

AQUATOX is distributed with a variety of self-contained studies (Table 1) that can be used as tutorial examples, templates, or starting points for developing new applications. They are color-coded here to give the user a rough idea of their applicability. There are four general classes of studies:

- **Nutrient studies** that are designed to examine the effects of organic matter, nitrogen, and phosphorus levels on primary productivity and the consequent effects on the food web.
- **Microcosm and mesocosm studies** in which the model is applied to experimental facilities or sites that are in themselves physical models with controlled boundary conditions; these range from simple aquaria to experimental streams to pond enclosures.
- **Chemical fate and effects studies** that examine bioaccumulation and the direct and indirect effects of organic chemicals on the food web as well as the persistence of those chemicals.
- **Studies intended for teaching purposes** that are not closely based on observed data, but that are included to illustrate particular AQUATOX features or site types.
- **Nearshore Marine Environment Studies** in which the model has been calibrated to biotic data representing the nearshore marine environment. (Blancher 2017)

The table below is organized by study type in the following order: nutrient studies, micro- and mesocosm studies, chemical fate and effects studies, and teaching studies. Well-calibrated studies¹ for each type are presented first.

Well-calibrated nutrient study	Roughly-calibrated nutrient study
Well-calibrated micro- or mesocosm study	Roughly-calibrated mesocosm study
Well-calibrated chemical fate/effects study	Roughly-calibrated chemical fate/effects study
Well-calibrated NME study	Study intended for teaching purposes

¹ In this case, the term “well calibrated” is a function of the available data to calibrate against and the goals of the study. The term does not necessarily mean that all state variables in the study have been calibrated against an extensive data set.

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Table 1. Description of Example Study Files for AQUATOX 3.1 NME

Study Name	Site Type	Location	Run time (h:mm; 2.66 GHz Quad CPU)	Notes
<i>Pass Marianne Reef, MS.aps</i> <i>(well-calibrated NME)</i>	Near-shore Marine Oyster	MS Sound	< 5 minutes for 3 years	Model calibration conforms well with observed oyster biomass. Magnitude of fish and invertebrate biomass estimates verified with Gulf locations (Grand Bay & Galveston Bay) Model driven with data from MODIS and Northern Gulf Institute studies. (Blancher 2017)
<i>MS_Sound_Soft Bottom.aps</i> (well-calibrated NME)	Near-shore Marine Soft	MS Sound	< 5 minutes for 3 years	Soft-bottom calibration in location near Cat Island, MS. Model calibrated to phytoplankton data from Northern Gulf Institute Studies. Magnitude of chl <i>a</i> predictions verified with MODIS data. Zooplankton, fish, secchi depth data also compared against model predictions.
<i>MS_Sound Exposed Beach.aps</i> (well-calibrated NME)	Near-shore Marine Beach	MS Sound	< 5 minutes for 3 years	Front-edge barrier-island calibration. Zoobenthos and fish biomass predictions compared to observed data from exposed beach habitats. (Blancher 2017)
<i>Hancock Marsh Edge.aps</i> <i>(well-calibrated NME)</i>	Near-shore Marine Marsh Edge	MS Sound	< 5 minutes for 3 years	Extensive fish and invertebrate biomass data are available for Hancock County marsh through the work of Larsen (2006). Predictions from the derived marsh-edge food-web model were compared to these data sets. (Blancher 2017)
<i>Blue Earth R.MN.aps</i> <i>(well-calibrated nutrient)</i> <i>Blue Earth R.MN BMP Criteria.aps</i>	River	Southern MN	0:14 for 2 yr 0:14 for 2 yr	The Blue Earth River drains a watershed in the Western Corn Belt Plains ecoregion that is 95% agricultural, planted in corn and soybeans. Suspended sediments are important most of the time; otherwise, algal blooms predominate. Study set up to evaluate nutrient reduction due to best management practices (BMPs).

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<i>Cahaba R AL.aps</i> <i>(well-calibrated nutrient)</i> <i>Cahaba R AL X2 TSS.aps</i>	River	Near Birmingham AL	0:47 for 2 yr 0:29 for 2 yr	A shallow stream incised in the southern Appalachians, located in a rapidly urbanizing area and receiving effluent from wastewater treatment plants. Good calibration data on periphyton, invertebrates, and fish. TSS is doubled to demonstrate embeddedness and impact on zoobenthos; it also decreases periphyton growth and speeds up simulation.
<i>Crow Wing R. MN.aps</i> <i>(well-calibrated nutrient)</i>	River	North central MN	0:13 for 2 yr	Shallow, relatively low-nutrient river that drains a predominantly forested watershed in the Northern Lakes and Forests ecoregion. Mile 72 is in the headwaters and drains numerous small lakes.
<i>DeGray Res AR.aps</i> <i>(well-calibrated nutrient)</i>	Reservoir	Near Hot Springs AR	0:16 for 2 yr	A mesotrophic-eutrophic impoundment of the Caddo River in the Ouachita Mountains ecoregion. Most of the watershed is forested. Study shows transient response to drowned forest shortly after dam construction. Uses sediment diagenesis model.
<i>Lake George NY.aps</i> <i>(Well-calibrated nutrient)</i> <i>Lake George NY smelt.aps</i>	Lake	Upstate NY	0:01 for 3 yr 0:03 for 13 yr	Mesotrophic end of large, deep lake in Adirondacks. Introduction of smelt changes food web and favors diatom blooms.
<i>Lower Boise R. ID Seg_1-3.als</i> <i>(Well-calibrated nutrient)</i> <i>Lower Boise R. ID Seg_1-3 Diel.als</i>	River River	Boise ID Boise ID	2:49 for 3 yr 2:35 for 1 yr	Three upstream linked segments of the lower Boise River, a shallow river with abundant periphyton. Flow is controlled by upstream releases and irrigation diversions. Two segments are low-nutrient and the third receives WTP effluent. Also has hourly simulation to predict diel oxygen, which is dominated by throughflow except during low flow.
<i>MN Rivers.als</i> <i>(Well-calibrated nutrient)</i>	Rivers	North, central, and southern MN	0:40 for 2 yr	Crow Wing, Rum, and Blue Earth Rivers as linked segments sharing the same parameter set (Park et al. 2005).

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<i>Onondaga Lake NY</i> <i>Sed Diagenesis.aps</i> (Well-calibrated nutrient)	Lake	North of Syracuse NY	0:01 for 2 yr (steady- state aerobic layer)	"Lake Onondaga is arguably the most polluted lake in the United States" from the preface of a book (Effler 1996), which served as the source of data for this study. The lake has significant nutrient inputs from wastewater treatment plant ("Metro") and combined sewers, successive algal blooms, hypoxia in hypolimnion, build-up of organic sediments in bottom, and high mercury levels and high salinity (the latter two are not modeled at present). Run with sediment diagenesis submodel (Di Toro 2001), with steady-state aerobic layers.
<i>Rum R MN.aps</i> (Well-calibrated nutrient)	River	north of St. Paul MN	0:13 for 2 yr	Rum River is a shallow river, with moderate nutrients and low suspended solids that drains forests and dairy farms in the North Central Hardwoods Forest ecoregion.
<i>Tenkiller Ferry Lake</i> <i>OK.als</i> (Well-calibrated nutrient)	Reser- voir	Eastern OK	0:51 for 2 yr	Linked segments representing a eutrophic reservoir impaired by nutrients and organics, especially from upstream poultry and swine farms; there are excessive algae, and the hypolimnion is anoxic during the summer. However, it is one of the most important recreational lakes in the state. The sediment diagenesis submodel is necessary to simulate the anoxic hypolimnion.
<i>Cheney Res KS.aps</i> (roughly-calibrated nutrient)	Reser- voir	Near Wichita KS	0:01 for 15 mn	City of Wichita acquires about 70 percent of its daily water supply from Cheney Reservoir. It is believed that objectionable tastes and odors in Cheney Reservoir result from cyanobacteria (blue-green algae), and there is concern with proliferation of algal growth. Both nutrients and suspended solids affect algal growth and could be a concern for taste-and-odor issues (USGS 2008).
<i>Lake Jesup FL.aps</i> (roughly-calibrated nutrient)	Lake	North of Orlando	0:01 for 7 yr	Lake Jesup is a large, shallow lake. Urban storm water and agricultural runoff impact the lake, as well as historic wastewater discharge. Blooms of the invasive cyanobacteria <i>Cylindrospermopsis</i> have been increasing.

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<i>Lake Pyhäjärvi</i> <i>Finland.aps</i> (roughly-calibrated nutrient)	Lake	SW Finland	0:04 for 10 yr	Mesotrophic boreal lake simulated by Anne Mäkynen, Jyväskylä University. The difference between observed and simulated phosphorus concentration corresponds perfectly with the mass removed by fishing.
<i>Farm Pond MO.aps</i> <i>Farm Pond MO</i> <i>Esfenval.aps</i> (Well-calibrated mesocosm)	Pond	Central MO	0:01 for 1 yr 0:01 for 1 yr	Generic pond built to USDA specifications. Esfenvalerate loadings are the worst-case scenario using runoff from an adjacent corn field predicted by the PRZM model.
<i>HCB Tank.aps</i> (Well-calibrated microcosm)	Aquari- um	Experime ntal lab	0:00:01 for 2 mn	Represents an experiment in which an aquarium tank containing macrophytes was dosed with hexachlorobenzene (Gobas et al. 1991).
<i>Ponds MN</i> <i>Chlorpyrifos.als</i> (Well-calibrated mesocosm)	Enclos- ures	Duluth MN	0:00:15 (perturbed & control) for 3 mn	Pond enclosures dosed with 0.5, 6, and 32 ug/L chlorpyrifos at an EPA lab.
<i>Expr Stream</i> <i>Esfenval.aps</i> (Roughly-calibrated mesocosm)	Stream	Idaho	0:15 for 10 mn (perturbed)	Based on Lower Boise River, this is a reach with a volume of 400 m ³ and a retention time of 0.1 day. Set up for constant dosing for a period of time. Study uses fixed time step so it can be used for detecting lowest effect levels.
<i>Ohio stream</i> <i>Chlorpyrifos</i> <i>constant.aps</i> (Roughly-calibrated mesocosm) <i>Ohio stream</i> <i>Chlorpyrifos</i> <i>pulsed.aps</i>	Stream	North central OH	0:07 for 2 yr	A small creek draining agricultural area, used as a generic study for various pesticides. One study has constant exposure and other has pesticide runoff during summer storms.

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Study Name	Site Type	Location	Run time (h:mm; 2.66 GHz Quad CPU)	Notes
<p><i>Coralville Res IA Dieldrin.aps</i></p> <p><i>(Well-calibrated chemical fate/effects)</i></p> <p><i>Coral Res IA Sens.aps</i></p>	Reservoir	Near Iowa City IA	<p>0:13 (perturbed)</p> <p>0:10 (control)</p> <p>for 9 yr</p> <p>2:41 for 1 yr</p>	<p>Coralville Reservoir is a large, shallow, eutrophic reservoir. The drainage area is over 90% agricultural, especially corn. Runoff carries large amounts of fertilizer, animal wastes, silt, and pesticides into the reservoir. By the early 1970's, the population of largemouth bass and fish other than buffalofish began to decline and residues of the pesticides aldrin and dieldrin greatly increased in tissue samples (Mauriello and Park 2002).</p> <p>Study set up for sensitivity analyses, 54 parameters.</p>
<p><i>Evers Res FL.aps</i></p> <p><i>(Well-calibrated chemical fate/effects)</i></p>	Reservoir	Bradenton FL	0:05 for 5 yr (perturbed)	A reservoir with increasing algal blooms, treated with copper sulfate and hydrogen peroxide. Simulated by Dr. Don Blancher, Sustainable Ecosystem Restoration, LLC
<p><i>Lake Ontario PCBs.aps</i></p> <p><i>(well-calibrated chemical fate/effects)</i></p>	Lake	US-Canada	1:55 for 4 yr	Demonstration of bioaccumulation simulation for numerous PCB congeners compared to data of (Oliver and Niimi 1988)see also (Burkhard 1998); this implementation uses Barber (2003) k2 estimation.
<p><i>Skensved Denmark TCE.aps</i></p> <p><i>(well-calibrated chemical fate/effects)</i></p> <p><i>Skensved Denmark Atrazine.aps</i></p>	Stream	Denmark	0:15 for 1 yr (perturbed)	<p>Studies produced by external researchers -- Simon Funder and Dr. Ursula McKnight of the Technical Univ. of Denmark,</p> <p>Groundwater with trichloroethene from a leaking tank is polluting a small stream. Researchers used AQUATOX to show the impacts are probably negligible. The same setup with atrazine does show some direct and indirect ecotoxicological effects. Concs. are near the no effects level so the option for a fixed time step was chosen.</p>

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<i>Clear Lake CA</i> <i>Fluridone.aps</i> (Roughly-calibrated chemical fate/effects)	Lake	Central CA	0:14 (both perturbed & control) for 3 yr	Roughly based on Clear Lake CA, a large, shallow, eutrophic lake with cyanobacteria blooms. Sonar (fluridone) has been used successfully in Clear Lake to eradicate <i>Hydrilla</i> . Although <i>Hydrilla</i> did not appear until 1994, the study is set up with 1970-1971 ecosystem data. Note that the fluridone loadings are for 1971 but without bracketing the simulation period with 0 loadings. The fluridone loadings are repeated in each of the three years. Also note that the entire lake was modeled for convenience; in reality, <i>Hydrilla</i> spread slowly, so only selected areas needed to be treated. Our simulation is therefore a worst-case scenario.
<i>East Fork Poplar Creek TN PCBs.aps</i> (Roughly-calibrated chemical fate/effects)	Stream	Oak Ridge TN	1:09 for 8 yr	A small stream that drains the Y-12 plant at Oak Ridge National Lab with PCB contamination. The simulation runs for eight years to illustrate gradual recovery.
<i>Galveston Bay TX.aps</i> (Roughly-calibrated estuary)	Estuary	Near Houston TX	0:11 for 3 yr	A shallow, productive bay that receives runoff from Central TX, including the Houston Ship Channel.
<i>Zollner Creek OR w chlorpyr dieldrin- pulse.aps</i> (roughly-calibrated chemical fate/effects)	Stream	Willamette Valley OR		The watershed is >90% agricultural, with row crops, orchards and vineyards, grain and grass fields, and large poultry farms. It is a USGS National Water Quality Assessment Program (NAWQA) site, and also a principal TMDL site. State criteria for chlorpyrifos and legacy dieldrin were exceeded (Williams and Bloom 2008).
<i>Impact of anadromous fish.aps</i> (Study intended for teaching purposes)	Lake	Based on Lake George NY	0:01 for 3 yr	Mesotrophic lake based on Lake George NY, with Chinook salmon representing anadromous fish. Nutrients are imported into lake.
<i>Nockamixon Res PA.aps</i> (Study intended for teaching purposes)	Reserv- oir	eastern PA	0:00:30 for 2 yr	Heavily impacted reservoir downstream of the Quakertown wastewater treatment plant outlet.

References

- Blancher, E. C., Park, R. A., Clough, J. S., Milroy, S. P., Graham, W. M., Rakocinski, C. F., Hendon, J. R., Wiggert, J. D., and Leaf, R. (2017). "Establishing nearshore marine secondary productivity baseline estimates for multiple habitats in coastal Mississippi and Alabama using AQUATOX 3.1 NME for use in the Deepwater Horizon natural resource damage assessment." *Ecological Modelling*, 359, 49–68.
- Burkhard, L. P. 1998. Comparison of Two Models for Predicting Bioaccumulation of Hydrophobic Organic Chemicals in a Great Lakes Food Web. *Environmental Toxicology and Chemistry* **17**:383-393.
- Effler, S. W., editor. 1996. *Limnological and Engineering Analysis of a Polluted Urban Lake*. Springer, New York.
- 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.
- Gobas, F. A. P. C., E. J. McNeil, L. Lovett-Doust, and G. D. Haffner. 1991. Bioconcentration of Chlorinated Aromatic Hydrocarbons in Aquatic Macrophytes (*Myriophyllum spicatum*). *Environmental Science & Technology* **25**:924-929.
- Larsen, K.M. 2006. Utilization of marsh edge and nonvegetated bottom habitats in western Mississippi sound by brown shrimp, *Farfantepenaeus aztecus*, with notes on associated nektonic assemblages. The University of Southern Mississippi. Master Degree Thesis. 63 pp.
- 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.
- 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.
- Oliver, B. G., and A. J. Niimi. 1988. Trophodynamic Analysis of Polychlorinated Biphenyl Congeners and Other Chlorinated Hydrocarbons in the Lake Ontario Ecosystem. *Environ. Sci. Technol.* **22**:388-397.
- Park, R. A., J. N. Carleton, J. S. Clough, and M. C. Wellman. 2009. AQUATOX Technical Note 1: A Calibrated Parameter Set for Simulation of Algae in Shallow Rivers. EPA-823-R-09-003, U.S. Environmental Protection Agency, Washington D.C.
- 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.
- Sourisseau, S., A. Bassères, F. Périé, and T. Caquet. 2008. Calibration, validation and sensitivity analysis of an ecosystem model applied to artificial streams. *Water Research* **42**:1167-1181.
- 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.
- USGS. 2008. The Cheney Reservoir and Watershed Study.