanobacterial blooms, and therefore is a possible water quality criterion.

Carleton, J. N., M. C. Wellman, P. A. Cocca, A. S. Donigian, R. A. Park, J. T. Love, and J. S. Clough. 2005. Nutrient Criteria Development with a Linked Modeling System: Methodology Development and Demonstration. Pages 1-25 *in* 2005 TMDL Conference. Water Environment Federation, Philadelphia PA.

This paper is an example of an approach to developing nutrient criteria with relatively minimal data and a linked mechanistic modeling system that consists of a watershed model and an ecological effects model. The watershed model HSPF and the aquatic ecosystem model AQUATOX are both part of U.S. EPA's BASINS 3.1 package. AQUATOX links aquatic nutrient concentrations with 'response variables' such as chlorophyll a and water clarity; HSPF, in turn, links land-use practices with nutrient concentrations.

Carousel, R. F., and R. C. Russo. 2001. Eutrophication Modeling Capabilities for Assessing Water Quality and Ecological Endpoints. Pages 345-372 *in* Fish Physiology,Toxicology, and Water Quality. U.S. Environmental Protection Agency, La Paz Mexico.

In a pilot study, the HSPF watershed model was linked to the CE-QUAL-W2 reservoir water quality model, which in turn was linked to AQUATOX to evaluate ecological impairments from nutrient and sediment runoff. The linked models were applied to the Tensas River Basin in Louisiana; the Basin was historically in bottomland hardwoods, but these were cleared so that 65% of the area is cropland. The water quality models were run with data from 1980 to 1992, including a calibration period and a verification period. The system was shown to be light-limited due to high TSS. With a 50% reduction in TSS and reductions in nutrients and organics representing changed land management the model predicted reduced chlorophyll *a* and changes in the benthic food chain, including benthic fishes. The authors conclude that higher trophic levels should be included in modeling lake ecosystems to provide an ecological endpoint.

Chen, H., L. Ma, W. Guo, Y. Yang, T. Guo, and C. Feng. 2013. Linking Water Quality and Quantity in Environmental Flow Assessment in Deteriorated Ecosystems: A Food Web View. PloS one 8:e70537.

Wetlands are subject to decreasing flow and increasing pollution due to human activities. A large wetland, including the largest natural lake in northern China, provides data for an integrated modeling study using multiple regression analysis, ECOPATH static food web analysis, and AQUATOX dynamic simulation of ecological responses. Differing water levels and nutrient and BOD loads were analyzed in 21 modeling scenarios.

Chen, W., X. Li, X. Chen, and F. Wang. 2012. Simulation of the response of eutrophic state to nutrient input in Lake Erhai using Aquatox model. Journal of Lake Sciences 24:362-370.

Abstract not available

Chen, Y., Z. Niu, and H. Zhang. 2012. Eutrophication assessment and management methodology of multiple pollution sources of a landscape lake in North China. Environmental Science and Pollution Research:1-13.

Urban lakes are subject to eutrophication from point sources and from nonpoint-source runoff. Several scenarios involving point-source reductions, nutrient retention and ecological restoration, and recycling of runoff water were simulated by AQUATOX linked to the Fluent hydrodynamic model. The results indicated that eutophication risks could be decreased and that significant improvements in water quality could be attained later. This environmental assessment and modeling approach is suitable for applications in other water regions.

Clouzot, L., C. Metcalfe, K. Kidd, and P. A. Vanrolleghem. 2011. Modeling the impact of endocrine disruptions on aquatic ecosystem: An experimental lake study. SETAC-Europe, Milan, Italy.

A PowerPoint presentation on simplifying and adapting the AQUATOX model in the WEST programming environment is based on De Laender's PhD thesis (*see below*). The objective was to develop a simple model to represent endocrine disruptors. The next step is to calibrate the model with data from the Canadian Experimental Lakes Area.

De Laender, F. 2007. Predicting effects of chemicals on freshwater ecosystems: model development, validation and application. PhD Thesis, Ghent University, Ghent, Belgium.

A dynamic ecosystem model was constructed in an object-oriented framework using the software package WEST and formulations from AQUATOX. Each object describes the growth of a model population in terms of its biomass concentration using differential equations. By connecting different objects and defining feeding relationships among them, a customized food web was designed. The number of populations that can be modelled is unlimited and available objects are: phytoplankton, macrophytes, zooplankton, planktivorous fish and piscivorous fish.

The following four papers illustrate the use of this model in testing alternative ecotoxicity formulations and in answering questions concerning its validation and application for assessment of ecological effects.

De Laender, F., K. A. C. De Schamphelaere, P. A. Vanrolleghem, and C. R. Janssen. 2008a. Comparison of different toxic effect sub-models in ecosystem modelling used for ecological effect assessments and water quality standard setting. Ecotoxicology and Environmental Safety 69:13-23.

De Laender, F., K. A. C. De Schamphelaere, P. A. Vanrolleghem, and C. R. Janssen. 2008b. Do we have to incorporate ecological interactions in the sensitivity assessment of ecosystems? An examination of a theoretical assumption underlying species sensitivity distribution models. Environment International 34:390-396.

De Laender, F., K. A. C. De Schamphelaere, P. A. Vanrolleghem, and C. R. Janssen. 2008c. Is ecosystem structure the target of concern in ecological effect assessments? Water Research 42:2395-2402.

De Laender, F., K. A. C. De Schamphelaere, P. A. Vanrolleghem, and C. R. Janssen. 2008d. Validation of an ecosystem modelling approach as a tool for ecological effect assessments. Chemosphere 71:529-545.

Donigian Jr, A. S., J. C. Imhoff, A. Mishra, P. Deliman, and E. Regan. 2010. A Watershed Modeling Framework for Military Installations: Assessment of the Hydrologic and Sediment Washoff Impacts of Military Management Alternatives.*in* 2nd Joint Federal Interagency Conference Las Vegas, NV.

A watershed modeling system for Fort Benning, GA using the U.S. EPA BASINS framework is described. Enhancements needed for analyses of impacts of military activities on watersheds were made to both HSPF and AQUATOX. At the time of the presentation at the conference, the widely used Ephemeroptera/Plecoptera/Tricoptera (mayfly, stonefly and caddisfly, or EPT) macroinvertebrate metric had been incorporated into AQUATOX.

Duda, P. B., J. L. Kittle, P. R. Hummel, M. H. Gray, and J. N. Carleton. 2009. Leveraging an Open Framework for Expanded Modeling Capabilities in BASINS 4.0. Proceedings of the Water Environment Federation 2009:441-450.

BASINS (Better Assessment Science Integrating Point and Nonpoint Sources) is an open-source system for use in performing watershed and water quality studies. AQUATOX is an integral part of BASINS, able to obtain time-series from the HSPF watershed model as boundary conditions for modeling receiving waters.

Echeverría, M., M. Wellman, R. Park, and J. Clough. 2003. Evaluation of AQUATOX for Ecological Risk Assessments in the U.S. EPA Office of Pesticide Programs. *in* SETAC NA 24th Annual Meeting in North America, Austin, Texas.

A comparative analysis was performed between the fate components of AQUATOX and EXAMS, the environmental fate and transport model used in the U.S. EPA Office of Pesticide Programs (OPP). Individual fate processes were tested, and the models were tested by simulating real chemical data. The results of individually testing each loss process indicate that, despite minor differences, fate processes are consistent between the two models. The results for the test chemicals show similar patterns of chemical concentration over time, but more disparity exists between the two models compared to the tests for the individual fate processes, probably due to propagated differences between the various fate processes and model assumptions. In addition, an example was developed to illustrate potential use of AQUATOX for evaluating integrated fate and effects in OPP. Results illustrate how AQUATOX output, including biomass concentrations and biological rates for control and perturbed simulations, could be used to inform the risk assessment process.

Erturk, A., R. A. Ambrose, and B. Rashleigh. 2007. Case Study: Dieldrin Attack in Dalyan Lagoon. Pages 329-386 *in* I. E. Gonenc, V. Koutitonsky, B. Rashleigh, R. A. Ambrose, and J. P. Wolfin, editors. Assessment of the fates and effects of toxic agents on water resources. Springer, Dordrecht, The Netherlands.

NATO sponsored an Advanced Study Institute in Istanbul, Turkey. It included a case study of a terrorist attack, where a chemical was assumed to be dumped into Sulunger Lake in Turkey. This chapter documents the response developed by the participants to this scenario, in terms of hydrodynamic transport, ecosystem effects, and decision making. WASP and EFDC were paired with AQUATOX in this exercise. The latter model provided a very detailed representation of the ecological effects of the toxicant, but required more detailed hydrodynamics than could be represented as a stand-alone model (the linked-segment capability was not yet available), so AQUATOX was coupled with WASP7. However, manually linking the two models required more than 8 hours of effort of three expert modelers. Suggestions are given as to how the linkage should be automated. Suggestions are also given as to how expansion of the chemical library could be supported by linkage with external chemical databases.

See also Rashleigh 2007

Funder, S. G. 2009. Risk Assessment of the Skensved Å Field Site: Review and Application of Surface Water Models. Bachelor's Thesis, Technical University of Denmark, Lyngby Denmark.

A trichloroethene (TCE) spill was found to infiltrate the surface water at a site in Denmark. Three surface water quality models developed by U.S. EPA (AQUATOX, QUAL2K, WASP) were evaluated based on four specific criteria (organic toxicant simulation, range of default values, simulation output and user friendliness) and one (AQUATOX) was selected for application to the field site. A quantitative risk assessment was then carried out using an integrated modeling approach. " It should be noted that in general the simulation output from AQUATOX was found to correspond very well with the actual measurements from the site (e.g. TCE concentrations, water levels).... however, it can be concluded that the TCE contamination is not a significant stressor to this ecosystem."

Several published papers with McKnight as senior author (below) carried the analyses further.

Giusti, E., S. Marsili-Libelli, and A. Gualchieri. 2011. Modelling a Coastal Lake for Flood and Quality Management.*in* 8th IWA Symposium on Systems Analysis and Integrated Assessment. International Water Association, San Sebastian, Spain.

This paper assesses the impacts of diverting flood water into Massaciuccoli Lake on the Tyrrhenian Coast, Italy. A volume dynamics module, developed in Simulink, was linked to an implementation of AQUATOX 3 with segments representing inflow channels as well as the lake. Synthetic input time series were developed using methods described in the next paper below. There was reasonable agreement between model output and observed data for nitrogen species and dissolved oxygen, but phosphorus data were not adequately explained. The calibrated model suggested that sediment release would not be triggered by flood waters but that addition of "clean" water might cause cyanobacteria to be replaced by green algae—the first step in ecosystem restoration.

Giusti, E., S. Marsili-Libelli, and S. Mattioli. 2011. A fuzzy quality index for the environmental assessment of a restored wetland. Water Science & Technology 63:2061-2070.

AQUATOX was used to study the feasibility of restoring a lake from drained wetland on the Tyrrhenian Coast, Italy. Synthetic water quality input data were developed by sampling drainage ditches and smoothing with a spline function. Flow was modeled as a Gamma distribution of rainfall coupled with a Markov chain of rainy and dry days. The model was run for 7 years with a 10% additional variability providing minimum and maximum loadings. In addition, perturbed scenarios were run to assess the robustness. Simulated nutrient removal was in quantitative agreement with literature values. Simulated phytoplankton blooms were in agreement with local observations. A fuzzy water quality index based on simulated chlorophyll *a*, dissolved oxygen, and total suspended solids represented model output and facilitated comparison of several scenarios and communication to stakeholders.

Huang, S., Y. Jia, and S. S. Wang. 2009. Two-dimensional numerical and eco-toxicological modeling of chemical spills. Frontiers of Environmental Science & Engineering in China 3:178-185.

An ecotoxicological model, based in part on AQUATOX, was developed at The National Center for Computational Hydroscience and Engineering, The University of Mississippi, Oxford, MS, and run with the results of a 2-D fate and transport model. Simulations indicated that the paired models are capable of predicting the acute effects of a chemical spill.

Imhoff, J. C., P. R. Hummel, A. S. Donigian Jr, and R. A. Park. 2010. Using US EPA BASINS Modeling System for Linking Hydrologic Models with an Ecological Model for Aquatic Endpoint Impact Assessments. *in* The 3rd USGS Modeling Conference.

Two of the models available in BASINS, HSPF and AQUATOX, are used to demonstrate the linkage between hydrologic and ecological models for conducting biological impact assessments. The methodology and results of a BASINS application on Fort Benning, GA, are presented as a case study. The study incorporates ruoff from military-specific land use categories and identifies impacts to aquatic biota such as the rare broadstripe shiner in the receiving waters.

Inthasaro, P., and W. Wu. 2012. A 1-D Aquatic Ecosystem/Ecotoxicology Model in Open Channels. Pages 1144-1147 *in* Biomedical Engineering and Biotechnology (iCBEB), 2012 International Conference on. IEEE.

Constructs from AQUATOX, including a basic food web structure with four trophic levels, were incorporated into a one-dimensional modeling package. The model simulates the bioaccumulation and toxic effects of chemicals in organisms. It has been tested by simulating PCB transport and bioaccumulation in the aquatic ecosystem of the Upper Hudson River, New York, with promising results.

Joyner, T. A., and R. V. Rohli. 2013. Atmospheric influences on water quality: a simulation of nutrient loading for the Pearl River Basin, USA. Environmental monitoring and assessment:1-10.

The Pearl River Basin in southern Mississippi and Louisiana was the focus of this study. "AQUATOX provided an excellent simulation of daily values for multiple water quality variables based solely on monthly time series records. The study found that climate does impact certain water quality variables in the studied segment of the [river]." The multidimensional and integrative nature of AQUATOX has many of the same capabilities as other models. However, the biological components included in AQUATOX enhance the utility and complexity of the model, providing potential biotic indicators of anthropogenic and natural changes within the ecosystem.

Karaaslan, Y., A. Akkoyunlu, F. Erturk, and E. Citil. 2013. The Effect of Toxic Organic Chemicals on Mogan Lake. International Journal of Environmental Research 7:595-604.

AQUATOX was loaded with data for one year from a lake and tributary creeks in Turkey, and calibrated and validated for two other years. Then data for 15 pesticides and PCB congeners were loaded from the AQUATOX library and the effects on phytoplankton and zooplankton were noted.

Lei, B., S. Huang, M. Qiao, T. Li, and Z. Wang. 2008. Prediction of the environmental fate and aquatic ecological impact of nitrobenzene in the Songhuajiang River using the modified AQUATOX model. Journal of Environmental Sciences 20:1-9.

The AQUATOX model was modified and adapted to simulate an accidental discharge of nitrobenzene and its potential ecological impacts. Nitrobenzene concentrations in flowing water, sediment, and biota were predicted with good agreement between model predictions and field observations. The perturbed and control simulations were compared; the model predicted biomass changes for diatoms and mussels, but no influence on other organisms. These results were interpreted as indicating that nitrobenzene pollution should have a limited impact on the benthos community in the river.

Lei, B. L., S. B. Huang, X. W. Jin, and Z. Wang. 2010. Deriving the aquatic predicted no-effect concentrations (PNECs) of three chlorophenols for the Taihu Lake, China. Journal of Environmental Science and Health, Part A 45:1823-1831.

The indirect effects of chemicals caused by interactions among species as well as direct effects were characterized by the ecological risk model AQUATOX. Predicted no effect concentration values in this study were smaller than ones from single species distributions, which suggested the influence of indirect effects characterized by the model. AQUATOX can reflect more realistic characteristics of the region, closer to the actual state of the environment, and can supply a more reasonable effect concentration compared to extrapolations based on single species toxicity tests.

Mauriello, D. A. and R. A. Park. 2002. An Adaptive Framework for Ecological Assessment and Management. Pages 509-514 *in* Integrated Assessment and Decision Support. International Environmental Modeling and Software Society, Manno Switzerland.

Adaptive Ecological Risk Analysis is an iterative process based on ecological modeling, the development and implementation of management alternatives, and the evaluation of their effectiveness. It depends heavily on the use of ecological models to perform both prospective and retrospective risk assessments and to analyze the outcomes of alternative management strategies. As an example of this approach, AQUATOX was used to examine the relative risks to the bass population of Coralville Reservoir in Iowa from the pesticide dieldrin. The objective of maintaining a viable recreational bass fishery was used to evaluate alternative strategies for reducing risks to the bass population. The model quantified the potential effectiveness of alternative management strategies and provided feedback for policy refinements.

Mauriello, D. A., D. Rodier, and F. S. Stay. 1998. Application of Simulation Models to the Ecological Risk Assessment Process. Pages 45-68 *in* M. C. Newman and C. Strojan, editors. Risk Assessment; Logic and Measurement. Ann Arbor Press, Chelsea Michigan.

Ecosystem experiments with 4-nonylphenol in pond enclosures in Duluth, Minnesota were simulated with two risk assessment models, LERAM and AQUATOX. The models represented the lethal and sublethal responses and recovery of a simple food web, including small fish. The close correspondence between the field studies and the modeling exercises demonstrates the capabilities of models designed specifically for estimating risks from toxic chemicals to aquatic ecosystems.

Mäkynen, A. 2009. AQUATOX – ecological risk assessment model – A tool for impact assessment for waters. Master's Thesis, University of Jyväskylä, Jyväskylä, Finland.

The goal was to test AQUATOX with data from a Finnish lake but without calibration. Total phosphorus, total nitrogen and chlorophyll a concentrations in constant and dynamic conditions were simulated for Lake Pyhäjärvi, Finland. The AQUATOX described relatively well the magnitude of nutrient and chlorophyll *a* concentrations under constant conditions, indicating its usefulness for planning work. However, calibration is needed in order to simulate temporal dynamics. If one includes removal of fish, then phosphorus mass balance can be achieved.

McKnight, U. S., S. G. Funder, J. J. Rasmussen, M. Finkel, P. J. Binning, and P. L. Bjerg. 2010a. An integrated model for assessing the risk of TCE groundwater contamination to human receptors and surface water ecosystems. Ecological Engineering 36:1126-1137.

The decision support system CARO-PLUS was coupled to AQUATOX in order to conduct both a quantitative human health risk assessment and an ecological risk assessment of a stream in Denmark polluted with TCE. AQUATOX was found to capture trends in TCE concentrations well, when compared with actual data. The model indicated that the TCE contamination does not have any significant effect on the stream ecosystem.

See Funder 2009 and the other papers with McKnight as senior author

McKnight, U. S., J. J. Rasmussen, S. G. Funder, M. Finkel, P. L. Bjerg, and P. J. Binning. 2010b. Integrated modelling for assessing the risk of groundwater contaminants to human health and surface water ecosystems *in* 7th International Groundwater Quality Conference, Zurich, Switzerland.

See Funder 2009 and the other papers with McKnight as senior author

McKnight, U. S., J. J. Rasmussen, B. Kronvang, P. L. Bjerg, and P. J. Binning. 2012. Integrated assessment of the impact of chemical stressors on surface water ecosystems. Science of the Total Environment 427-428:319-331.

This is similar to the other McKnight papers, except that AQUATOX results are compared with empirical methods. The model indicates that stream discharge rather than toxicity is limiting benthic biomass. It presents a strong argument for combining bioassessment and modelling techniques in evaluating field sites with multiple stressors.

See Funder 2009 and the other papers with McKnight as senior author

Mead, J. V. 2007. An Empirical and Modeling Analysis of the Spatial Structure and Trophic Energy Flow Through a Small Temperate Stream. PhD thesis, Syracuse University, Syracuse NY.

Periphyton production in a small stream in Upstate New York was simulated using AQUATOX. Also, invertebrate parameters from AQUATOX were used in the application of a newly developed, spatially explicit, invertebrate model of the stream.

Moermond, C., and A. Koelmans. 1999. Nutrients and contaminants: study with AQUATOX into the interaction between contaminants and communities in model ecosystems and shallow lakes. [report in Dutch] Aquatic Ecology and Water Quality Management Group, Wageningen University, Wageningen, The Netherlands.

No abstract available

Morkoç, E., V. Tüfekçi, H. Tüfekçi, L. Tolun, F. T. Karakoç, and T. Güvensel. 2009. Effects of land-based sources on water quality in the Omerli reservoir (Istanbul, Turkey). Environmental Geology 57:1035-1045.

Omerli Reservoir is an important source of drinking water for Istanbul. AQUATOX was run with three inflow scenarios: 1) all existing inflows are discharging into the lake (present situation with simulated results consistent with data); 2) none is discharging (with a significant decrease in simulated pollutants); and 3) all are discharging except one channel (with a small improvement in simulated water quality due to wastewater bypassing the lake). The conclusion, based on predicted nutrients, dissolved oxygen, chlorophyll *a,* and nuisance algae, was that wastewater should bypass the reservoir in order to significantly improve the water quality.

Park, R. A., J. J. Anderson, G. L. Swartzman, R. Morison, and J. M. Emlen. 1988. Assessment of Risks of Toxic Pollutants to Aquatic Organisms and Ecosystems Using a Sequential Modeling Approach. Pages 153-165 Fate and Effects of Pollutants on Aquatic Organisms and Ecosystems. U.S. Environmental Protection Agency, Athens, Ga.

This is the first published reference to AQUATOX.

Park, R. A., E. C. Blancher, S. A. Sklenar, and J. L. Wood. 2002. Modeling the Effects of Multiple Stressors on a Use-Impaired River *in* Society of Environmental Toxicology and Chemistry, Salt Lake City.

See Blancher et al. 2002

Park, R. A. and J. S. Clough. 2005. Validation of AQUATOX with Nonylphenol Field Data (Unpublished Report). U.S. Environmental Protection Agency, Washington, DC.

AQUATOX simulated the fate and effects of 4-nonylphenol in littoral mesocosms in Duluth, Minnesota. The close visual correspondence between the field data and the model results served as a partial validation of the model.

Park, R. A., J. S. Clough, and M. C. Wellman. 2007. AQUATOX: Modeling Fate of Toxic Organics in the Galveston Bay Ecosystem. ***in*** **Proceedings of the Eighth Biennial State of the Bay Symposium, January 23-25, 2007, Galveston Texas.**

Water balance is computed using the salt balance approach. Saltwater inflow occurs to replace water that is admixed from one layer (usually the lower) to the other layer, producing—along with freshwater discharge—the observed salinities of the two layers at the mouth of the estuary. Validation of estuarine bioaccumulation in AQUATOX was obtained using data on PCB concentrations observed in New Bedford Harbor, MA. The observed PCB concentrations in water and bottom sediment were used in a simulation of Galveston Bay, and the predicted concentrations in biota were compared with the observed concentrations. With the exception of obvious differences between shrimp and lobsters and surf clams and hard clams, the mean predicted PCB concentrations fell within the error bounds of the observed data.

Park, R. A., J. S. Clough, and M. C. Wellman. 2008. AQUATOX: Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems. Ecological Modelling 213:1-15.

This is the definitive, peer-reviewed paper on AQUATOX, with numerous examples of applications. Supplemental material includes all 450 equations as of 2008.

Park, R. A., J. S. Clough, M. C. Wellman, and A. S. Donigian. 2005. Nutrient Criteria Development with a Linked Modeling System: Calibration of AQUATOX Across a Nutrient Gradient. Pages 885-902 ***in*** **TMDL 2005. Water Environment Federation, Philadelphia, Penn.**

This paper discusses one aspect of a project that uses the watershed model HSPF and the aquatic ecosystem model AQUATOX, which are both part of U.S. EPA's BASINS package. AQUATOX was calibrated across a nutrient gradient in order to develop an ecoregional implementation of the model. By developing a robust parameter set for algae and cyanobacteria that are adapted either to the nutrient-rich, turbid Blue Earth River, to the nutrient-poor, clear Crow Wing River, or to the Rum River with intermediate nutrient conditions and low turbidity, the model is more likely to represent changing conditions and not require extensive site calibration in future applications. By simultaneously calibrating for all three rivers, the model is shown to represent a broad range of conditions in Minnesota rivers without site-specific calibration and, as such, is suitable for ecoregional applications where monitoring data are sparse.

See also Carleton et al. 2005, 2009

Park, R. A., B. Firlie, R. Camacho, K. Sappington, M. Coombs, and D. A. Mauriello. 1995. AQUATOX, A General Fate and Effects Model for Aquatic Ecosystems. Pages (3)7-(3)17 Proceedings for the Toxic Substances in Water Environments: Assessment and Control. Water Environment Federation, Arlington, Virginia.

This paper is the first general description of the AQUATOX model.

Rashleigh, B. 2003. Application of AQUATOX, a process-based model for ecological assessment, to Contentnea Creek in North Carolina. Journal of Freshwater Ecology 18:515-522.

AQUATOX Release 1, Ver.1.69 was applied to Contentnea Creek, a coastal plain stream in North Carolina. The model was used to assess sensitivity of four fish groups to six habitat factors: temperature, nutrients, sediment, dissolved oxygen, detrital loading, and pH. It was judged to have lower sensitivities to sediment and dissolved oxygen, and it lacked multiple age classes and spatial relationships—but the author knew that those deficiencies would be corrected in the next version.

Rashleigh, B. 2007. Assessment of lake ecosystem response to toxic events with the AQUATOX model. Pages 291-299 *in* I. E. Gonenc, V. Koutitonsky, B. Rashleigh, R. A. Ambrose, and J. P. Wolflin, editors. Assessment of the fate and effects of toxic agents on water resources. Springer, Dordrecht, The Netherlands.

As part of a NATO-sponsored Advanced Study Institute, a hypothetical terrorist attack involving addition of dieldrin to Coralville Reservoir, Iowa, at two different times of the year was simulated using AQUATOX. The model represented time-varying bioacumulation and toxic effects on the food web. It also facilitated understanding of two endpoints: clearance of the chemical in fish tissue and recovery of fish biomass over time.

See also Erturk et al. 2007

Rashleigh, B., M. Barber, and D. Walters. 2009. Foodweb modeling for polychlorinated biphenyls (PCBs) in the Twelvemile Creek Arm of Lake Hartwell, South Carolina, USA. Ecological Modelling 220:254-264.

The AQUATOX model (Release 3.1) was parameterized and applied to the Twelvemile Creek Arm (TCA) of Lake Hartwell in South Carolina, which is of primary interest due to PCB releases upstream. “This application of AQUATOX to the TCA allowed us to meet our objective of providing an updated simulation with future forecasts. As expected, differences in toxicant concentrations among species were due to differences in diet, and PCB concentration in largemouth bass declined most slowly, due to their large size and carnivorous diet. There was reasonable agreement of the observed PCB concentrations, although it may be difficult to match observed data based on low sample numbers with high variability.”

Rashleigh, B., M. C. Barber, and D. M. Walters. 2005. Foodweb modeling for PCBs in the Twelvemile Creek Arm of Lake Hartwell. Pages 301-304 *in* Georgia Water Resources Conference, Athens, Georgia.

This is an earlier paper on the application described in the 2009 paper above.

Rashleigh, B., R. Park, J. Clough, R. Bringolf, P. Lasier, and M. Wellman. 2012. P73—Modeling bioaccumulation as a potential route of riverine foodweb exposures to PFOS. Reproductive Toxicology 33:626.

AQUATOX is one of the few models available for simulating the effects of Perfluoroctane sulfonate (PFOS) in aquatic ecosystems. Bioaccumulation in animals is modeled as a function of perfluoroalkyl chain length. The model has been applied in an estuarine system and is currently being applied to a river using linked segments.

Rayne, S., and M. G. Ikonomou. 2005. Polybrominated diphenyl ethers in an advanced wastewater treatment plant. Part 2: Potential effects on a unique aquatic system. Journal of Environmental Engineering and Science 4:369-383.

A rudimentary limnological model was developed with AQUATOX using an example lake study and site-specific data from the literature. Physicochemical properties for seven PHDE congeners were input to the model. Halflives were estimated for the congeners using BIOWIN; they were not field-checked. AQUATOX predicted insightful relative temporal patterns in both water and sediments. Time to reach steady state ranged from 3 years to "never," depending on bromination.

Scholz-Starke, B., R. Ottermanns, U. Rings, T. Floehr, H. Hollert, J. Hou, B. Li, L. L. Wu, X. Yuan, and K. Strauch. 2013. An integrated approach to model the biomagnification of organic pollutants in aquatic food webs of the Yangtze Three Gorges Reservoir ecosystem using adapted pollution scenarios. Environmental Science and Pollution Research:1-18.

This paper describes a hugely ambitious German-Chinese cooperative project that takes full advantage of the analytical power of the latest release of the AQUATOX model. The model is being used in an integrative approach to better understand the eutrophication due to nutrients and the bioaccumulation and biomagnification of organic pollutants entering the newly impounded Three Gorges Reservoir in China. The model provides a framework to seamlessly connect eight modules ranging from hydrodynamics to ecotoxicology and risk assessment. At this stage of the application one can already state that the model is suitable to evaluate ecological, toxicological, and hydrological scenarios for the reservoir and to recommend specific management actions to protect aquatic organisms and human consumers.

Schramm, H. L., M. S. Cox, T. E. Tietjen, and A. W. Ezell. 2009. Nutrient dynamics in the Lower Mississippi River Floodplain: comparing present and historic hydrologic conditions. Wetlands 29:476-487.

The existing Cahaba River, Alabama, AQUATOX study was adapted to represent nutrient uptake and release during inundation of the floodplain by the Lower Mississippi River.

Two macrophytes and a macroalga in the model library were added as surrogates for wetland plants, providing increased surface area for periphyton that in turn take up nutrients from the water column. The model was run with present conditions and with conditions presumed to have occurred with historic flooding. Nutrient sequestration and release, including denitrification, were simulated for both scenarios. Although available within AQUATOX, the Wisconsin Bioenergetics model was run separately to represent fish growth and nutrient sequestration.

Smith, D., J. Warwick, and C. Fritsen. 2011. Modeling Nutrient Dynamics and Benthic Algal Relationships on the South Fork Humboldt River, NV. Pages 1147-1150. World Environmental and Water Resources Congress 2011.

The application of AQUATOX to an arid, regulated river subject to releases from an upstream reservoir is described. The model was used to simulate nutrient loadings and benthic algal impacts on dissolved oxygen. The authors state: "A limited preliminary calibration of AQUATOX 3 resulted in excellent overall agreement between predicted and downstream gross primary productivity (>40 g O2 m-2 d-1) and diel dissolved oxygen swings (<4 to 19 mg/L)."

Sourisseau, S., A. Bassères, F. Périé, and T. Caquet. 2007. Calibration, validation and sensitivity analysis of an ecosystem model applied to artificial streams. Water Res. doi:10.1016/j.watres.2007.08.039.

In this often-cited study, AQUATOX was used to simulate dynamics of various aggregated algal and invertebrate compartments in artificial streams designed for measuring the effects of pollutants on aquatic communities. Calibration and validation of the model were performed using data from separate stream channels. Multivariate sensitivity analysis identified those parameters that exert a prominent role in the outputs of the model. The calibrated model was able to adequately describe the dynamics of most of the simulated biological compartments. Using data from other streams, between-streams natural variability was shown to explain discrepancies between observed and simulated data. The model was shown to be highly sensitive to parameters for temperature limitation, maximum rate of photosynthesis, and maximum consumption.

Taner, M. U., J. N. Carleton, and M. Wellman. 2011. Integrated model projections of climate change impacts on a North American lake. Ecological Modelling 222:3380- 3393.

The potential impacts of climate change on Lake Onondaga, New York, were assessed using linked watershed, thermal balance, and ecosystem models. Output from a global circulation model were used to drive the HSPF-CATS watershed model and the UFILS4 lake stratification model. Outputs from these models are drivers for the AQUATOX ecosystem model. The integrated models predict prolonged periods of thermal stratification due to warming of lake waters and a general increase in primary production and zooplankton biomass in response to climate change. Phytoplankton blooms, especially of green algae, are predicted to increase in frequency and duration; cyanobacteria are predicted to increase by 25%, but to remain a small constituent of the plankton. The zooplankton *Bosmina* is predicted to increase dramatically. In general, zebra mussels are projected to increase and chironomids to decrease with climate change. Fish exhibit high seasonal variability without any clear trend.

Tsegaye, T., and M. Wagaw. 2006. Stream Water Quality Modeling Using AQUATOX: Hester Creek and Flint Brown River of Northern Alabama. American Society of Agronomy-Crop Science Society of America, Indianapolis, Indiana.

AQUATOX can be used for assessment of nutrient and sediment pollution; examples are given for two watersheds in northern Alabama. However, accurate data on discharge, nutrients, and TSS at multiple points in the watershed are critical for calibration. The model has great potential to estimate recovery times for fish and invertebrates after reducing pollutant loads.

U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. EPA-823-R-00-008, Washington, DC.

Three validation studies were performed using AQUATOX Release 1: Lake Onondaga, New York; Coralville Reservoir, Iowa (run without modeling the impacts of dieldrin and other pesticides); and bioaccumulation of PCBs in the Lake Onterio food web.

U.S. Environmental Protection Agency. 2001. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports Addendum: Formulation, Calibration, and Validation of a Periphyton Submodel for AQUATOX Release 1.1. EPA-823-R-01-008, Washington, DC.

Constructs were added in AQUATOX Release 1.1 to better represent periphyton than in Release 1. This new submodel was successfully calibrated with artificial channel data and validated with *in situ* stream data from Walker Branch, Tennessee. A single parameter set was developed to fit twenty treatments in a factorial experiment involving nutrients, light levels, and presence and absence of grazing snails in stream-side channels and stream enclosures. The calibrated model fit nineteen treatments where relative bias and F tests showed that the predicted and observed values were from similar distributions. The model was also partially validated with independent data from the stream channel.

Welty, N., D. Hyndman, and L. Panayotoff. 2004. Eco-hydrologic Modeling of Nutrients, Oxygen, and Temperature Across a Range of Michigan Streams. Page 1175 *in* AGU Fall Meeting Abstracts.

Several streams in Michigan were chosen on the basis of land use and data availability to model water quality; these included the Muskegon River and Grand Traverse Bay watersheds. AQUATOX was used to simulate changing concentrations of nutrients, other solutes, and sediments in the water, as well as the biota. Preliminary modeling results compare favorably with observations.

Yifan, Y., Z. Yongqing, and L. Weiqing. 2009. Simulation study on blue-green algae blooms in Dianshan Lake and its impact factors [In Chinese]. Environmental Pollution & Control 6:016.

AQUATOX was employed to simulate the ecology of Dianshan Lake. The effects of retention time, nutrients, pH, water temperature, wind, and light on algal growth, especially of blue-greens (cyanobacteria), were analyzed. The temporal distribution of nutrients and algal growth were well simulated by the model, and the mechanisms of blue-green algal (cyanobacteria) blooms could be analyzed.

Zhang, L., J. Liu, Y. Li, and Y. Zhao. 2013. Applying AQUATOX in determining the ecological risk assessment of polychlorinated biphenyl contamination in Baiyangdian Lake, North China. Ecological Modelling 265:239-249.

With calibration of AQUATOX, the reference simulation of Baiyangdian Lake was not significantly different from observed biomass. Sensitivity analysis demonstrated the potential contribution of the direct and indirect effects of physiological parameters. The model was highly sensitive to parameters related to temperature limitations and respiration rates. Risk estimation demonstrated that the model successfully represented direct toxic effect risks of PCBs on each population and the indirect ecological effects that were distributed throughout the pelagic-benthic food web. This study demonstrated that AQUATOX could be used as a generic ecosystem effects model by which to estimate ecological risks of chemicals on specific aquatic ecosystems.

ZHU, Y.-q., W.-q. LIN, and S.-q. LU. 2011. Study on Application of Water Quality and Ecological Model in Olympic Rowing-Canoeing Park. [In Chinese] Environmental Science and Technology 1:004.

Zijian, L. B. H. S. W. 2009. Theories and Methods of Ecological Risk Assessment. [In Chinese]Progress in Chemistry:Z1.

Zouiten, H., C. Á. Díaz, A. G. Gómez, J. A. R. Cortezón, and J. G. Alba. 2013. An advanced tool for eutrophication modeling in coastal lagoons: Application to the Victoria lagoon in the north of Spain. Ecological Modelling 265:99-113.

Ecological risk assessment should consider indirect effects as well as direct effects of chemicals on aquatic ecosystems. AQUATOX was effective in this application.

"AQUATOX is the most comprehensive of the general ecological risk models presently available. It is capable of representing the combined environmental fate and effects of toxic chemicals and their impacts on aquatic ecosystems. The model has been widely applied."