

ECOTOX TOOLBOX

User's Manual

v. 1.0

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July 12, 2026

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1. OVERVIEW

1.1 Toolbox Summary

The EcoTox Toolbox (the Toolbox) is an R Shiny application for modeling the bioavailability, bioaccumulation and effects of environmental stressors with a focus on inorganic stressors. Currently, the Toolbox has a model applicable to Al but additional models will be added in the near future:

1. Aluminum

- **Chronic *Ceriodaphnia dubia* Al MLR Model:** A multiple linear regression (MLR) bioavailability model that accounts for the effects of hardness, dissolved organic carbon (DOC), and pH on Al bioavailability and predicts effects of Al on *C. dubia* reproduction (DeForest et al., 2020).

This manual provides information on online access, Toolbox organization and capabilities, example user workflows, a technical overview of each model, and details on the underlying equations and parameterization of each Tool.

2. ACCESS TO THE TOOLBOX AND CITATION

The EcoTox Toolbox is an R shiny app that can be freely accessed via the EcoTox LLC website (<https://www.ecotoxllc.com>). If you have any issues with access or app functionality at any time, please contact the Toolbox administrator (KevinBrix@EcoTox.onmicrosoft.com).

If you use the Toolbox to support analyses in reports or peer reviewed publications, please consider citing it:

Brix, K.V. 2026. EcoTox Toolbox, v1.0. EcoTox LLC, Miami, Florida

As mentioned, access to the Toolbox is free and the only thing being requested in return is to fairly cite it's use. Additionally, if the Tool being used is a direct adaptation of a model from the peer-reviewed literature, please cite the primary source for the model as well to properly acknowledge the scientists that developed the model.

3. OVERVIEW OF TOOLBOX WORKFLOWS

3.1 Selecting a Stressor and Tool from the Toolbox

When the Toolbox opens you will see a **Title Page** that includes information on the appropriate citation when the Toolbox is used in reports or papers. You can then navigate to the **Main Page** (or any of the other pages) by clicking on the tabs in the top toolbar. On the left-hand side of the **Main Page** is a sidebar user interface (UI). The first option is a dropdown window that allows you to **Select Stressor** (currently only Aluminum). Depending

on the stressor selected, different stressor-specific options appear below to **Select Tool**. Depending on the Tool selected additional dropdown windows may appear that allow you to navigate to the specific model you are interested in using. The remainder of Section 3 provides information on general workflows for each of the tools. Details on the technical basis for specific tools are provided in subsequent sections.

3.2 *Ceriodaphnia dubia* MLR Model - Aluminum

The *C. dubia* Al MLR model allows you to estimate effects on *C. dubia* reproduction while also accounting for the effects of hardness, pH, and DOC on Al bioavailability (DeForest et al., 2020). In the left sidebar UI, users will see two **Input Modes** to run the model; **Single Sample** and **Upload Excel File**. In single sample mode, enter hardness (mg L⁻¹ as CaCO₃), pH (standard units), and DOC (mg L⁻¹) concentrations into the windows in the sidebar and press Run Model. Results will be provided in a Model Outputs table. Results can be exported as an Excel file via the Download Results button. Upload Excel File mode allows the user to import data for multiple samples and run them through the model simultaneously. A Download Import Template button allows you to export a data import template. Once data are entered click Browse and select the import file for analysis. You will see summary information on the import in **Input Summary**. It is **critical** to carefully review the data you have uploaded from a file before running the model to ensure it has properly loaded. Once you are satisfied, press **Run Model** and results will be plotted in the figure. The **X-axis Selector** allows you to plot the data as a time series (**Date**) or by **Site ID** which plots data using sites as a categorical variable. For both options, multiple sites can be plotted on the same figure. **Download Results** allows the user to export an Excel file with model inputs and results in tabular form. You can also export figures as png files. If you place the cursor in the upper right-hand corner of each plot, it will activate a series of controls to change your view of a specific plot. Clicking the camera image allows you to export the png file to any location you want.

Note that when you run the model you will see a green indicator saying the results are current. If you then change the data inputs, you will see this indicator turn yellow and state that inputs have changed and data export options have been disabled until the model is run again. This prevents accidental paired export of model outputs from one data set and model inputs from a data set subsequently loaded into the app but without the model being run again. The model also has guardrails establish to prevent predictions outside the environmental conditions over which it was parameterized.

4. TECHNICAL OVERVIEW OF MODELS

This section provides a technical overview of the models in the EcoTox Toolbox.

4.1 *Ceriodaphnia dubia* Chronic Al MLR Model

The *Ceriodaphnia dubia* chronic MLR model for Al predicts the EC20 for *C. dubia* reproduction while taking into account the effects of hardness, pH, and DOC on Al bioavailability. Data from 30 chronic *C. dubia* tests were used to develop the model using ln-transformed data. Several different model forms were evaluated in DeForest et al. (2020) with the final selected model having the general form:

$$\ln(EC20) = a + b \times \ln(DOC) + c \times pH + d \times \ln(Hard) - e \times \ln(Hard) \times pH$$

where, EC20 is the total Al concentration ($\mu\text{g L}^{-1}$) causing a 20% effect on *C. dubia* reproduction, and DOC (mg L^{-1}), pH, and hardness (mg L^{-1} as CaCO_3) represent the water quality conditions at which the EC20 is being estimated. The EC20, DOC, and hardness are ln-transformed in the model but both inputs and outputs are provided as untransformed data.

The *C. dubia* MLR parameterization is summarized below (Table 1).

Table 1. Summary of *C. dubia* MLR Parameterization

Parameter	<i>C. dubia</i>
Intercept	-9.272
ln DOC	0.619
pH	2.021
ln Hardness	2.581
ln Hardness x pH	-0.307
Adj. R ²	0.91
Predicted R ²	0.89

5. REFERENCES

DeForest, D.K., Brix, K.V., Tear, L.M., Cardwell, A.S., Stubblefield, W.A., Nordheim, E., Adams, W.J., 2020. Updated multiple linear regression (MLR) models for predicting chronic aluminum toxicity to freshwater aquatic organisms and development water quality guidelines. *Environ. Toxicol. Chem.* 39, 1724-1736.