Lab 1: A Tour Through the AQUATOX Screens

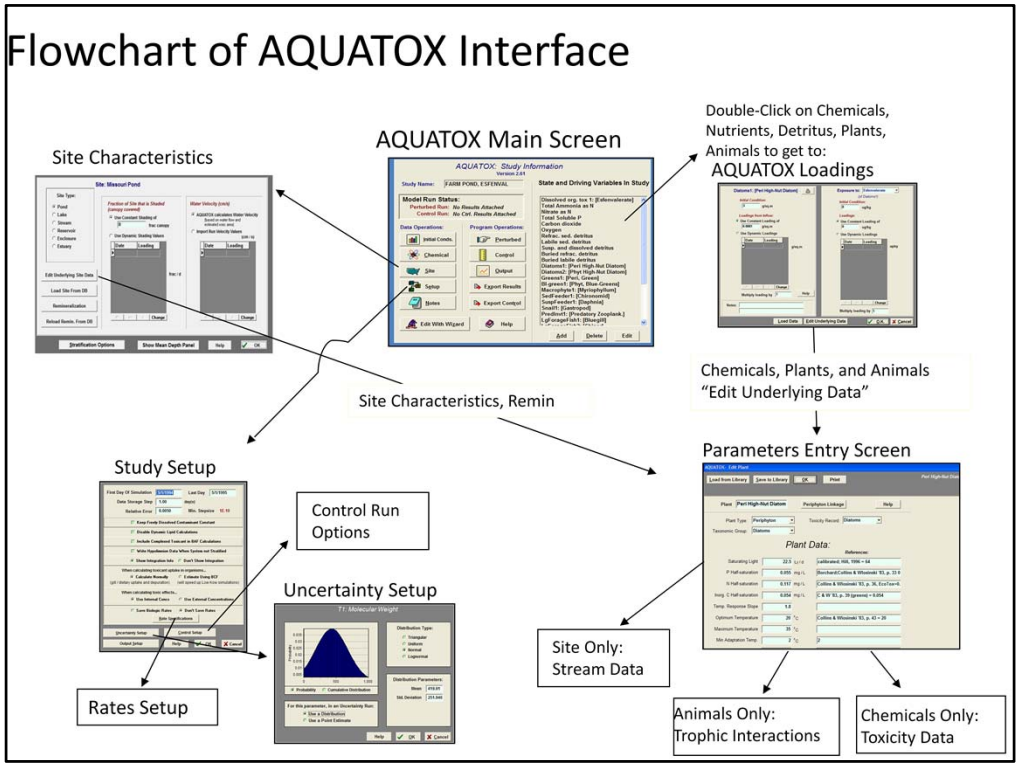
- ❑ Main Screen
- ❑ Toolbar
- ❑ Simulation Window
- ❑ Initial Conditions
- ❑ Chemical Screen
- ❑ Site Screen
- ❑ Stream Data
- ❑ Remineralization Data
- ❑ Setup Screen
- ❑ Rates Screen
- ❑ Libraries
- ❑ Uncertainty Screen
- ❑ Output Setup
- ❑ Control Setup Screen
- ❑ Help File
- ❑ Wizard
- ❑ Run Buttons
- ❑ Export of Results
- ❑ State Variable List (Chemicals, Nutrients, Organics, Plants, Animals, etc.)

This lab is not intended to describe the functionality of any of these screens in particular, but rather to get you used to navigating through AQUATOX and provide an overview of model and interface design. We will start by loading **FarmPond MO Esfenvalerate.aps** into AQUATOX as a basis for exploring these screens. In the next few pages we will run a few experiments with this simulation.

START THE SIMULATION NOW so the results will be available for after we have reviewed the interface. You can interact with the software while the simulation is running.

Questions to answer on your own as you explore the screens:

- What period is simulated?
- What rates are being saved?
- What is the mean temperature for the site?
- What is the mean light?
- What is the pH?
- What is the ammonia loading?
- What is the nitrate loading? Source?
- Does water volume vary?
- What is mean wind speed?
- What is the source of the esfenvalerate loadings?



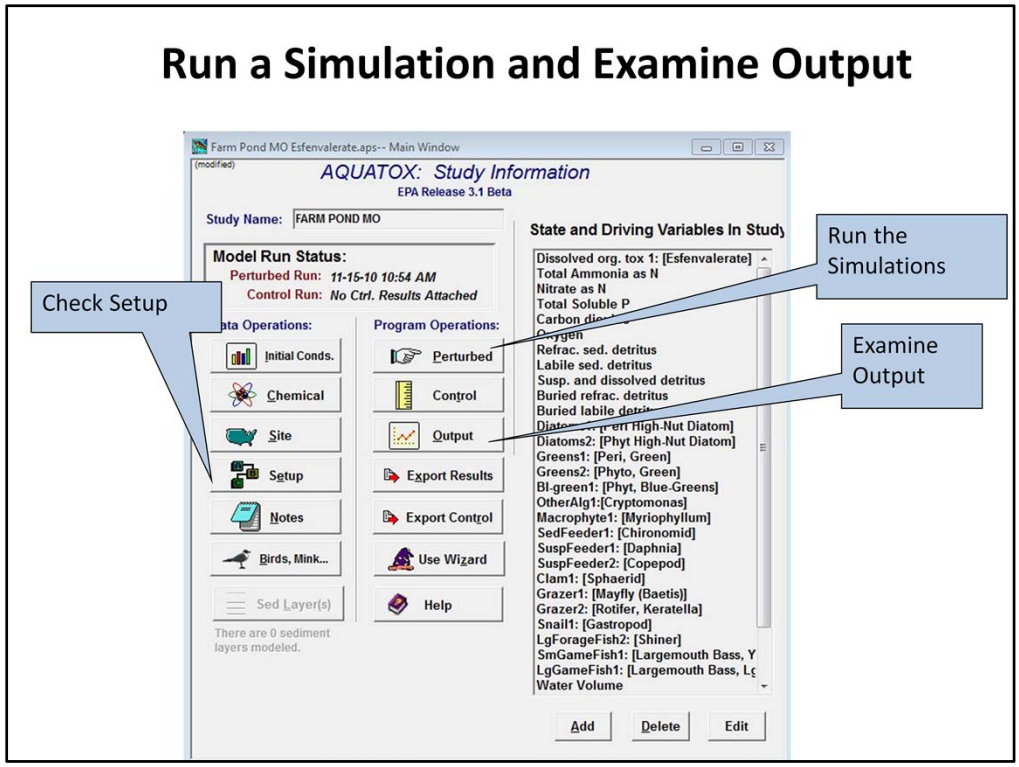
This page provides a general overview of the navigation through the AQUATOX Interface.

Double-click on the state variable list to bring up initial conditions and loadings for each state variable. For animals, chemicals, and plants, you can move from the loadings screen down into the "underlying data" which is a list of parameters that describe the organisms.

Other important buttons on the main interface include the "Site" button which brings you to site type and characteristics. From here you can move down into "site underlying data" or site parameters and characteristics and "Remineralization" which are parameters pertaining to the organic matter.

Finally, the "Setup" button is important to note as it allows the user to change the characteristics of a study run (e.g. time-period and differential equations solver options). The study setup screen is also where settings for control runs, uncertainty setup, and the saving of differential equation rates may be specified.

Run a Simulation and Examine Output



We spent a few minutes going through each of the AQUATOX screens that show all of the model input that comprise this particular simulation. We also ran the simulation while exploring those screens. The next thing to do is to examine results.

The Many Types of AQUATOX Output

(in order of output list)

- Concentrations of State Variables
  - toxicants in water
  - nutrients and gasses
  - organic matter, plants, invertebrates, fish
- Physical Characteristic State Variables
  - water volume, temperature, wind, light, pH
- Mass of Toxicants within State Variables (normalized to water volume)
  - T1-T20 in organic matter, plants, invertebrates, and fish
- Additional Model Calculations
  - Secchi depth, chlorophyll *a*, velocity, TN, TP, BOD
- Biological metrics
  - % EPT, Chironomids, Amphipods, % Blue-Greens, Diatoms, Greens, Gross Primary Production, Turnover, Trophic State Indices

State variables are organized in order of trophic level, starting with organic matter and working upward through plants, invertebrates, and fish.

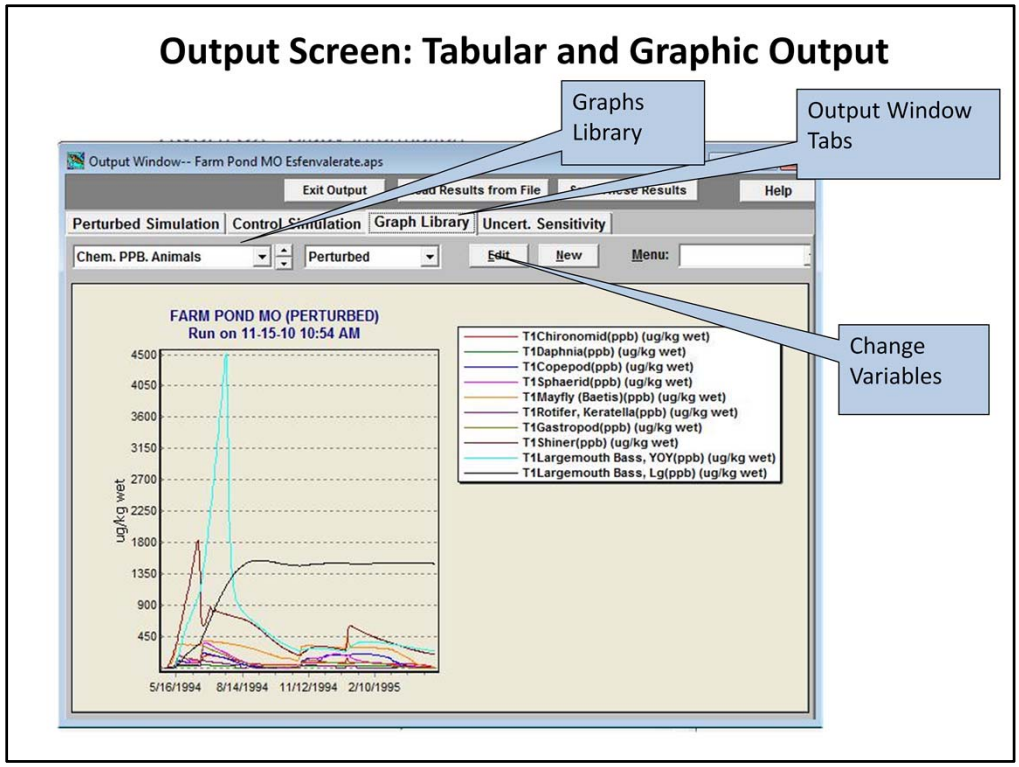
When a toxicant is included in a simulation, the amount of output in a simulation more than triples. Additional chemical output includes the toxicant dissolved in water, the mass of toxicants in state variables normalized to the water volume (units of μg/L), the concentration of toxicants in state variables (PPB), and bioaccumulation factors for organisms.

Because there are so many types of AQUATOX output you may use the “filter” option whenever looking through this list to reduce the amount of output. Try filtering on units (“mg/L” or “g/m2”) or on partial state variable names (“peri” “phyto”). Only state variables that include your sub-string will be displayed, making it far easier to find the output you wish to graph.

The Many Types of AQUATOX Output
(continued)

- Sediment diagenesis state variables
- Toxicant PPB
  - T1-T20 (PPB) in organic matter, plants, invertebrates, and fish
- Nitrogen and Phosphorus Mass Tracking Variables
- Bioaccumulation Factors
- Uptake, Depuration, and Bioconcentration Factors
- State Variable Rates
- Limitations to Photosynthesis
- Observed data imported by user

Output facilitates detailed analyses of simulated responses. Mass loadings and losses and mass balances are output for nutrients. K1, K2, and BCFs are output for toxicants. The ability to output in tabular and graphical form all the state-variable rates and the limitations to photosynthesis is especially powerful.



We will work together and look at the tabular output then produce a simple graph that shows the toxicant concentration in the water column.

After that, please spend 5-10 minutes working with the output screens to familiarize yourself with the interface. Please be sure to ask us if you have any questions. Some exercises you can work on:

• First try to produce a graph of the water column concentration of Esfenvalerate predicted within this simulation. *Hint: T1 stands for "Toxicant 1" which in this case is Esfenvalerate so the result to graph is "T1 H2O (ug/L)"*
• Can you produce an output table with parts per billion output for Esfenvalerate throughout the food-chain? Is there evidence of biomagnification through the food-chain?
• Can you produce a graph that displays parts per billion output for Esfenvalerate in all animals (*Chironomid* through Largemouth Bass Lg)?
• To help answer "why are the parts per billion output for Gastropod falling to zero" graph the Gastropod state variable.
• If time permits, explore graphs containing other output categories (i.e. detrital state variables, bioaccumulation factors).