# Applying AQUATOX to Aquatic Mesocosms for Higher-Tier Pesticide Risk Assessment

Damian Preziosi (Integral Consulting Inc), Daniel Dawson (Integral Consulting Inc), Laura Mudge (Integral Consulting Inc), Robert Pastorok (Integral Consulting Inc), Brandon Sackmann (GSI International), Conner Schultz (Integral Consulting Inc), Chiara Accolla (Waterborne Environmental Inc.), Ann Kathrin Lörracher (Mesocosm GmbH), Klaus Peter Ebke (Mesocosm GmbH), Amelie Schmolke (Waterborne Environmental Inc.), Nika Galic (Syngenta Crop Protection), Roman Ashauer (Syngenta Crop Protection AG and University of York)

## INTRODUCTION

- Aquatic system modelling (ASM) complements empirical approaches to higher-tier pesticide risk assessment, but past applications to mesocosm studies are rare.

**KEY QUESTION: How well can an AQUATOX ecosystem model represent a biological community in a mesocosm system?**

- Four separate teams developed different models of a small artificial pond (i.e., a mesocosm), experimentally treated with an agricultural fungicide.
- We developed an ecosystem model within the USEPA-sponsored AQUATOX software (Figure 1) with 28 biota representing either species or functional groups.
- A calibration of the model to control mesocosm data by manually adjusting biological parameters resulted in a reasonable visual "fit" of simulated biota trajectories to observed study data.
- Here we describe a semi-automated calibration of the model to exposure data from the fungicide-treated mesocosms.

## METHODS

- Three months of study data for pesticide-treated mesocosms
- Adjusted LC/EC$_{50}$ of 2 biota (Cyclopidae, Daphniidae) with clear observed effects and 2 biota (Diatom Phytoplankton, Diatom Periphyton) with large differences between modelled and observed outcomes
- Supervised uncertainty evaluation using both statistical and mechanistic approaches
    - Series of Monte Carlo (MC) simulations generated by sampling distributions for dose-response parameter (i.e., LC/EC$_{50}$) values using a Latin Hypercube Design.
    - Simulation outputs from one MC series manually used to determine sampled parameter ranges for next MC series.
    - Criteria: Average Mean Error (AME) between modelled and measured biomass data on corresponding sample days
        - Mean Error per biota, day= abs (%effect$_{observed}$ - %effect$_{simulated}$)
        - AME = average (Mean Error per all biota, over all days)
    - Final calibration values selected through hierarchical process
- Model performance evaluated with calibrated LC/EC$_{50}$ values

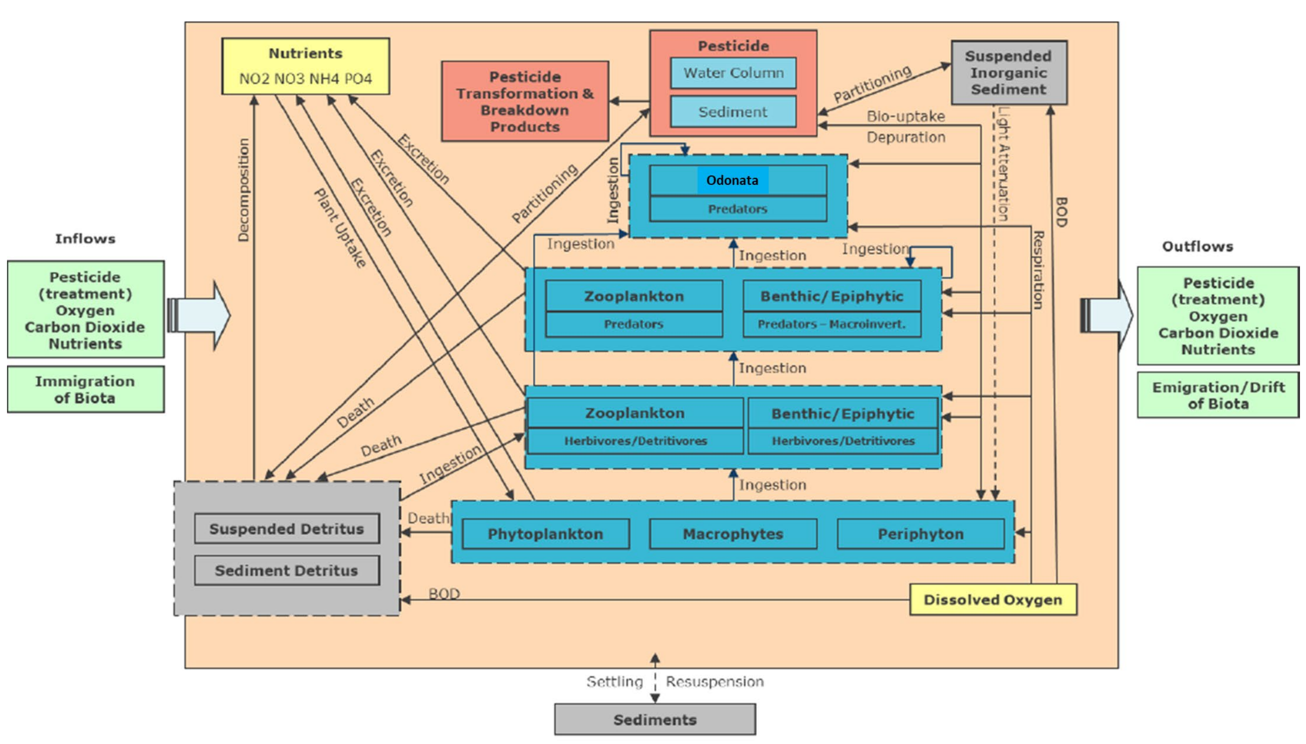


**Figure 1.** Conceptual representation of AQUATOX mesocosm model. Each biotic compartment contains species and/or functional groups.

## RESULTS

Best calibration values for LC/EC$_{50}$:

- Predatory Copepods (Cyclopidae): 9.55 ug/l
- Daphniidae: 35.67 ug/l
- Diatom Phytoplankton: 31.90 ug/l
- Diatom Periphyton: 120 ug/L†

**Legend**

- = Lower than default data
- = Higher than default data

† Manually adjusted outside of MC-process

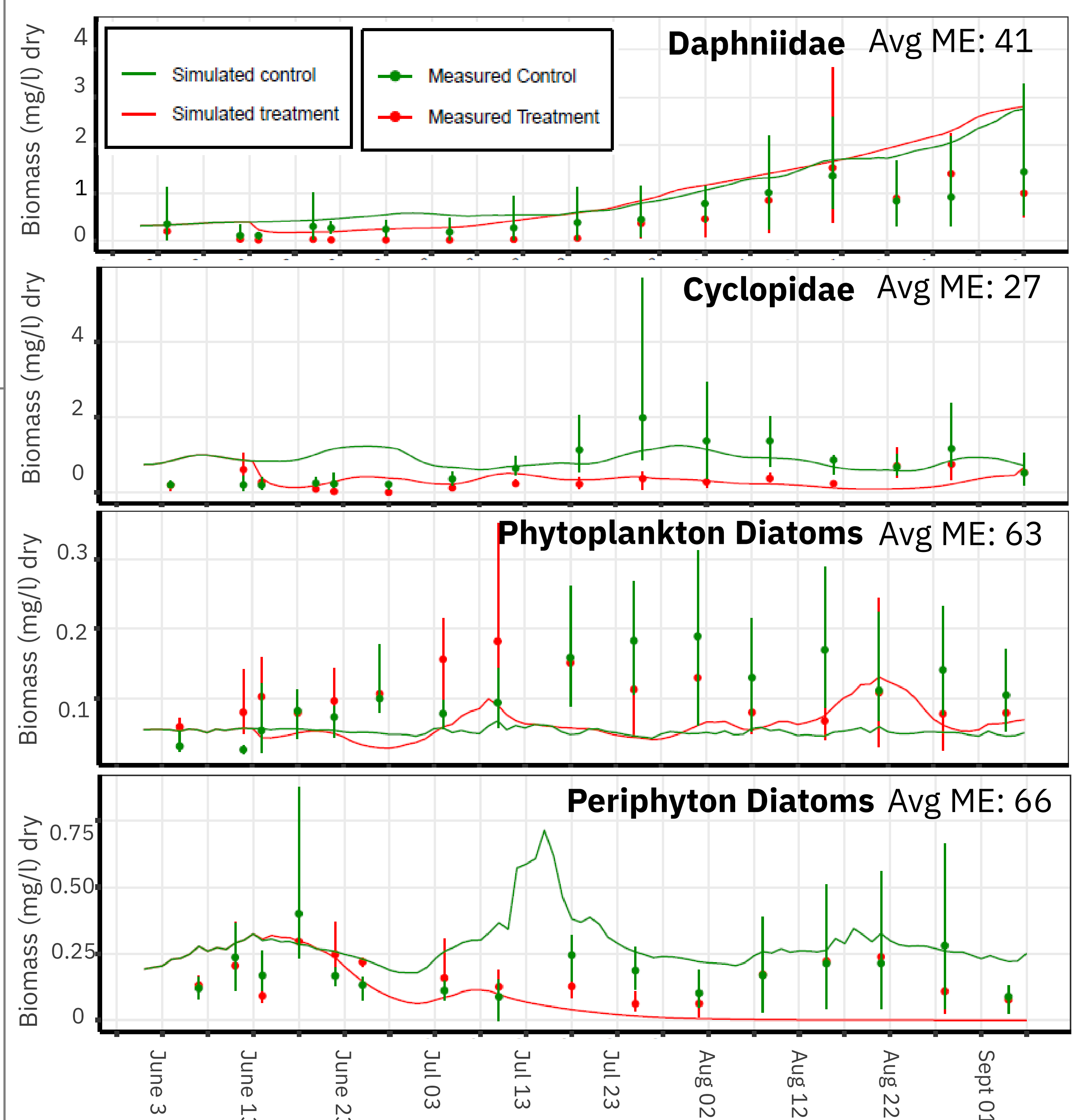


**Figure 2:** Modeled versus observed biomass for species adjusted by calibration. Note that the periphyton diatom group EC50 was manually adjusted outside the MC approach. Patterns of population trajectory and quantitative measures of effect size differences (AME) show that the model reasonably captured the pesticide effects.

## DISCUSSION

- It is critical to establish the credibility of aquatic system modelling in representing ecological processes and outcomes, especially if it is to be used for regulatory risk assessment.
- Automated and hybrid approaches to calibration/validation allow both uncertainty and professional judgement to inform the calibration process.
- The AQUATOX model was able to reasonably reproduce observed patterns for some biota, especially those with calibrated LC/EC$_{50}$ values.
- Some biota were **poorly** captured by the model, likely due to poor fits during control calibration because of high inter-annual variation, and high variability between replicates.
- Better alignment of study sampling designs with model design and data needs may lead to better replication of mesocosm systems by aquatic system modelling.