Mathematics Education and Simulations:
How Relevant Are They?

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ABSTRACT

The fast advancement in Information Technology coupled with immense improvement in advanced knowledge in mathematical sciences related to water resources has rendered computer simulation models to become an important and reliable tool in the understanding, planning and management of water resource systems. This understanding of aquatic environmental and its ecosystem components and processes, vis a vis simulation models would provide a better frame work for the proper management of such ecosystem components and processes, such as reservoir operations, coastal zone processes and wetlands dynamics, for example. The applicability of simulation models and mathematical sciences towards solving real life problems has helped to respond positively to the call for relevancy of modern university education in general, and mathematics education in particular. This paper will briefly explore the extents to which simulation models have been developed, and successfully applied in answering to the demands put upon them, and the perceived directions that simulation models will proceed, in the broad context of mathematics education at both the undergraduate and graduate level, in the new millennium dominated by information technology.

SIMULATION MODELS FOR AQUATIC ECOSYSTEMS

The discharge of excessive quantity of domestic, industrial and agricultural wastes has rendered the coastal zones incapable of properly assimilating these wastes, thus becoming grossly polluted and hence posing immense stress on water quality, marine ecosystems and other coastal resources. Hence, integrated coastal zone resources management is urgently needed to conserve and enhance existing coastal resources. Positively responding to this urgent demand, computer modelling and simulations has become a useful management tool in this regards to assess the impacts of development on the morphology, water quality and ecosystems in the coastal zones and to provide appropriate remedial options, where possible. The performance and capability of several popular yet inexpensive simulation models such as QUAL2E, WASP6, AQUATOX, AQUASEA, E_FISH and MIKE SWMM, will be briefly discussed to illustrate how successful they are applied to coastal environments with particular reference to the simulation of marine eutrophication and ecosystem dynamics, sediment transport and morphology, harmful bacteria and aquatic ecotoxicology. The introduction of such models in undergraduate and post graduate curriculum for teaching and

research has progressed satisfactorily leading to, hopefully, more active research in this area. We briefly explore some highly successful simulation models developed by the USEPA (Unites States Environment Protection Agency) that might be gainfully adapted into modern mathematics curriculum elsewhere too.

WASP6

WASP6 is an enhanced Windows version of the USEPA Water Quality Analysis Simulation Program WASP. WASP6 (Wool *et al.*, 2001) had been developed to aid modelers in the implementation of WASP (Koh and Lee, 1995; Koh *et al*, 2001). WASP6 has features including a pre-processor, a rapid data processor, and a graphical post-processor that enable the modeler to run WASP more quickly and easily and evaluate model results both numerically and graphically. With WASP6, model execution can be performed up to ten times faster than the previous USEPA DOS version of WASP. Nonetheless, WASP6 uses the same algorithms to solve water quality problems as those used in the DOS version of WASP6.

WASP6 contains 1) a user-friendly Windows-based interface, 2) a pre-processor to assist modelers in the processing of data into a format that can be used in WASP6. 3) a High-speed WASP6 Eutrophication and organic chemical model processors, and 4) a graphical post-processor for the viewing of WASP6 results and comparison to field data (Figure 1).

Because of the architecture utilized in the design of WASP6, it is going to be relatively easy to develop other kinetic modules for WASP6. Currently, there is a plan on the development of an enhanced eutrophication model that will include the addition of the following state variables: 2 additional algal groups, salinity, full heat balance, coliforms, second BOD group, and sediment digenesis model.

Figure 1. WASP6: Modeling of water quality in inland waters like rivers and small lakes, and estuarine system

AQUAWEB

Several studies have assessed contaminants, their bioaccumulation and their potential adverse effects on wildlife and wetland ecosystems. Available data indicates a wide array of organic contaminants, including pesticides, polychlorinated biphenyls (PCBs) and polycyclic aromatic hydrocarbons (PAHs). Fishes sampled from northern and southern Everglades during 1970-73 and again in 80's through December 1995, for example, were found to contain traces of PCBs with concentrations ranging from 50 to 260 µg/kg.

In order to evaluate the potential exposures and their harmful effects on wildlife, we need to assess and quantify the transfer of the contaminant through the food web. For that purpose, an aquatic food web AQUAWEB was assembled for the graminoid-dominated areas of the Everglades, consisting of sedimented detritus, phytoplankton, zooplankton and 3 fish compartments. A mass balance toxicant bioaccumulation model is constructed for PCBs using a steady-state representation of the aquatic food web. The main objective is to calculate total PCBs concentrations in all compartments, to assess model sensitivity and to assess contaminant transfer routes to see which route is more dominant. The model was successfully applied to predict residue levels of total PCBs in fish species with results falling in the range of field data reported. There is a general increase in contamination further up the food web from the primary producers to the top predators. These results conform to the theory of food web exposure being the dominant sources of PCBs for top predators. It is observed that the model is extremely sensitive to variation of lipid content. The model results might be used as a guide in protecting wild live in the Everglades and other wetland regions by setting regulation on permissible levels of contamination in water and fish tissues, since the consumption of foods, particularly fish, is second only to industrial exposure as a source of PCBs to human .The model can be modified for other contaminants.

AQUATOX

AQUATOX (ver.1.69, release 1; USEPA, 2000a, b; Park *et al*., 1995) models both nutrients and toxic chemicals and is designed to be a general, realistic dynamic model of the combined fate and effects of nutrients and pollutants in aquatic ecosystems. The model has been implemented for streams, ponds, lakes and reservoirs. Average daily conditions are modelled. The eutrophication model construct is rather complete and can be used to study the effects of nutrient enrichment on various trophic levels. Eight compartments of organic matter are modeled (refractory and labile detritus, either dissolved, suspended, surface or buried sediment) and include all non-living organic material, dissolved and particulate, and also the associated decomposers (bacteria and fungi). The food web consists of several species of algae (blue–green, green, diatom), macrophytes and different groups of zooplankton, zoo benthos and different types of fish. Advective vertical transport of phytoplankton, photosynthesis, respiration, excretion or photorespiration, non-predatory mortality, washout and sinking are taken into account. Change in biomass is modeled as a function of consumption, excretion, defecation, mortality, respiration, predation and other processes. Kinetic sorption and desorption is used to describe the partitioning of an organic chemical among the phases of the ecosystem. For fish, a quasi-equilibrium partition is used, resulting in a lag in uptake. Contaminant association with DOC is included. Biodegradation of pollutants is modeled as a function of pH, temperature, nutrient availability and light. Direct and indirect effects of temperature can be examined since realistic temperature responses are used.

AQUATOX includes the effects of the contaminants on the ecosystem. Direct toxicity leading to mortality is quantified using the Weibull distribution and is based on internal concentrations for all organisms. This mortality leads to several indirect effects of the toxicants: e.g. decrease of grazing and predation pressure, increase in decomposition of detritus and recycling of nutrients from dead organisms causing oxygen consumption and eventually oxygen depletion. AQUATOX further accounts for sub lethal toxicant stress affecting phytoplankton growth and settling rates, and rates of consumption, defecation, and egestion by animals. AQUATOX was validated using data from three different water bodies, including a dataset on PCB transfer in the Lake Ontario food web (USEPA, 2000b). Recently, the model was implemented for Dutch shallow lakes to study the flows of a pesticide, a PCB and a PAH as a function of lake trophic state (Moermond and Koelmans, 1999).

PARALLEL ALGORITHM FOR A POPULATION MODEL

Complex ecosystem simulation models such as those used for the prediction of global warming and spreading of deserts require high computer memory and fast computational speed for efficient execution. Constraints imposed by limited memory and speed often put restriction on model resolutions that may result in unsatisfactory model output. The study of the Unionid mussel communities in the United States of America, using age-structured spatially explicit modeling approach, for example, was hampered by the limited capacity of the PC. However, special features of the mussel life cycle make it possible to construct an efficient parallel algorithm to model the dynamics of various mussel communities found in the various river systems in North America.

The Unionid mussels are native to North America, with a rich diversity of species. They can be found in many of the river systems in North America living in many different types of environment. Their spatial-temporal distribution dynamics have previously been studied theoretically by Lee and DeAngelis (1997) and Lee *et al*. (1998). However, since the early 1900's the mussel communities in North America have been declining rapidly due to anthropogenic activities such as:-

1. Over-harvesting of mussel communities in certain parts of North America;
2. Indiscriminate discharge of industrial or mining waste into the river systems;
3. Impoundment of rivers to create reservoirs for power and water supply; and
4. Accidental introduction of foreign prey and competitor species into North America river system.

The native Unionid mussels have life spans ranging from 9-60 years (Stein, 1971; Lewandowski and Stanczykowska, 1975; Burky, 1983; Jirka, 1986) with a distinct parasitic stage in their life cycle. They are sessile creatures and are dependent on host fish during their larval parasitic stage for food and shelter. In addition, the host fish also plays a major role in the spread of the mussel communities into different areas of the river. The mussels' life cycle is shown graphically in Figure 2.

Adult Male Mussel

Fertilization

Adult Female Mussel

Release

Parasitic Larval

Juvenile Mussel

Drop off

Glochidia attached to Fish Host
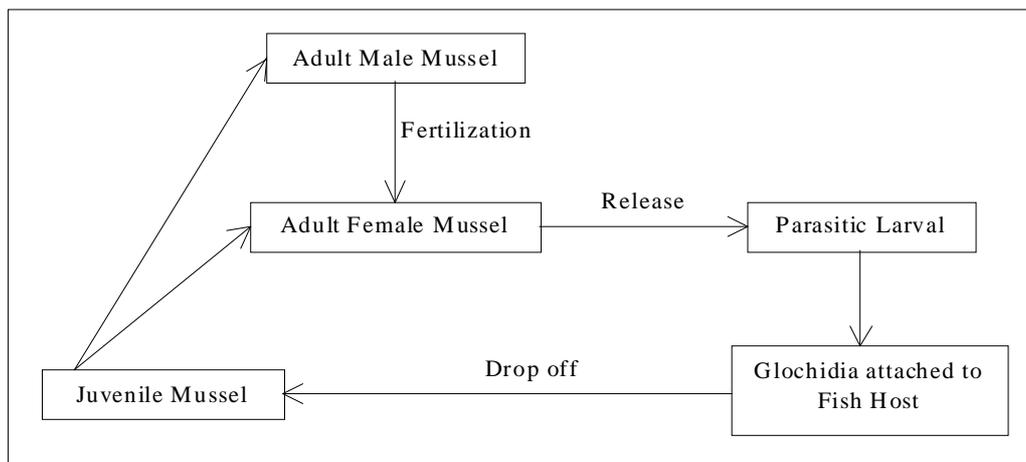
Figure 2. Life cycle of the Unionids.

After fertilization, the eggs are incubated in the female mussels prior to being released into the water. The close approach of a fish will often triggered a "pregnant" female mussel to release its parasitic larvae. The larvae, called glochidia, will attach themselves to the fish and will consequently be dispersed by the fish host away from the location of the parents. Different species of mussels have different species of fish as host (Fuller, 1974). Density-dependent competition may occur among glochidia for fish hosts (Stein, 1971; Fuller, 1974). Upon maturity, the glochidia will simply detached itself from its fish host and begin life as a juvenile mussel in a new location in the river.

The mathematical model used in this study is based on the Roughgarden *et al.* (1985) concept of a single open marine population with space-limited recruitment, adapted to include features such as age-structure modeling, density dependence and spatial dispersal. Deterministic equations are used to describe the physiological growth and the probability of survival of the mussels. Dispersal of the glochidia is assumed to occur through the random movements of the fish hosts.

The computer algorithm is designed to parallelize the river system into discrete cells (Lee *et al*, 2001). A hypothetical river system was created with 4000 distinct cells. Each cell in the river system was then assigned a micro-processor in a parallel computer, to simulate its local mussel community. In addition each cell can have up to a maximum of 15 different age classes and 35 different species of Unionid mussels. Overall, the entire river system is modeled as a set of contiguous spatial cells with varying habitat suitability characterized by 5 physical environmental parameters.

The main motivation for the construction of a parallel algorithm to model the mussel communities is the lack of movement among the mussels. The mussels in generally are sessile creatures and found in low-density communities. In addition the mussels are also subjected to very little inter or intra-specific competition in most parts of the river system. An assignment of each age class of each species in each cell (called age class cohort) to a processor is quite similar to the approach used by Ramachandramurthi *et al.* (1996) in their parallel algorithm of physiologically structured population models. The assignment of a community of mussels living together within a spatial boundary (a spatial cell) to a processor is called cell-to-processor assignment. This is convenient,

as mussel communities from different cells in the model do not interact with each other except during the breeding season, just as in nature.

It is also assumed that the characteristics affecting the mussels are uniform throughout a given cells. Glochidia released by a mussel in cell i can settle in any other suitable cell, including cell i. The distance the glochidia/juvenile travels is determined by its fish host. A random normal distribution probability function is used to determine the distance and direction of settlement. The cells in the main river branch are numbered sequentially first, followed by the cells in the tributaries. However, each cell is allowed to have only one tributary. Figure 3 shows graphically the division of a river and its tributaries into cells in the algorithm.
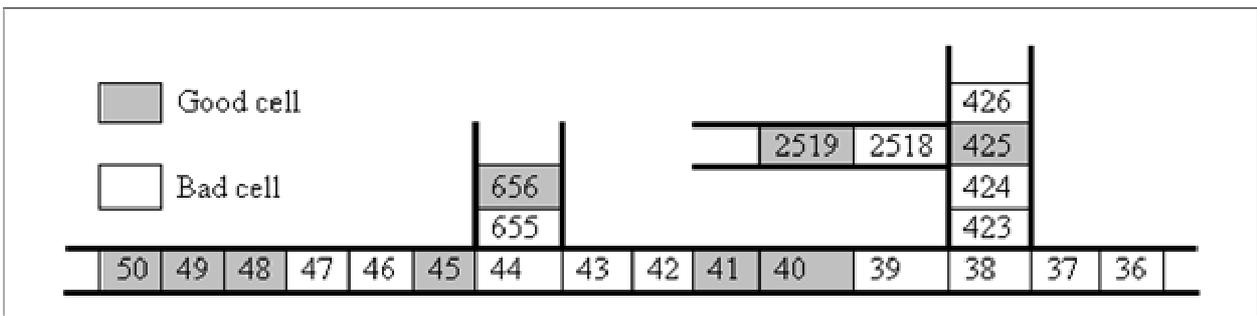
Figure 3. Schematic of a river cells division.

The dynamics of the mussels in all cells are computed simultaneously in each time step. The growth in mass of each mussel cohort, the availability of free-space in the cells and the probability of survival from one age class to another respectively are some of the physical functions that are computed each time step. Last but not least the design of this parallel algorithm also minimises the communication between the individual micro-processors. Hence to achieve this, communication between micro-processors are only permitted during dispersion/settling period of the glochidia/juvenile period of the life-cycle of a mussel. This physical inter-processor communication is restricted to occur only at three discrete annual reproductive events in a year.

Overall, it must be noted that this parallel algorithm does face a problem in load balancing in the usage of micro-processors due to the highly variable mussel densities in each cell as well as the existence of "empty" cells. Empty cells are defined as cell without any mussel population. The more micro-processors that are active simultaneously, the greater will be the efficiency of a parallel algorithm over a sequential algorithm (Leighton, 1992).

This research effort, though preliminary, does provide some incentives to promote more advance applications in the field of parallel computing, as well as to stimulate related activities in Mathematics curriculum developments.

THE FLORIDA EVERGLADES GEER MODELS

The Florida Everglades is the largest remaining sub-tropical wilderness in the continental United States, and is currently the last remaining habitat for 68 federally listed threatened or endangered

species, including the American crocodile and the Florida panther. However, it is facing many problems, which prompted the US Congress to authorize and fund an ecological restoration plan known as GEER (Greater Everglades Ecological Restoration). In this regards, fish community ecology and dynamics have become a core area of interest in many modeling projects within the framework of GEER. The effects of water level and seasonal temperature fluctuations on fish community, the impacts of trophic interactions, the path way and extent of toxicant bioaccumulation and the transfer of toxicant from lower trophic levels to higher trophic levels are core areas of interests. This Everglades Fish Model provides a crucial link to the *Everglades Landscape Model* (ELM) dan *Across-Trophic-Level System Simulation* (ATLSS) (DeAngelis, 2001). It is hoped that more will be done in the near future to utilize the immense facility of modern IT, as applied to ELM and ATLSS, to advance basic science, to stimulate active graduate programs, as well as to help provide solutions to the ills of modernization. One such benefit that is immediately useful would be to extend these models for applications to the recent endeavour to rehabilitate several major rivers and their associated basins in Malaysia, and to utilize this exercise to promote proactive joint research with GEER partners. We briefly discuss some modest achievements in the modelling of fish ecology in the Everglades in pursue of this joint collaboration.

THE FLORIDA EVERGLADES FISH MODEL E_FISH

Seasonal temperature fluctuations have been noted to have significant effects on fish community, which in turn will bring about wide ranging consequences to other ecosystems in the Everglades. Al-Rabai'ah *et al.*, (2002a) has performed simulations, using mathematical modeling techniques, to assess the effects of seasonal temperature on fish density in the Everglades as shown in Figure 4, which shows satisfactory results based upon comparison with data obtained from the literature, which indicate significant sensitivity of fish ecology to temperature. Hence any serious attempt to model Everglades fish ecology should include temperature effects in the models, particularly when other stressors are implicated, as is clearly shown in the case of Daphnia population dynamics subject to multiple environmental stressors (Koh *et al*, 1997).
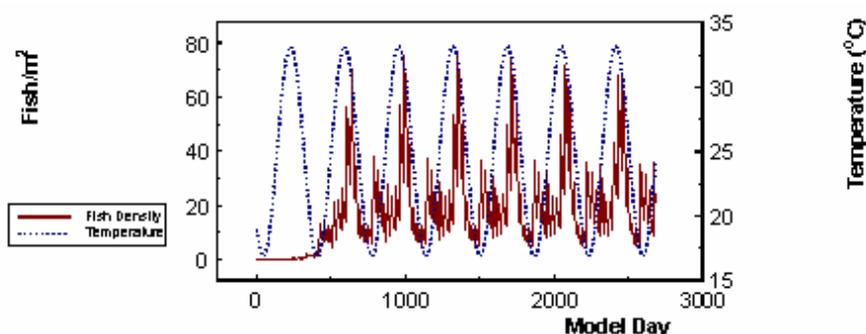
Figure 4. Fish density in marsh areas of Florida Everglades for small fish, with temperature effects.

In addition to temperature, hydrological changes and trophic interactions too play an important role in fish community dynamics. Computer simulations taking into consideration different water level scenarios (Al-Rabai'ah *et al.*, 2001) show clearly that a 10 cm increase in mean water level would induce significantly different fish densities in the Everglades as shown in Figure 5, showing the

sensitivity of fish ecology in the Florida Everglades to changes in water level. These simulation results are potentially helpful when applied to future hydrological projects to manage the hydrology in that area, as well as in Malaysia.
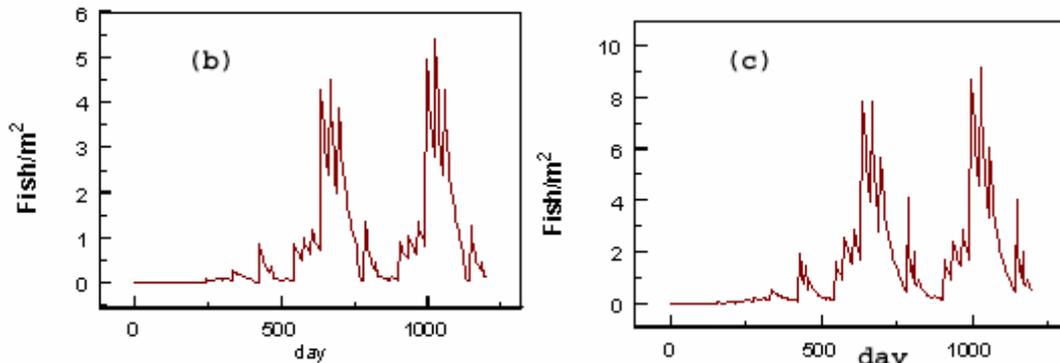
Figure 5. The Everglades small fish population density at three different mean water depths (D) left: D = 0.6 m, right: D = 0.7 m.

Furthermore, other area of interest includes an analysis of the pathway of toxicant transfer from lower trophic levels to higher trophic levels, which can be simulated by a toxicant-bioaccumulation model. Al-Rabai'ah *et al*. (2002b) described a PCBs-bioaccumulation model that closely mimics data collected from the field. The ability of this toxicant model to accurately predict contaminant transfer in a complex food web indicates that it could be an important planning and management tool in toxicological study for developing targets, evaluating contaminant-based remediation strategies, and performing biological risk assessment (EPA, 1992).

CONCLUSION

An attempt has been made to demonstrate the applicability of simulation models and mathematical sciences to address some urgent issues related to the degradation and restoration of the environment and its ecosystem. It is hoped that this paper would provide some incentives to help stimulate more active research in this area and to propel a constant effort to review mathematics curriculum to make it more relevant and responsive to the changing needs of the time.

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REFERENCES

Al-Rabai'ah, H.A., Koh, H.L., DeAngelis, D. and Lee, H.L. (2001). Modeling fish community dynamics in Florida Everglades: Role of hydroperiods and trophic interaction, Asian Wetland Symposium 2001, 27-30 August 2001, Penang, Malaysia.

Al-Rabai'ah, H.A., Koh, H.L., DeAngelis, D. and Lee, H.L. (2002a). Modeling fish community dynamics in Florida Everglades: Role of Temperature Variations. Water Sci. Tech., accepted.

Al-Rabai'ah, H.A., Koh, H.L., DeAngelis, D. and Lee, H.L. (2002b). A Bioaccumulation Model of PCBs in an Everglades Aquatic Food Web. Constructed Wetlands and Waste Stabilization Ponds Research Project: "8th International Conference on Wetlands Systems for Water Pollution Control". 16 - 19 September 2002, Arusha, Tanzania (accepted).

Burky, A.J. (1983). Physiological ecology of freshwater bivalve. In: W.D. Russell-Hunter (Editor), The Mollusca. Vol. 6: Ecology, Academic Press, New York, pp 281-237.

DeAngelis, D.L. (2001). The Use of Landscape Models in Planning Restoration of The Florida Everglades. Proceedings of the National Workshop on Ecological and Environmental Modeling (ECOMOD 2001), to appear.

EPA (1992). Framework for ecological risk assessment. EPA/630/R-92/001. USEPA, Washington, D.C.

Fuller, S.L.H. (1974). Clams and mussels (Mollusca: Bivalvia). In: C.W. Hart, Jr., and S.L.H. Fuller (Editors), Pollution ecology of freshwater invertebrates, Academic Press, New York, pp 215-273.

Jirka, K.L. (1986). Reproduction biology and comparative growth rates of selected species of freshwater mussels (Bivalvia: Unionidae) in the New and Greenbriar rivers, Virginia and West Virginia. M.S. thesis, Virginia Polytechnic Institute and State University, Blacksburg.

Koh, H.L. and H.L. Lee. 2001. Modeling water quality in Sg. Lebum, Johor, Malaysia. Recent Advances in Marine Science and Technology, 2000, ed. Narendra Saxena, p.199-208. PACON International, USA, June 2001.

Koh, H.L., Hallam, T.G. and Lee, H.L. (1997). Combined effects of environmental and chemical stressors on a model Daphnia population. Ecological Modelling 103: 19-32, Elsevier Sciences B.V., London.

Koh, H.L., P.E. Lim and H.L. Lee. 1995. Water quality modelling for an estuary in Johore. Water Qual. Res. J. Canada 30(1): 45-52.

Lee, H.L., DeAngelis, D.L. and Koh, H.L.(1998). Modeling Spatial Distribution of The Unionid Mussels and the Core-Satellite Hypothesis. Wat. Sci. Tech. Vol. 38,No. 7,pp.73-79.

Lee, H.L. and DeAngelis, D.L. (1997). A simulation study of the spatio-temporal dynamics of the unionid mussels. Ecological Modelling, 95(2-3), pp 171-180.

Lee, H. L., Halloy, C. and Koh, H. L. (2001). Parallel Algorithm for an Age-Structures Population Model. Proceedings of the National Workshop on Ecological and Environmental Modeling (ECOMOD 2001), to appear.

Leighton, F.T. (1992). Introduction to Parallel Algorithms and Architectures: Arrays, Trees, Hypercubes. Morgan Kaufmann Publishers, San Mateo, California.

Lewandowski, K. and Stanczykowska, A. (1975). The occurrence and role of bivalves of the family Unionidae in Mikolajskie Lake. Ekol. Pol., 23(2):317-334.

Moermond C. T. A. and Koelmans A. A. (1999) Nutrients and contaminants. Scenario studies with AQUATOX on the interaction between contaminants and communities in modelecosystems and shallow lakes . Report commissioned by RIZA. Wageningen University, Wageningen, The Netherlands.

Park R. A., Firlie B., Camacho R., Sappington K., Coombs M. and Mauriello K. D. (1995) AQUATOX, a general fate and effects model for aquatic ecosystems. In *Proceedings for the Toxic Substances in Water Environments: Assessment and Control, Water Environment Federation*, pp. (3)7–(3)-17.

Ramachandramurthi, S., Hallam, T.G. and Nichols, J.A. (1996). Parallel simulation of individual-based, physiologically structured population models. Mathematical and Computer Modelling.

Roughgarden, J., Iwasa, Y. and Baxter, C. (1985). Demographic theory for an open marine population with space-limited recruitment. Ecology, 66(1):54-67.

Stein, C.B. (1971). Naiad life cycles:their significant in the conservation of the fauna. In: S.E. Jorgenson and R.W. Sharp (Editors), Proceedings of a symposium on rare and endangered mollusks (Naiads) of United States, Ohio State University, Columbus.

USEPA (2000a) *Aquatox for Windows. A Modular Fate and Effects Model for Aquatic Ecosystem, Release 1, Vol. 2. Technical Documentation.* EPA-823-R-00-007, Chicago, IL.

USEPA (2000b) Aquatox for Windows. A Modular Fate and Effects Model for Aquatic Ecosystem, Release 1, Vol. 3. Model validation reports. EPA-823-R-00-008, Chicago IL.

Wool, T., Ambrose, R., Martin, J. and Comer, E. (2001). Water Quality Analysis Simulation Program (WASP). Version 6.0, User Manual, USEPA - Region 4.