

TRACE Document

This is a TRACE document ("TRANSPARENT and Comprehensive model Evaluation") which provides supporting evidence that our model presented in:

C. Accolla , A. Schmolke, A. Jacobson, C. Roy, V. E. Forbes, R. Brain, N. Galic
Modeling pesticide effects on multiple threatened and endangered Cyprinid fish
species: the role of life-history traits and ecology

was thoughtfully designed, correctly implemented, thoroughly tested, well understood, and appropriately used for its intended purpose.

The rationale of this document follows:

Schmolke A, Thorbek P, DeAngelis DL, Grimm V. 2010. Ecological modelling supporting environmental decision making: a strategy for the future. *Trends in Ecology and Evolution* 25: 479-486.

and uses the updated standard terminology and document structure in:

Grimm V, Augusiak J, Focks A, Frank B, Gabsi F, Johnston ASA, Kułakowska K, Liu C, Martin BT, Meli M, Radchuk V, Schmolke A, Thorbek P, Railsback SF. 2014. Towards better modelling and decision support: documenting model development, testing, and analysis using TRACE. *Ecological Modelling*

and

Augusiak J, Van den Brink PJ, Grimm V. 2014. Merging validation and evaluation of ecological models to 'evaluation': a review of terminology and a practical approach. *Ecological Modelling*.

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1 Problem formulation

This TRACE element provides supporting information on: The decision-making context in which the model will be used; the types of model clients or stakeholders addressed; a precise specification of the question(s) that should be answered with the model, including a specification of necessary model outputs; and a statement of the domain of applicability of the model, including the extent of acceptable extrapolations.

The goal of this project is to develop, implement and evaluate a population model representing a set of fish species. In particular, we focus on listed species belonging to the family of Cyprinidae. The model is based on Dynamic Energy Budget (DEB) theory (Kooijman, 2010), which describes the energy flow within an individual organism, and is developed for risk assessment purposes. Our model is modular, and can be applied to multiple species of Cyprinidae taking into account differences on environmental drivers (e.g. temperature and diet), and on life cycles (e.g. reproduction strategies, stage-specific survival rates). For the purposes of this study, we primarily focused on four species of Cyprinidae: Humpback chub, Spikedace, Devils River minnow and Topeka shiner. As a case study, we represent the population-level effects of chlorothalonil exposure. Chlorothalonil is a broad-spectrum fungicide that has effects on fishes, invertebrates and plants. Therefore, it affects fish directly (lethal and sub-lethal effects), and indirectly through a decrease of food availability. We use chronic studies on the fathead minnow (FHM) to model effects on fish survival, reproductive efficiency, and hatching success (Schults et al., 1980; Yellowlees, 2016). We use data on invertebrates to calculate exposure-driven food depletion (see table 12)).

The model can be easily modified to represent other species of Cyprinidae and different exposure scenarios, resulting in a powerful tool to explore the effects of chemical exposure on listed species.

2 Model description - ODD: Overview, Design concepts, Details

This TRACE element provides supporting information on the model. It provides a detailed written model description. For individual/agent-based and other simulation models, the ODD protocol is recommended as standard format. For complex submodels it should include concise explanations of the underlying rationale. Model users should learn what the model is, how it works, and what guided its design.

Summary:

Here we present the complete model description following the ODD (Overview, Design concepts, Details) designed for describing individual-based models.

The model description follows the ODD protocol (Grimm et al., 2020). The model was implemented in Netlogo. The code is available in supplemental material.

2.1 Purpose and patterns

The purpose of the model is to represent the population dynamics of multiple listed fish species, and to estimate the population-level effects of time-variable exposures under realistic habitat conditions. At the individual level, the metabolic processes are based on the Dynamic Energy Budget (DEB) theory (Figure 1, Kooijman 2010), and are driven by temperature and resource availability. Population dynamics emerge from individual interactions and is affected by environmental stochasticity. Chemical effects are based on laboratory data and take into account relevant effect endpoints, such as fish mortality, hatching success, egg production, and decrease of food availability.

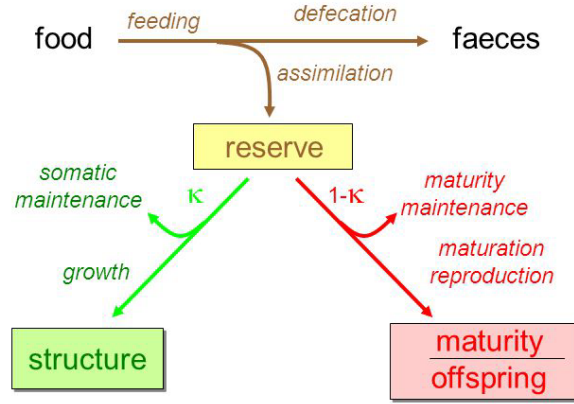


Figure 1: Schematic representation of the DEB model. Energy enters the organism through the feeding process. Part of it is assimilated into the reserve, which acts as an energy buffer. The rest is lost with defecation. A fixed fraction, κ , of the assimilated energy is then allocated to growth and somatic maintenance, whereas the fraction $1 - \kappa$ goes to maturity maintenance and maturation or, once the organism reaches puberty, reproduction.

2.2 Entities, state variables and scales

Entities in the model are individuals and their environment. We do not model males and females separately. Each species is characterized by a species-specific set of DEB-parameters and mortality rates. The individuals are represented by four state variables, defined within DEB theory:

1. structure, expressed as length L [cm];
2. scaled reserve, U_E [$d \text{ cm}^2$], which serves as an intermediate storage of energy between feeding and mobilization;
3. scaled maturity, U_H [$d \text{ cm}^2$], which regulates transitions between the three developmental stages (embryo, juvenile, adult);
4. cumulative reproduction, U_R [$d \text{ cm}^2$], expressed as a scaled buffer of energy that is converted into eggs during reproduction events ;

The scaled values of U_H^b , U_H^j and U_H^p are given by the parametrized values E_H^b , E_H^j , E_H^p divided by $\{p_{Am}\}$.

In addition, individuals are characterized by their age in days [d] and by the number of eggs they produce in each reproduction season [#]. Environment is defined by two forcing variables: the temperature profile [$^{\circ}\text{C}$] and the amount of resource [J] (see 2.7 and 2.6).

Time is represented continuously (ordinary differential equations). However, the model implementation is based on discrete time steps set at 1 (daily time step) or 24 (hourly time step) depending on the species. The choice depends on how accurately the model captures the switches linked to scaled maturity U_H . Moreover, some procedures are run with a smaller time step (egg production and GUTS model). The model is not spatially explicit.

Table 1: Dimensions

-	no dimension	L	length (individual)	e	energy
t	time	l	length (environment)	T	temperature
#	number	m	mass		

Table 2: State variables

DEB notation	Interpretation	Dimensions	Code notation
U_E	Scaled reserve	tL^2	U_E
U_H	Scaled maturity	tL^2	U_H
U_R	Reproduction buffer	tL^2	U_R
L	Volumetric structural length	L	L

2.3 Process Overview and scheduling

The model represents the agents (fish) and their environment. At the beginning of each day, temperature, resource, chemical exposure and density-dependent embryo mortality values are defined. If the simulated year is stochastically defined as a dry year, an extra mortality is applied to those individuals that are younger than 1 year old. The age of the individuals is updated if needed, and their metabolic fluxes calculated at each time step following the DEB equations. DEB theory assumes that biomass is divided into structure, which requires maintenance, and reserve, which can fuel metabolic processes and does not require maintenance. Structural biomass is expressed through the structural length, L :

$$L = l_m \cdot \delta_m \quad (1)$$

where l_m is the measured length and δ_m is the shape coefficient. Structural length determines the actual size of the organism, as well as the processes of feeding and somatic maintenance: feeding rate is proportional to the surface area of the individual and scales with L^2 , whereas maintenance costs are proportional to L^3 . The wet weight of the organism is given by:

$$W_w = L^3 + \left(U_E \{ \dot{p}_{Am} \} + U_R \{ \dot{p}_{Am} \} \right) \frac{\omega_E}{d_E \mu_E}. \quad (2)$$

Part of the energy ingested with food is assimilated into the reserve compartment, from which it is mobilized for the needs of the organism. A fraction κ of this energy is used for growth and somatic maintenance (sections 2.7.2 and 2.7.5). The remaining $1 - \kappa$ energy goes to increase maturity and to maturity maintenance. Maturity specifies the development status of the individual and maturity maintenance is proportional to the level of maturity. Once the organism reaches puberty, the energy previously allocated to maturation fuels reproduction (egg formation) (section 2.7.3). Somatic and maturity maintenance have priority over growth and maturation/reproduction.

We use a variation of the standard DEB model: the *abj* model. The *abj* model is a general model used to represent the life cycle of fish, which takes into account the metabolic acceleration that occurs in early life stages (Kooijman and Lika, 2014). This acceleration in growth is called "type M", and takes place during a short period of time starting at birth and ending before puberty (at a transition called "metamorphosis"

in DEB theory). During this time, fish are considered as V1-morphs: their shape changes during growth, and their assimilation surface is proportional to their volume V^1 . Before and after acceleration, organisms are considered to be isomorph as in the standard DEB model (that is, the organism does not change its shape during growth, and the surface is proportional to $V^{2/3}$). To take into account this modification, we apply to $\{p_{Am}\}$, $\{F_m\}$ and \dot{v} a shape correction function (section 2.7.8).

Individual state variables are updated based on a set of differential equations. The implementation follows Martin et al., 2012. Reproduction and death are discrete events. Death after birth can occur because of background mortality, density dependence (among eggs and larvae), droughts or chemical exposure. Moreover, only a fraction of spawned eggs survive (section 2.7.7). Reproduction is a discrete event and happens once a year during the reproduction period (section 2.7.4).

If the organisms are exposed to the chemical, lethal and sub-lethal effects are evaluated (section 2.7.9).

Since the species are listed, data about population sizes are rare. Our goal was to compare species-specific population dynamics with and without chemical stressors, therefore population sizes have been adjusted in order to have a stable dynamics without exposure.

The following pseudo-code describes the scheduling process. State variables are updated at the end of each time step.

Setup initial conditions (parameter values, environmental properties)

At the beginning of each day

Setup the day of the year

If the day is 366 (end of the year)

→ define if the next year is a "bad" year for recruitment

→ If chemical-exposure module is on, upload chemical-exposure data for the next year

Calculate temperature and temperature correction factor.

Update resource

If the day is the birthday of an agent → increase its age of one year

If there is density-dependence (DD) → calculate DD-embryo mortality

If chemical-exposure module is on → read chemical-exposure values for the current day and calculate mortality thresholds.

At each time step

Calculate the shape correction function (abj model)

Calculate change in reserve

Assimilation and decrease the resource available of the amount of eaten food

Mobilization

If not mature → Calculate change in maturity

If mature → Calculate change in reproduction buffer

If enough energy to reproduce and reproduction conditions are met → Reproduce

Calculate energy investment for offspring (bisection method)
If chemical-exposure module is on → calculate sub-lethal effects on reproduction
Create new offspring
If chemical-exposure module is on → calculate morality thresholds on new hatched individuals
If density-dependent module is on → calculate density-dependent mortality on embryos
If chemical-exposure module is on → Implement the GUTS model on juveniles and adults, the GUTS model for hatching on embryos, and the TKTD model (sub-lethal effects on reproduction)
Calculate change in Length
Calculate background mortality
Update variables and plots

2.4 Design concepts

Basic principles

Key processes in the model are based on Dynamic Energy Based theory (Kooijman, 2010), which aims to capture the quantitative aspects of metabolism. It is explicitly based on the principles of conservation of energy and matter. Environmental fluctuations are represented through food oscillations, temperature variability, and stochastic drought events. Eggs and larvae (embryo stage in DEB) experience density dependence. The chemical effects are modeled by representing (i) lethal effects on embryos, juveniles and adults (GUTS models), (ii) sub-lethal effects describing a decrease of reproduction efficiency (TKTD model), and (iii) a decrease on the food function (indirect effects).

Emergence

Population dynamics emerges from the interactions between environmental rules, density dependence, stressors and DEB equations.

Adaptation, Objectives, Learning, Prediction, Sensing

The model does not include adaptive behavior nor decision making scenarios; in particular, DEB parameters vary among individuals but remain constant over an individual's lifespan. There are not learning processes, predictions capabilities or sensing-based decisions.

Interaction

Individuals interact through density-dependent mortality and, if chemical-related indirect effects apply, intra-specific competition for food.

Stochasticity

Stochastic processes are: the background mortality, the allocation of the chemical tolerance threshold of each individual, the definition of bad recruitment years, the decrease in recruitment during the bad years, and the scatter added to some of the DEB parameters. This scatter is implemented by applying a small variation to the parameter $\{\dot{p}_{Am}\}$, that is the maximum assimilation efficiency per unit of surface, following the method outlined in Kooijman et al., 2018 and implemented by Martin et al., 2012. Since $\{\dot{p}_{Am}\}$ is used to calculate other parameters ($\{j_{XAm}\}$, $[E_m]$, $\{\dot{p}_{XAm}\}$, g , L_m), the variability will be extended to them, as well as to $U_{H^b}^b$, $U_{H^j}^j$ and $U_{H^p}^p$. The scatter term is the realization of a log-normal distribution of mean 0 and standard deviation 10%.

Collectives

We do not simulate any kind of aggregation.

Observation

Several plots are produced by the model. One plot shows the exposure profile. Two figures represent the population size over time with or without exposure. Two other plots show the ratio between the average exposed population abundance over the average non-exposed population abundance for different exposure magnification factors (EMF) or for different modeled exposure sub-models. Averages are calculated over time (5 years of exposure) and over replicates. Another plot shows the population biomass averaged over the exposure years.

2.5 Initialization

Simulations are initialized in year one and on the first day of the reproduction period: day 90 for Spikedace, day 80 for Humpback chub, day 1 for Devils River minnow and day 150 for Topeka shiner (day 1 being January 1st). These days have been chosen in order to start during the reproductive period and create the initial cohort of individuals. This cohort of embryos is created using the bisection method (Martin et al., 2012). The initial number of individuals is 50. The values of DEB parameters are defined in the *add – my – pet* portal. Initial values for environmental parameters are shown in table 8.

2.6 Input data

We implement three different temperature profiles to represent the three modeled habitats: Little Colorado River (LCR) for chubs and daces, Devils River for the minnows, and Midwestern habitat for shiners (figure 2). The water temperature of the LCR is given by the daily average for the period 2015-2020 ([LCR temperature profile](#), US Geological Survey at the station ABV mouth NR desert view, AZ). Data on Devils River temperature are available only as monthly averages (Mcmillan, 2011). However, we found daily mean values sampled in a downstream warmer station of the Rio Grande River from 2011 to 2020 ([RG temperature profile](#), US Geological Survey at the station Rio Grande Village, TX). We corrected Rio Grande values by the difference between monthly average temperatures in the two sites (Rio Grande and Devils River). Finally, the temperature profile for the Midwestern habitat is based on the temperature profile implemented by Schmolke et al., 2019.

Since rates depend on temperature, some of the DEB parameters are corrected for temperature effects (Arrhenius correction). These are:

1. maximum surface area specific assimilation rate, $\{\dot{p}_{Am}\}$;
2. conductance rate, \dot{v} ;
3. volume specific maintenance rate, $[\dot{p}_M]$;
4. maturity maintenance coefficient, k_j .

The Arrhenius correction is given by the equation (3) (Kooijman, 2010):

$$C_T = \exp^{\frac{T_A}{T_{ref}} - \frac{T_A}{T}} \quad (3)$$

where T_A is the Arrhenius temperature, T_{ref} is a chosen reference temperature and T the actual absolute temperature.

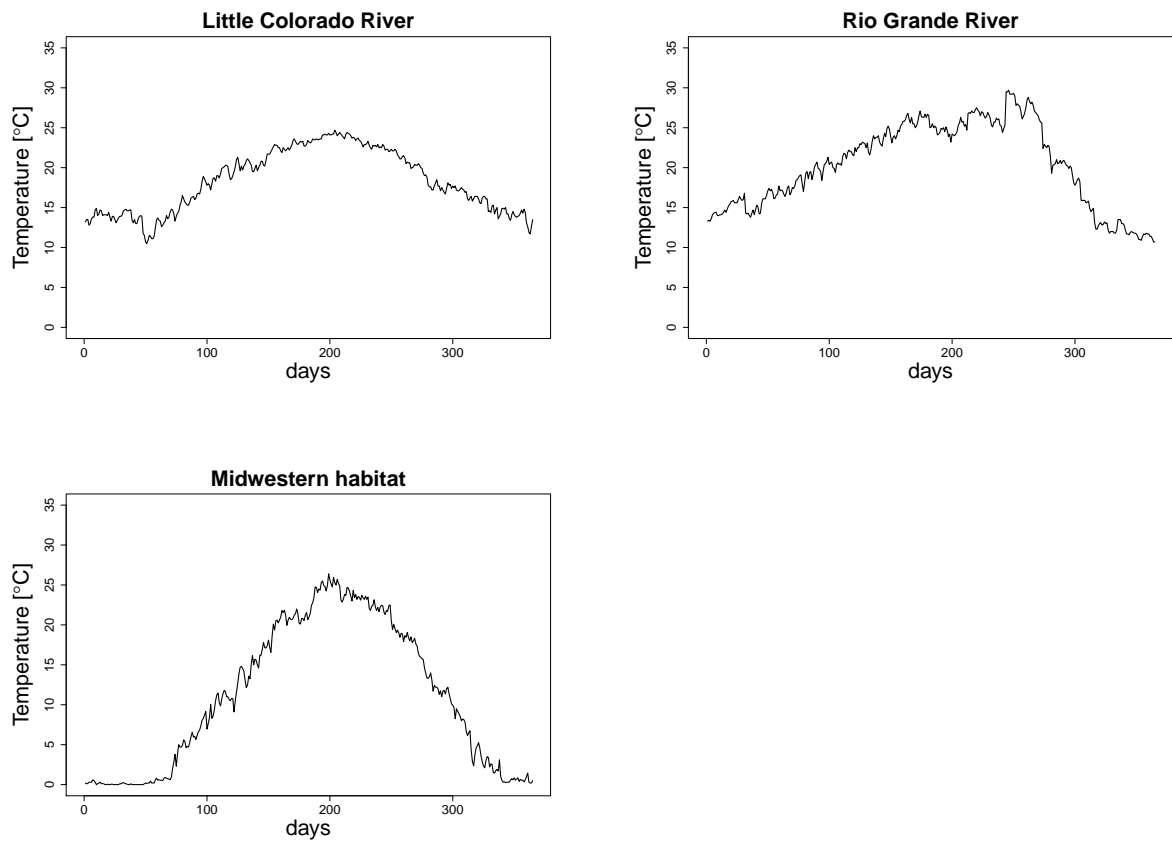


Figure 2: The three temperature profiles used for (a) Humpback chub and Spikedace, (b) Devils River minnow, and (c) Topeka shiner

2.7 Submodels

2.7.1 Resource dynamics

We consider three different diet functions for the three habitats. In the three cases, the resource, X , is represented by a generic sinus function that has one or two peaks, depending on the represented habitat:

$$\frac{dX}{dt} = r[K(\tau) - X] \quad (4)$$

where

$$\begin{cases} K(\tau) = X_{max} - \frac{X_{max} - X_{min}}{2} \left[1 + \left(\sin\left(\frac{\pi\tau}{Z} + \gamma\right) \right)^\theta \right], & 0 \leq \tau < Z \\ K(\tau) = X_{max} - \frac{X_{max} - X_{min}}{2} \left[1 - \left(\sin\left(\frac{\pi(\tau-Z)}{Y-Z} - \gamma\right) \right)^\theta \right], & Z \leq \tau < Y \end{cases} \quad (5)$$

X is the amount of resource (or food) in $[J]$, X_{max} and X_{min} are the maximum and minimum values between which the function oscillates, Z is the beginning of the growing season for food and Y is the number of days in a year. The parameter θ gives the steepness of the sinusoidal function, whereas γ translates the function on the x axis (time). The resource X_t is adjusted every time an individual eats (within the same time step):

$$X_t = X_t - X_{eaten} \quad (6)$$

$$X_{eaten} = S_{A_i} \cdot \frac{\dot{p}_{Am_i}}{\kappa_X} \frac{T_{corr}}{Vol * timestep} \quad (7)$$

where N is the total number of individuals, Vol is the space volume (1 in our case), κ_X is the assimilation efficiency and T_{corr} the temperature correction factor. Then, every time step the resource is updated:

$$X_{t+\Delta t} = X_t + dX \cdot dt \quad (8)$$

$$dX = r_* \cdot (K(\tau)X) \quad (9)$$

Finally, we do not allow the organisms to eat all the food: a part of it, called *limit*, is "invisible" to individuals. This prevents the depletion of all the resource.

2.7.2 Calculate delta energy reserve

The change in the scaled energy reserve U_E (with $U_E = E/\{p_A m\}$) of an individual is determined by the difference of the scaled assimilation and mobilization fluxes:

$$\frac{dU_E}{dt} = S_A - S_C. \quad (10)$$

The scaled assimilation S_A is given by:

$$S_A = fL^2 \quad (11)$$

where f is the scaled functional response (see later for more details)

$$f = \frac{x}{1+x} \quad (12)$$

$$x = \frac{X - limit}{K_{ind}}. \quad (13)$$

Therefore, $f = 1$ represents an *ad libitum* feeding scenario. If $U_H < U_H^b$ (before birth), then $f = 0$. In this case, the change in reserve will be defined only by the mobilization flux:

$$\frac{dU_E}{dt} = -S_C. \quad (14)$$

The scaled mobilization flux is given by:

$$S_C = L^2 \frac{g^e}{g + e} \left(1 + \frac{L\dot{k}_M}{\dot{v}} \right) \quad (15)$$

where e is the scaled reserve density [-], g is the energy investment ratio [-] and \dot{k}_M is the somatic maintenance rate coefficient [t^{-1}]:

$$e = \frac{\dot{v}U_E}{L^3} \quad (16)$$

$$g = \frac{[E_G]}{\kappa[E_m]} \quad (17)$$

$$\dot{k}_M = \frac{[\dot{p}_M]}{[E_G]}. \quad (18)$$

2.7.3 Calculate delta maturity and delta reproduction buffer

Maturation represents the development of an individual that grows in complexity (immune system, reproductive system, etc.). In the unscaled model, this process is characterized by two thresholds: E_H^b , energy of birth, and E_H^p , energy of puberty. When the maturity E_H [J] reaches the value E_H^b , the individual ends its embryo stage to enter the juvenile stage and it starts eating. Puberty begins when $E_H = E_H^p$ and is characterized by the beginning of energy allocation to reproduction. E_H^p is also the maximum level of maturity: once reached, maturation stops and all the energy allocated to this branch is used for maturity maintenance and for reproduction.

In the scaled model, we work with the scaled maturity level $U_H = E_H / \{p_{Am}\}$ and the scaled energy allocated to reproduction $U_R = E_R / \{p_{Am}\}$, which are set to 0 at the beginning of an individual's life. These values change as follows:

$$\begin{cases} \frac{dU_H}{dt} = (1 - \kappa)S_C - \dot{k}_j U_H, & \frac{dU_R}{dt} = 0, & \text{if } U_H < U_H^p \\ \frac{dU_H}{dt} = 0, & \frac{dU_R}{dt} = (1 - \kappa)S_C - \dot{k}_j U_H^p, & \text{if } U_H = U_H^p \end{cases} \quad (19)$$

2.7.4 Reproduction submodel

In DEB theory the reserve density of the offspring, at the moment of hatching, equals the reserve density of the mother at conception. The cost of producing an egg is U_0 [J], and the annual mean reproduction rate [t^{-1}] is:

$$\dot{R} = \frac{\kappa_R U_R}{U_0} \quad (20)$$

with κ_R [-] equal to the fraction of reproduction energy fixed in eggs.

Individuals can reproduce when they have enough energy to produce offspring with an initial energy density at hatching equal to the energy density of the mother at conception. To determine when an individual can reproduce, we run the bisection method once to estimate the energy of hypothetical eggs.

Each mature individual creates hypothetical eggs with the initial energy reserves set to the available energy in the reproduction buffer $\kappa_R U_R$ of the mother. The initial length of embryos is fixed small *a priori* (L_0 , see table 3). The embryonic period of the hypothetical offspring is then simulated until one of two conditions is met: (i) if the scaled reserve density (e) of the hypothetical offspring falls below that of the mother, then the simulation is stopped and the mother does not reproduce in that time step; (ii) if the hypothetical embryo reaches the energy needed for birth, then the mother reproduces in the current time step.

The next phase of the reproduction submodel is to determine the exact amount of energy a mother will invest in the eggs. This is determined numerically using the bisection method a second time. The initial bounds for the bisection method are set to 0 and $\kappa_R U_R$ of the mother. Simulations are run until the offspring e is within 5% of the mother's scaled reserves in the simulated time step, and when maturity hits the threshold for birth $U_H > U_H^b$. Eggs are then created with initial reserves set to the estimation from the previous step. These eggs will hatch and thus begin exogenous feeding (Martin et al., 2012 ODD document).

DEB theory assumes that as soon as the organism has enough energy to produce one offspring, it does so. However, Cyprinidae usually reproduce in a precise period of time, which is late March-August, but usually stops in May for Humpback chub (Gorman and Stone, 1999, FWS), April-June for the Spikedace U.S. Fish and Wildlife Service, 1988, January-August for Devils River minnow (Hubbs et al., 2005), and May-July for Topeka shiner (Kerns and Bonneau, 2002). The spawning event happens in a different day for each individual, which is randomly chosen in the reproductive season. We implement spawning as a single event per year, as justified below, and consider species-specific differences in the spawning period:

- chubs can potentially spawn many times during the reproductive season, but data on the number of reproductive events and on clutch size are lacking. In LCR, spawning starts in late-March, peaks in mid-April, and wanes in mid-May (Gorman and Stone, 1999). In our model, the reproductive period is between day 80 and day 135.
- minnows can potentially reproduce multiple times during the spawning season. Some estimates of the clutch size exist (about 107-147 oocytes, Mcmillan, 2011), but they are not in agreement with DEB predictions (about 102 eggs in the whole year).

In the model, we implement reproduction as a one-year event to prevent having too small clutch sizes. The reproductive period is between day 1 and day 230.

- David L. Propst et al., 1986 reports that also daces reproduce mostly once during the spawning season. The reproductive period is usually April-June (U.S. Fish and Wildlife Service, 1988) or April-May (Gori et al., 2014). In the model, the reproductive period goes from day 90 to day 180.
- the reproductive period of shiners goes from May to July: Dahle, 2001 reports that reproduction takes place from the 15 of May to August 6. Similarly, Kerns and Bonneau, 2002 reports that reproduction happens from May 23 to July 31. In the model, the reproductive period goes from day 135 to day 212.

2.7.5 Calculate delta length

In DEB theory growth is possible only after all the maintenance costs have been paid. Maintenance processes include many processes such as maintenance of concentration gradients across membranes, protein turnover, a mean level of muscle tension, movement, production of hairs, feathers and maturity

maintenance. These processes require energy, and growth (as well as maturation/reproduction) happens only if there is any energy left. The equation for the delta length is:

$$\frac{dL}{dt} = \frac{1}{3} \left(\frac{\dot{v}S_C}{gL^2} - \dot{k}_M L \right). \quad (21)$$

2.7.6 Starvation

Death from starvation occurs because resources are limited and individuals indirectly interact through feeding competition. This density-dependent mortality is an emergent property. DEB theory takes into account four different patterns to represent starvation. The most common in animals such as fish implies that during prolonged starvation all the mobilization flux is diverted to pay maintenance. This corresponds to the third strategy described by Kooijman, 2010. Under this condition, $S_A = 0$ and therefore the reserve is depleted:

$$\frac{dU_E}{dt} = S_A - S_C = -S_C \quad (22)$$

If organisms face mild starvation for a relatively short period of time, there are no changes in the allocation rules. However, if the mobilized energy allocated to soma is not enough, growth is set to 0 and part of the energy allocated to maturation or reproduction is diverted to pay somatic maintenance. This happens when:

$$e < \frac{L}{L_m}. \quad (23)$$

L_m is the maximum length an individual can reach:

$$L_m = \frac{\dot{v}}{\dot{k}_M g} \quad (24)$$

If growth is set to 0, that means that (Kooijman, 2010):

$$\frac{dl}{dt} = \frac{dL}{dt} \frac{1}{L_m} = \frac{\dot{k}_M g}{3} \frac{e - l}{e + g} = 0. \quad (25)$$

Resolving equation (25) gives $e = l$. Knowing this condition and the relation (24), from equation (15) we obtain:

$$S_C = eL^2. \quad (26)$$

Moreover, from equation (21) it results that under starvation S_C is as follows:

$$\kappa S_C = \frac{\dot{k}_M \kappa g L^3}{\dot{v}}. \quad (27)$$

κS_C is the amount of mobilized energy needed to pay somatic maintenance. The rest can be allocated to maturation or reproduction:

$$energy_{available} = (1 - \kappa)energy_{mobilized} - \text{maturity maintenance} + \Delta(E) \quad (28)$$

$$\Delta(E) = energy_{mobilized} - (\text{energy needed to pay somatic maintenance}) \quad (29)$$

which leads to the expression:

$$\frac{dU_H}{dt} = (1 - \kappa)S_C - k_j U_H - \kappa L^2 \left(\frac{L}{L_M} - e \right), \quad \frac{dU_R}{dt} = 0, \quad \text{if } U_H < U_H^p \quad (30)$$

$$\frac{dU_R}{dt} = (1 - \kappa)S_C - k_j U_H^p - \kappa L^2 \left(\frac{L}{L_M} - e \right), \quad \frac{dU_H}{dt} = 0, \quad \text{if } U_H > U_H^p \quad (31)$$

Therefore, when starvation occurs, growth is set to 0 and we calculate again the energy for $\frac{dU_{H/R}}{dt}$. If $\frac{dU_H}{dt} < 0$ or $\frac{dU_R}{dt} < 0$, that is when maintenance costs cannot be paid, death occurs.

In the model the food level is high enough to avoid starvation in absence of the stressor. Therefore, starvation can occur only as a result of exposure (indirect effect, see section 2).

2.7.7 Mortality

There are four sources of mortality: background mortality, density-dependent mortality of embryos, reduced recruitment due to drought events, and mortality due to exposure (see 2.7.9).

1. Background mortality

Background mortality rates were applied stochastically in the model, using a uniform distribution. Mortality rates for eggs, adults and juveniles were adjusted during the model calibration and are reported in tables 4-7.

2. Density-dependent mortality

Cannibalism on eggs and larvae during the reproduction period is a common feature among different species of Cyprinidae (Campbell et al., 2016; Mills, 1981; Phillips, Gibson, and Fries, 2011). We implement density dependence as a Ricker function, assuming that survival of embryos decreases with increasing adult biomass as done in the model of Schmolke et al., 2019:

$$s_{egg}(B) = s_{egg}(0)e^{-\gamma B} \quad (32)$$

where B is the adult biomass and γ is the steepness of the function, and $s_{egg}(0)$ is the background mortality of eggs (see tables in section 2.8)

3. Drought-induced mortality

The modeled species are particularly affected by habitat degradation and droughts (Echo-Hawk and Garrett, 2015; Gori et al., 2014; U.S. Fish and Wildlife Service, 2002). Drought frequency and extent are simulated on the basis of data found in Christensen and Lettenmaier, 2007 and Udall and Overpeck, 2017 (see section 3). Brouder, 2001 used an empirical relationship to describe the recruitment of roundtail chub as a function of the maximum mean daily discharge in a defined year in the Verde River (Gila River basin):

$$\log_{10} Y = 0.601(\log_{10} X) - 1.288 \quad (33)$$

where Y is the mean CPUE (catch per unit effort) of age-1 roundtail chub in a defined year, and X is the maximum mean daily discharge in the previous year. We used this empirical equation to calculate the recruitment for flow values of 6.5 or 15 BCM, which give the result of 2.1 and 1.27, that is 19% and 11% of the mean CPUE of age-1 individuals in about 10 years (Brouder, 2001, figure 2(b)). In the model setup, we define a stochastic list (called *bad – year*) that has values between 1 and 25, and a variable

called $y - stoch$ that is set equal to 1. Once a year, we calculate the difference between the year and $y - stoch$. If this difference is equal to the first element of the list $bad - year$, then a drought event happens and an extra mortality is applied to those individuals that are younger than 1 year old. This extra mortality rate is randomly chosen between 81% and 89% (uniform distribution). Then, $y - stoch$ is set equal to the current year, the code reads the following item in the list $bad - year$ and the implementation is repeated. For example, if the first elements of $bad - year$ are [3, 10, 4, ...], a drought happens at year 4 of the simulation ($4 - 1 = 3$). Then, $y - stoch$ is set equal to 4, and the next low recruitment happens at the year 14 ($14 - 4 = 10$).

2.7.8 Shape and temperature corrections

Two corrections are needed. The first one is the multiplication by the *shape correction* function (sc). This function is equal to 1 for isomorph organisms, which are those individuals that do not change their shape during growth. Their surface is proportional to their volume to the power of $2/3$ ($V^{2/3}$). On the contrary, if shape changes during growth, two other morphisms are possible: V0-morphs (surface area proportional to V^0) and V1-morphs (surface proportional to V^1). Fishes have a unique life cycle and their growth shows an acceleration during a short period of time, between birth and puberty (called "metamorphosis" in DEB theory). During this time, they are considered as V1-morphs. From a mathematical point of view, this translates into a slight modification of DEB theory by multiplying the maximum specific assimilation rate ($\{\dot{p}_{Am}\}$), the specific searching rate ($\{\dot{F}_m\}$), the specific surface area-linked somatic maintenance rate ($\{\dot{p}_T\}$, equal to 0 in our model) and the energy conductance (\dot{v}) by sc .

$$sc = 1 \quad \text{if} \quad U_H < U_H^b \quad (34)$$

$$sc = \frac{L}{L_b} \quad \text{if} \quad U_H^b \leq U_H < U_H^j \quad (35)$$

$$sc = \frac{L_j}{L_b} \quad \text{if} \quad U_H \geq U_H^j \quad (36)$$

$$(37)$$

L_b and L_j are the lengths at birth and metamorphosis. In our code, this means that we have to multiply $\{\dot{J}_{XAm}\}$, $\{\dot{F}_m\}$, \dot{v} , S_A and S_C by the sc factor.

The second modification is the multiplication of the assimilation rate by the correction for temperature, T_{corr} . Every energy flow is influenced by this modification, since temperature affects all the metabolic rates. In our code, this means that dU_E , dU_H , dU_R , dL , $d\dot{q}$, $d\dot{h}$ are multiplied by the temperature correction factor.

2.7.9 Stressor effects

We represent direct and indirect effects due to exposure to chlorothalonil, a fungicide toxic for fish, invertebrates and plants. Data on effects of chlorothalonil were obtained from the report by Schults et al., 1980.

1. Direct effects

Lethal effects

Lethal effects are modeled using the General Unified Threshold model of Survival (GUTS), which is an accepted risk assessment refinement option for predicting survival based on standard lab experiments (Jager et al., 2011). The GUTS model is based on two steps: first the calculation of the internal chemical concentration of the individual, which changes dynamically; second the evaluation of the

internal concentration, to define if it is high enough to cause the individual's death. Because internal concentrations within the organisms were not measured in the study, we express the dynamics of the internal concentration or damage (D_i) as dependent of the external concentration in the water (C_w) through the dominant rate constant k_d :

$$\frac{dD_i}{dt} = k_d \cdot (C_w - D_i) \quad (38)$$

Once defined the internal concentration of the chemical, we can use two ways to represent individual death. In GUTS-IT, the individuals differ in their sensitivity to the chemical, or their "individual tolerance". The second approach considers mortality due to toxicant stress as a stochastic process. All individuals are equal, and death is stochastic. This approach is called SD, "stochastic death" (Jager and Ashauer, 2018). In the model, we implemented GUTS-IT to simulate lethal effects of pesticide exposure because it provided a better fit to available study data, with a smaller AIK value (645.48 vs 782.36) (figure 5 in section 6). The GUTS parameters used for chlorothalonil are derived by fitting the GUTS models to available data from laboratory toxicity studies conducted with fathead minnow (see section 6). This was done on Matlab, using the 2020 version of the code downloaded at <http://www.openguts.info/download.html>. Outputs of the GUTS fits that have been used as input in our model (implemented in NetLogo) are the parameters k_d (dominant rate of the reduced model), mw (median of the log-logistic distribution of thresholds), and Fs (spread factor of the thresholds distribution).

The threshold distribution describing the individual tolerance to damage is log-logistic. In the NetLogo code, each fish draws a threshold concentration from this distribution using the equation:

$$F(t) = \frac{1}{1 + \left(\frac{D_i}{mw}\right)^{-\beta}} \quad (39)$$

where mw is the median of the threshold distribution and β is the shape parameter (see table 9), calculated as

$$\beta = \frac{\log_{10} 39}{\log_{10} Fs}. \quad (40)$$

This draw is done at the beginning of the simulation, or after an egg is spawned during the simulation. The individual threshold value does not change during the whole life cycle. The GUTS-IT sub-model is applied in sub-daily time steps to achieve a monotonous function $\frac{dD_i(t)}{dt}$.

We consider effects on hatching as a decrease in survival between day 0 and day 4 (the time needed to hatch). A second GUTS-IT model is calibrated on the experimental data on hatching (generation F_1) from the same laboratory toxicity studies conducted with fathead minnow. Data on one control (solvent) are omitted. The procedure is the same as described for juvenile and adult mortality.

Sub-lethal effects

Reported sub-lethal effects concern a decrease in reproduction efficiency (Schults et al., 1980). Data show that the eggs per female of FHM are 95%, 20%, 11% and 2% of the eggs spawned in the control experiment when the fish is exposed to 1.4, 3, 6.5, and 16 $\mu\text{g/L}$ of chlorothalonil, respectively. We use these data and the results of the GUTS-IT fit for juveniles and adults to parametrize the following TKTD model:

$$\frac{dD_i}{dt} = k_d(C_{ext} - D_i) \quad (41)$$

$$s = \frac{1}{c_T}(D_i - c_0) \quad (42)$$

$$\kappa_R = (1 - s)\kappa_R \quad (43)$$

where D_i is the scaled damage (or scaled internal concentration), κ_R is the reproduction efficiency, s is the stress level, c_0 is the threshold, i.e. the no effect concentration, c_T is the tolerance gradient, that is the sensitivity to the toxicant at concentration levels above c_0 , and k_d is the dominant constant rate parametrized by the GUTS-IT fit (see [Lethal effects](#)). Parameter values are reported in table 11.

2. Indirect effects

Invertebrates are the major food items of most of the species of Cyprinidae (see section 3.1). Because chlorothalonil affects a wide range of organisms, including aquatic invertebrates, we expect that fish will also experience a decrease in food availability as a consequence of exposure. To represent the effects on invertebrates we used a collection of LC50 and EC50 values calculated for 19 different species exposed to chlorothalonil (table 12). These endpoints were mainly measured after 48-hour, with a couple of data points obtained after four days, one after a 24-hour and one after a 96-hour. We used these data to build an SSD (Species Sensitivity Distribution) and considered this function as a proxy of effect level. If $x\%$ of the species are above their LC50/EC50, then the food availability is reduced by the same $x\%$. To choose the right distribution, we used the SSD toolbox Version 1.0 developed by the EPA and fitted the data with six SSD functions: normal, logistic, triangular, Gumbel, Weibull, and Burr. The Weibull function had the best goodness of fit (highest p-value) and the second-lowest value of AIC (Akaike Information Criterion), just after the triangular distribution. Based on these results, we chose to represent the SSD curve with the Weibull function (which is continuous, on the contrary of the triangular distribution). Equation 4 gives the cumulative distribution function for the Weibull distribution.

$$CDF_W = 1 - \exp\left(-\left(\frac{x}{\lambda}\right)^k\right) \quad (44)$$

where x is the chemical concentration, λ and k are equal to 182.8936 and 1.081 respectively.

2.8 Tables

Table 3: Parameters that have the same values for the four species

DEB notation	Interpretation	Value	Dimensions	Code notation	Source
$\{F_m\}$	Surface area-specific maximum search rate	6.5	$t^{-1}l^3L^{-2}$	F_m	Kooijman, 2010
κ_X	Fraction of food energy fixed in reserve	0.8	-	$kappa_X$	Kooijman, 2010
κ_R	Reproduction efficiency	0.95	-	$kappa_R$	Kooijman, 2010
k_J	Maturity maintenance rate coefficient	0.002	t^{-1}	k_J	Kooijman, 2010
T_A	Arrhenius temperature	8000.0	T	T_A	AddMyPet (see species tables)
s_G	Gompertz stress coefficient	0.0001	-	s_G	AddMyPet (see species tables)
L_0	Structural length at embryo formation	0.0001	L	L_0	Martin et al., 2010
T_{ref}	Reference temperature	293.15	T	T_ref	Kooijman, 2010
d_E	Specific density of reserve	0.2	mL^{-3}	d_E	Kooijman, 2010
μ_E	Chemical potential of reserve	550000	$e\ mol^{-1}$	mu_E	Kooijman, 2010
ω_E	Molecular weight of reserve	23.9	$m\ mol^{-1}$	$omega_E$	Kooijman, 2010
μ_X	Chemical potential of food	525000	$emol^{-1}$	mu_X	Kooijman, 2010

Table 4: Parameters values for Topeka shiner

DEB notation	Interpretation	Dimensions	Code notation	Value TS	Source
κ	Fraction of energy allocated to soma	-	<i>kappa</i>	0.96612	Kooijman and Augustine (2020)
$\{p_{Am}\}$	Surface-area specific maximum assimilation rate	$eL^{-2}t^{-1}$	<i>pA_m_surf</i>	262.651	Kooijman and Augustine (2020)
\dot{v}	Energy conductance	Lt^{-1}	<i>v</i>	0.025042	Kooijman and Augustine (2020)
$[p_M]$	Volume-specific maintenance rate	$eL^{-3}t^{-1}$	<i>pM_vol</i>	295.649	Kooijman and Augustine (2020)
U_H^b	Scaled maturity at birth	tL^2	<i>Ub_h</i>	9.78e-5	Kooijman and Augustine (2020)
U_H^j	Scaled maturity at metamorphosis	tL^2	<i>Uj_h</i>	1.4278	Kooijman and Augustine (2020)
U_H^p	Scaled maturity at puberty	tL^2	<i>Up_h</i>	0.5863	Kooijman and Augustine (2020)
$[E_G]$	Volume-specific cost of growth	eL^{-3}	<i>E_G_vol</i>	5237.44	Kooijman and Augustine (2020)
δ_m	Shape correction factor	-	<i>del_M</i>	0.18706	Kooijman and Augustine (2020)
z	Zoom factor	-	<i>z</i>	0.85829	Kooijman and Augustine (2020)
<i>lifespan</i>	maximum age	days	<i>lifespan</i>	1095	Kooijman and Augustine (2020)
Code notation	Interpretation	Dimensions	Value TS		Source
<i>egg - survival</i>	Survival rate for eggs	t^{-1}	0.085		This study
<i>juvenile - mortality - rate</i>	Juvenile mortality rate	t^{-1}	0.004		This study
<i>adult - mortality - rate</i>	Adult mortality	t^{-1}	0.0025		This study
<i>gamma_dd_egg_survival</i>	Coef for DD function	g^{-1}	0.25		This study
<i>DailySurvival_Egg_Larva0</i>	embryo survival rate for DD	t^{-1}	1		This study
<i>area</i>	area in which DD occurs	m^2	1000		This study

Table 5: Parameters values for Devils River minnow

DEB notation	Interpretation	Dimensions	Code notation	Value DRM	Source
κ	Fraction of energy allocated to soma	-	<i>kappa</i>	0.95841	Augustine (2020)
$\{p_{Am}\}$	Surface-area specific maximum assimilation rate	$eL^{-2}t^{-1}$	<i>pA_m_surf</i>	52.4104	Augustine (2020)
\dot{v}	Energy conductance	Lt^{-1}	<i>v</i>	0.020708	Augustine (2020)
$[p_M]$	Volume-specific maintenance rate	$eL^{-3}t^{-1}$	<i>pM_vol</i>	45.31	Augustine (2020)
U_H^b	Scaled maturity at birth	tL^2	<i>Ub_h</i>	0.0061	Augustine (2020)
U_H^j	Scaled maturity at metamorphosis	tL^2	<i>Uj_h</i>	0.0062	Augustine (2020)
U_H^p	Scaled maturity at puberty	tL^2	<i>Up_h</i>	0.8128	Augustine (2020)
$[E_G]$	Volume-specific cost of growth	eL^{-3}	<i>E_G_vol</i>	5235.66	Augustine (2020)
δ_m	Shape correction factor	-	<i>del_M</i>	0.1627	Augustine (2020)
z	Zoom factor	-	<i>z</i>	1.1086	Augustine (2020)
<i>lifespan</i>	maximum age	days	<i>lifespan</i>	730	Augustine (2020)
Code notation	Interpretation	Dimensions	Value DRM		Source
<i>egg - survival</i>	Survival rate for eggs	t^{-1}	0.3		This study
<i>juvenile - mortality - rate</i>	Juvenile mortality rate	t^{-1}	0.004		This study
<i>adult - mortality - rate</i>	Adult mortality	t^{-1}	0.0025		This study
<i>gamma_dd_egg_survival</i>	Coef for DD function	g^{-1}	0.1		This study
<i>DailySurvival_Egg_Larva0</i>	embryo survival rate for DD	t^{-1}	1		This study
<i>area</i>	area in which DD occurs	m^2	1000		This study

Table 6: Parameters values for Humpback chub

DEB notation	Interpretation	Dimensions	Code notation	Value HC	Source
κ	Fraction of energy allocated to soma	-	<i>kappa</i>	0.97579	Augustine (2020)
$\{\dot{p}_{Am}\}$	Surface-area specific maximum assimilation rate	$eL^{-2}t^{-1}$	<i>pA_m_surf</i>	244.101	Augustine (2020)
\dot{v}	Energy conductance	Lt^{-1}	<i>v</i>	0.020708	Augustine (2020)
$[\dot{p}_M]$	Volume-specific maintenance rate	$eL^{-3}t^{-1}$	<i>pM_vol</i>	105.962	Augustine (2020)
U_H^b	Scaled maturity at birth	tL^2	<i>Ub_h</i>	5.846e-4	Augustine (2020)
U_H^j	Scaled maturity at metamorphosis	tL^2	<i>Uj_h</i>	0.0112	Augustine (2020)
U_H^p	Scaled maturity at puberty	tL^2	<i>Up_h</i>	49.1191	Augustine (2020)
$[E_G]$	Volume-specific cost of growth	eL^{-3}	<i>E_G_vol</i>	5200	Augustine (2020)
δ_m	Shape correction factor	-	<i>del_M</i>	0.14848	Augustine (2020)
z	Zoom factor	-	<i>z</i>	2.2479	Augustine (2020)
<i>lifespan</i>	maximum age	days	<i>lifespan</i>	1825	Augustine (2020)
Code notation	Interpretation	Dimensions	Value HC		Source
<i>egg - survival</i>	Survival rate for eggs	t^{-1}	0.1		This study
<i>juvenile - mortality - rate</i>	Juvenile mortality rate	t^{-1}	0.004		This study
<i>adult - mortality - rate</i>	Adult mortality	t^{-1}	0.0025		This study
<i>gamma_dd_egg_survival</i>	Coef for DD function	g^{-1}	0.005		This study
<i>DailySurvival_Egg_Larva0</i>	embryo survival rate for DD	t^{-1}	1		This study
<i>area</i>	area in which DD occurs	m^2	1000		This study

Table 7: Parameters values for Spikedace

DEB notation	Interpretation	Dimensions	Code notation	Value SD	Source
κ	Fraction of energy allocated to soma	-	<i>kappa</i>	0.86937	Kooijman and Augustine (2020)
$\{p_{Am}\}$	Surface-area specific maximum assimilation rate	$eL^{-2}t^{-1}$	<i>pA_m_surf</i>	164.604	Kooijman and Augustine (2020)
\dot{v}	Energy conductance	Lt^{-1}	<i>v</i>	0.02254	Kooijman and Augustine (2020)
$[p_M]$	Volume-specific maintenance rate	$eL^{-3}t^{-1}$	<i>pM_vol</i>	183.867	Kooijman and Augustine (2020)
U_H^b	Scaled maturity at birth	tL^2	<i>Ub_h</i>	0.0038	Kooijman and Augustine (2020)
U_H^j	Scaled maturity at metamorphosis	tL^2	<i>Uj_h</i>	0.0213	Kooijman and Augustine (2020)
U_H^p	Scaled maturity at puberty	tL^2	<i>Up_h</i>	3.1287	Kooijman and Augustine (2020)
$[E_G]$	Volume-specific cost of growth	eL^{-3}	<i>E_G_vol</i>	5228.09	Kooijman and Augustine (2020)
δ_m	Shape correction factor	-	<i>del_M</i>	0.14483	Kooijman and Augustine (2020)
z	Zoom factor	-	<i>z</i>	0.77829	Kooijman and Augustine (2020)
<i>lifespan</i>	maximum age	days	<i>lifespan</i>	1460	Kooijman and Augustine (2020)
Code notation	Interpretation	Dimensions	Value SD		Source
<i>egg - survival</i>	Survival rate for eggs	t^{-1}	0.1		This study
<i>juvenile - mortality - rate</i>	Juvenile mortality rate	t^{-1}	0.004		This study
<i>adult - mortality - rate</i>	Adult mortality	t^{-1}	0.0025		This study
<i>gamma_dd_egg_survival</i>	Coef for DD function	g^{-1}	0.1		This study
<i>DailySurvival_Egg_Larva0</i>	embryo survival rate for DD	t^{-1}	1		This study
<i>area</i>	area in which DD occurs	m^2	1000		This study

Table 8: Environmental parameters. HC = Humpback chub, SD = Spikedace, TS = Topeka shiner, DRM = Devils River minnow.

Parameter	Interpretation	HC	SD	TS	DRM	Unit	Code
r_X	resource growth rate	1.5				t^{-1}	rX
X_{max}	maximum of the food sinus function	$4.69 \cdot 10^8$	$3.16 \cdot 10^8$	$5.05 \cdot 10^8$	$1.01 \cdot 10^8$	$e\ l^{-3}$	$X - max$
X_{min}	minimum of the food sinus	$1.17 \cdot 10^8$	$7.91 \cdot 10^7$	$1.26 \cdot 10^8$	$2.52 \cdot 10^7$	$e\ l^{-3}$	$X - min$
$limit$	Lower limit of the available resource detected by individuals	$5.87 \cdot 10^7$	$3.96 \cdot 10^7$	$6.3 \cdot 10^7$	$1.26 \cdot 10^7$	$e\ l^{-3}$	$limit$
T_{in}	Initial temperature	16.5	16	18.1	13.3	C	–
N_{in}	Initial number of individuals (embryo)	50				–	N_{in}

Table 9: GUTS-IT parameters for juvenile and adult survival

Parameter	Interpretation	value	Unit	Code
k_d	dominant rate of the reduced model	0.107	t^{-1}	kd
mw	median log-logistic distribution	10.57	$\mu g/L$	mw
Fs	spread factor of the thresholds distribution	1.875	–	Fs
β	shape parameter for the distribution of thresholds	5.83	–	$beta$

Table 10: GUTS-IT parameters for hatching mortality

Parameter	Interpretation	value	Unit	Code
k_d	dominant rate of the reduced model	11.29	t^{-1}	$kd - h$
mw	median log-logistic distribution	5.218	$\mu g/L$	$mw - h$
Fs	spread factor of the thresholds distribution	10.46	–	-
β	shape parameter for the distribution of thresholds	1.56	–	$beta - h$

Table 11: TKTD parameters for sub-lethal effects

Parameter	Interpretation	value	Unit	Code
k_d	dominant rate of the reduced model	0.107	t^{-1}	kd
c_T	tolerance gradient	2	$\mu g/L$	c_T
c_0	threshold	1.4	$\mu g/L$	c_0

Table 12: Data used to build the SSD function (indirect effects)

Organism	Life stage	Endpoint	µg/L	Reference
<i>Astacopsis gouldi</i>	0.13g	4d-LC50	12	Davies, Cook, and Goenarso, 1994
<i>Paratya australiensis</i>	0.05-0.15g	4d-LC50	16	Davies, Cook, and Goenarso, 1994
<i>Brachionus calyciflorus</i>	<24h	24h-EC50	24	Hamer and Gemtle, 1999
<i>Leptocerus</i>	Larva	48h-EC50	38	Hamer and Gemtle, 1999
<i>Brachionus calyciflorus</i>	<24h	24h-EC50	24	Hamer and Gemtle, 1999
<i>Palaemonetes pugio</i>	Larva	96h-EC50	38	Key, Meyer, and Chung, 2003
<i>Daphnia magna</i>	NR	48h-EC50	24	Ernst et al., 1991
<i>Crangonyx pseudogracilis</i>	Juvenile	48h-EC50	38	Hamer and Gemtle, 1999
<i>Chydorus</i>	Adult	48h-EC50	24	Hamer and Gemtle, 1999
<i>Chironomus riparius</i>	Larva	48h-EC50	38	Hamer and Gemtle, 1999
<i>Planorbis</i>	NR	48h-EC50	24	Hamer and Gemtle, 1999
<i>Erpobdella</i>	NR	48h-EC50	38	Hamer and Gemtle, 1999
Hamer and Gemtle, 1999 <i>Planaria</i>	NR	48h-EC50	38	Hamer and Gemtle, 1999
<i>Gammarus pulex</i>	Juvenile	48h-EC50	38	Hamer and Gemtle, 1999
<i>Hyalella azteca</i>	Adult	48h-EC50	38	Hamer and Gemtle, 1999
<i>Lymnaea stagnalis</i>	NR	48h-EC50	38	Hamer and Gemtle, 1999
<i>Macrocylops fuscus</i>	Adult	48h-EC50	38	Hamer and Gemtle, 1999
<i>Ostracoda</i>	NR	48h-EC50	38	Hamer and Gemtle, 1999
<i>Asellus aquaticus</i>	Juvenile	48h-EC50	38	Hamer and Gemtle, 1999
<i>Cloeon dipterum</i>	Nymph	48h-EC50	38	Hamer and Gemtle, 1999

3 Data evaluation

This TRACE element provides supporting information on: The quality and sources of numerical and qualitative data used to parameterize the model, both directly and inversely via calibration, and of the observed patterns that were used to design the overall model structure. This critical evaluation will allow model users to assess the scope and the uncertainty of the data and knowledge on which the model is based.

Summary: We provide here an overview of the data used to represent the resource dynamics, the drought-induced mortality on agents younger than 1 year, and the stressor effects.

3.1 Resource dynamics

Cyprinidae are opportunistic organisms, and switch diet depending on season and turbidity. Diet is mainly composed by diatoms, algae, amorphous detritus, Chironomidae, Simuliidae, terrestrial vegetation and other aquatic invertebrates (Seegert et al., 2014; Greger and Deacon, 1988; Echo-Hawk and Garrett, 2015; Mcmillan, 2011). Studies in the Colorado River show that the diet of Speckled Dace is dominated by Chironomidae, Simuliidae and other aquatic invertebrates (Seegert et al., 2014). Clear-water seasons are usually characterized by higher primary production (e.g. diatoms) and consequently higher invertebrate production, whereas during the monsoon season (late summer- early fall) the higher turbidity makes it harder for fish to detect scarce invertebrates prey items, and diet is dominated by terrestrially sourced carbon and amorphous detritus. Similar oscillations are shown by studies on chubs living in Jordan Creek (IL), where invertebrates are less common late in the year (July-January) than in spring (March-June, with a maximum sampled in May-June) (Angermeier, 1982). Therefore, Cyprinidae experience resource depression between July and October, and eat more terrestrial items. A decrease in invertebrate densities between late spring and early autumn is also reported in the Virgin River (Greger and Deacon, 1988), and in an Iberian stream (Magalhaes and Magalhães, 1993). The assumed food function for the Little Colorado River takes into account these results and is based on data from Angermeier, 1982. In the model, the food function has a peak around April-May and decreases in July, with a minimum value at the end of October. This function is used for chubs and daces (figure 3(a)).

Studies in the Devils River show that Devils River minnows (Rio Grande Basin) eat primarily detritus and algae (filamentous green algae, blue-green algae and diatoms), with some seasonality patterns in the type of algae (Mcmillan, 2011). Data show a more heterogeneous diet in summer, and sometimes in winter (Pinto creek). Usually, a more heterogeneous diet suggests resource depression. In the model, the food function has a minimum around January-February and a second minimum between July and August. Because of the absence of data concerning diet seasonality or starvation, we consider a hypothetical food function without strong oscillations (figure 3(b)).

A previous model representing Topeka shiner (TS) in Midwestern head water pools used data on TS gut contents to make the assumption that the diet is characterized by microzooplankton, Rotifera, Copepoda, Cladocera, Chironomidae, Ephemoptera, Trichoptera, Periphyton and detritus (Schmolke et al., 2019). Relative concentration of these items have been calculated from figures 17-19 in the Appendix A of Schmolke et al., 2019, and used to adjust the sinus function. Maximum peaks are in June and in December (figure 3(c)).

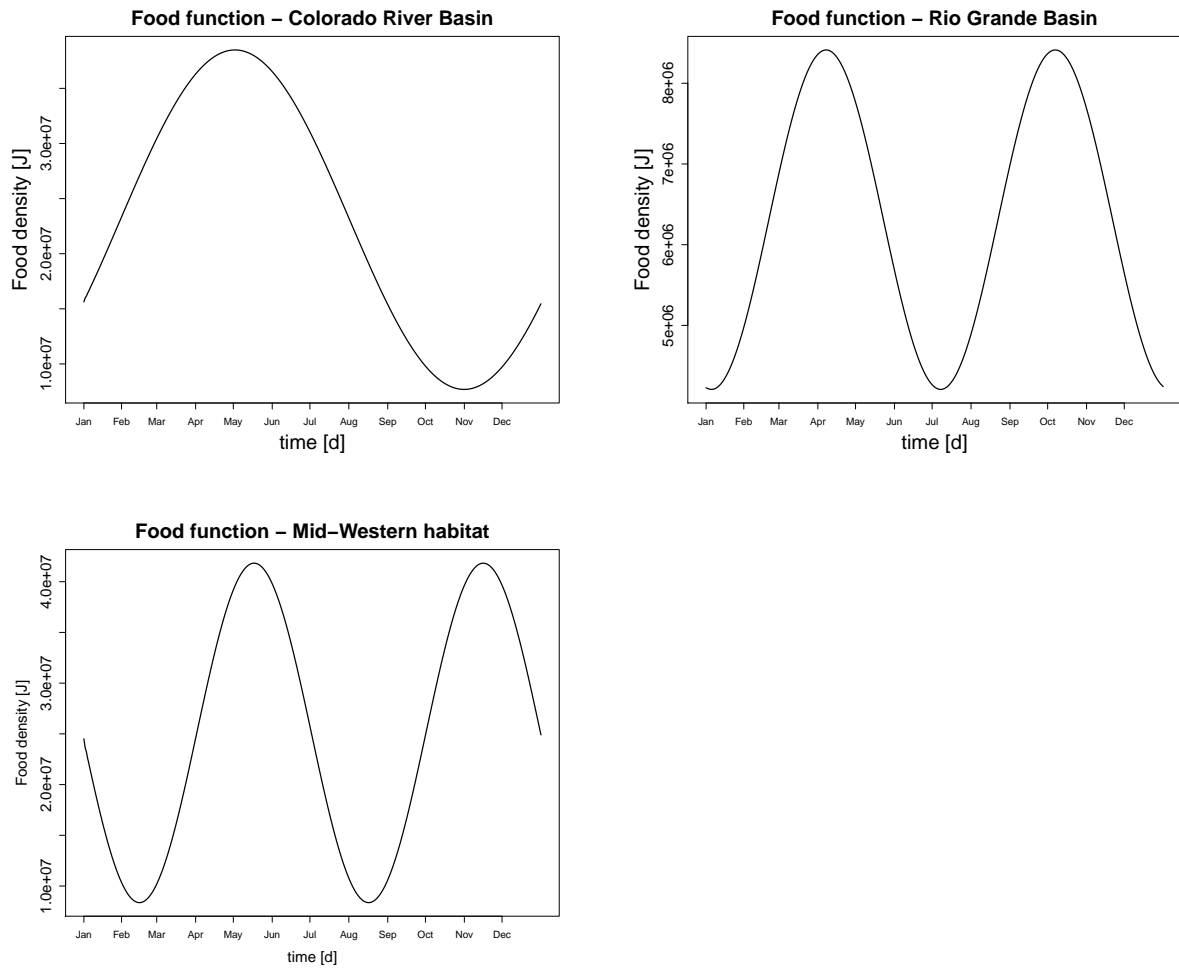


Figure 3: The three food profiles used (a) for Humpback chub and Spikedace, (b) Devils River minnow, and (c) Topeka shiner

3.2 Drought-induced mortality

Alterations to the natural hydrograph (e.g., water storage and diversion dams) have reduced or eliminated flooding, which is an important abiotic factor regulating stream fish assemblages (Brouder, 2001). For example, data suggests that the long-term average flow of the Colorado River is getting lower with respect to its historical range (1906-2003) (Christensen and Lettenmaier, 2007). Udall and Overpeck, 2017 report about a drought lasting from 2000 to at least 2014. In a dry year, the annual mean flow of the Colorado River is usually lower than 15.15 billion cubic meters (BCM) (Udall and Overpeck, 2017), with low-flow years having an average flow between 6.5 and 15 BCM (Christensen and Lettenmaier, 2007). Data during the period 1905-2005 show that drought events can occur every 1 to 25 years (Christensen and Lettenmaier, 2007, figure 2). Because there is a strong positive relationship between maximum mean daily discharge and fish recruitment (Brouder, 2001), in the model we link dry events to reduced recruitment, as explained in section 2.7.7. Because we found only these data to represent environmental stochasticity, we model this process in the same way for the four species.

3.3 Stressor effects

The study of Schults et al., 1980 reports chronic toxicity effects of chlorothalonil on fathead minnow (*Pimephales promelas*). Mean measured exposure concentrations are 0.6, 1.4, 3.0, 6.5 and 16 $\mu\text{g/L}$. The test starts with 200 fertilized eggs for each exposure concentration, and is split into distinct stages in order to accurately measure the hatching, survival, growth and reproductive success of the individuals. There are two replicate vessels of each test concentration, solvent control and dilution water control. Available data are:

- embryo hatching success of F_0 generation (expressed in percentages);
- survival of the F_0 generation between hatching and day 35 (post-hatch), and between hatching and day 64 (expressed in percentages);
- survival of the F_0 generation between day 64 and day 172 (expressed in total number of survivors);
- survival of the F_0 generation between day 172 and day 283 (expressed in total number of survivors);
- total length and weight of the F_0 generation after 35, 64, 283 days;
- reproduction success of the F_0 generation (eggs per spawn);
- embryo hatching success of the F_1 generation;
- survival of the F_1 generation after 34 days;
- total length and weight of the F_1 generation after 34 days.

3.3.1 GUTS model

Inputs for the fit of the GUTS model are data showing the number of surviving organisms over time for the different exposure concentrations. We used data on F_0 survival to represent juvenile and adult mortality, and data on embryo hatching success of the F_1 generation to represent embryo mortality. For juveniles and adults, we used the data on survivals from time $t_0 = 4$ days (hatching) to 35, 64, 172 and 283 days post-hatch. We considered an initial number of 100 hatched larvae for each test concentration and for the control. Data concerning survival at day 172 (283) were reported as number of surviving

individuals from day 64 (172) to day 172 (283). We therefore use a proportion to calculate the number of survivors adapted to our case:

$$s_{172} = s_{64} \frac{s_R}{tot_R} \quad (45)$$

where s_{64} is the number of survivors we calculated in the previous step (considering a starting point of 200 individuals), tot_R is the number of individuals selected in the report at day 64 to continue the exposure experiment, and s_R is the number of survivors counted in the report from day 64 to day 172. A similar calculation is performed for s_{283} . The GUTS parametrization gives the values of the parameters k_d, mw, Fs , reported in table 9. The results are shown on figure 5.

For the second GUTS model representing hatching mortality, we consider data on F_1 (second column of the table 15) because this is the most conservative choice. Data show a slightly higher effect than for F_0 generation, and using F_1 corresponds to assuming exposure of the eggs prior to spawning in contrast to assuming onset of exposure at time of spawning (even if the GUTS model cannot take into account exposure of the mother prior to egg laying). Since we want to represent only the effect of the chemical, we have recalculated the hatching success without taking into consideration any background mortality (third column in table 15).

3.3.2 TKTD model for sub-lethal effects

Data on reproduction efficiency show that the eggs per female of FHM are 95%, 20%, 11% and 2% of the eggs spawned in the control experiment when the fish is exposed to 1.4, 3, 6.5, and 16 $\mu\text{g/L}$ of chlorothalonil, respectively (Schults et al., 1980). To setup the TKTD model, we assume that c_0 is equal to the reported NOEC (1.4 $\mu\text{g/L}$). Values of the stress levels are given by the experiment (0.05%, 80%, 89% and 98%). One of the control experiment (solvent) and the data at the lower concentration 0.6 $\mu\text{g/L}$ are not used because of quality concerns (Yellowlees, 2016). c_T is calculated by using the program *optim* (R), which optimizes the following equation :

$$0 = \sum \left(\frac{D - NOEC}{s} - c_T \right)^2. \quad (46)$$

3.3.3 Indirect effects

The following figures show the fit of the Weibull function to the LC50 and EC50 data used to represent effects on invertebrate.

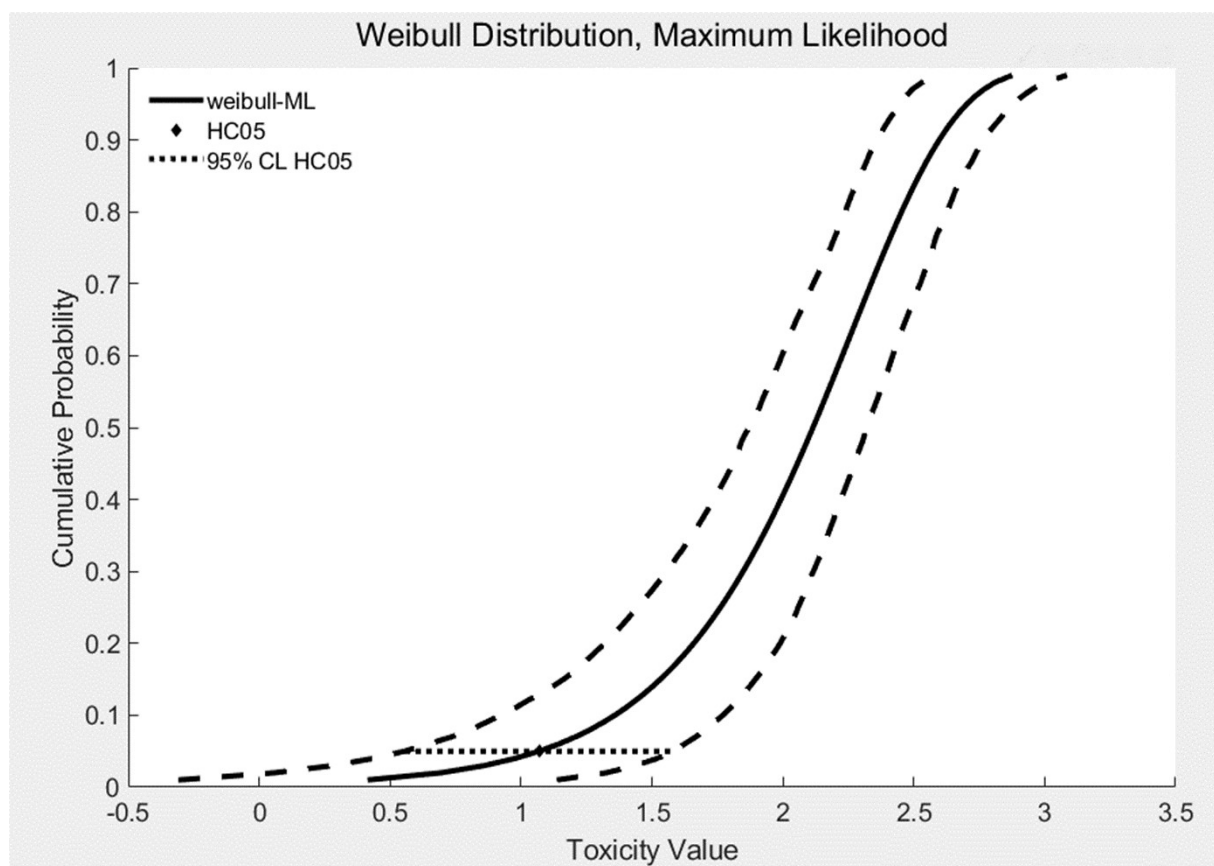


Figure 4: Weibull distribution fitted to the data on invertebrate toxicity endpoints

4 Conceptual model evaluation

This TRACE element provides supporting information on: The simplifying assumptions underlying a model's design, both with regard to empirical knowledge and general, basic principles. This critical evaluation allows model users to understand that model design was not ad hoc but based on carefully scrutinized considerations.

Summary:

Consideration of modeled metabolic processes was based on Dynamic Energy Budget theory that postulates how resources are assimilated and allocated to metabolic endpoints. It is based on first principles of conservation of energy and matter and follows strict assumptions of how energy fluxes are distributed in the organism.

The conceptual model is based on DEB theory (figure 1), which is also described under 2.3. The effect sub-models are TKTD models, which are recognized as an appropriate approach to select in the refined risk assessment. The scheduling of processes and events is described in the pseudo-code in the same paragraph. Assumptions for the model were developed from the data sources available (or missing) about the species and other species, and are presented along with the data used.

5 Implementation verification

This TRACE element provides supporting information on: (1) whether the computer code implementing the model has been thoroughly tested for programming errors, (2) whether the implemented model performs as indicated by the model description, and (3) how the software has been designed and documented to provide necessary usability tools (interfaces, automation of experiments, etc.) and to facilitate future installation, modification, and maintenance.

Summary:

Model implementation was verified in a series of tests to ensure that the code reproduced the concepts described in the 2.3 and 2.4. Verification was performed by using modeling platform tools for syntax checking, in addition to visual testing, print statements, spot testing with agent monitors, stress tests, test programs, and code reimplementations.

Model code was tested to verify that the model behaves as expected and as planned. The model was implemented in NetLogo and parts were implemented using Matlab (MATLAB R2016b) or R (R 4.1.1). All these languages offer several tools that enable the developer to check whether the implemented syntax is correct.

Implementation testing was done on several levels:

1. Syntax checking. Using software tools, which check for syntax errors such as forgetting a bracket. These errors are immediately picked up by the software without a possibility to proceed with simulations until the syntax has been corrected. Run-time errors are not syntax errors, but represent events that the software cannot deal with. This, for instance, includes divisions by zero or producing numbers that are too large for storing. Even though run-time errors cannot directly pinpoint to the problem, they offer helpful directions and explanations of the issue.
2. Visual testing of model outputs. Visual testing was continuously used to look for errors that may be

unlikely to be detected soon, if ever, via other methods. Individual properties, e.g. length, number of eggs, and overall population dynamics have all been monitored for checking whether model behaves as expected. Food levels have been adjusted to avoid starvation and recruitment has been adjusted to avoid the death of too many adults by starvation.

3. Print statements. Using the print statements allowed for a visual check and manual calculation of the right functioning of all the submodels. We programmed the model to print the value of some variables at different times to check that the model was behaving in the expected way. Basic examples are: writing the number of agents at every time step to check that they are actually dying and leaving the model; writing some particular energy values (such as energy at birth); write the time of a specific event, e.g. reproduction; give messages if erroneous values arose (e.g. wrong length measurements, wrong energy levels, etc.). Print statements were also used to locate issues such that they would have a role of markers in the code, e.g. if not printed, that meant that the code lines were not reached or a particular error was (not) made.
4. Spot tests with Agent Monitors. The agent monitors were used for quickly seeing agent state variable values and testing key calculations, like transitions between life stages, age and length measurements.
5. Stress tests. Stress tests were performed by using extreme values of parameters and comparing simulation output to expectations. For example, chemical concentrations were changed to check the GUTS models; reproduction-related parameters were shut off to check the population dynamics; test on food levels were made.
6. Test programs. At some cases, it was convenient to write a separate short program under simplified conditions that served only to test a particular algorithm or procedure. For instance, the GUTS implementation and the SSD curve were first coded in a secondary program.
7. Simulations experiments. Several controlled simulation experiments were performed, in which the model or its parts were simplified so that the outcome of each experiment could be predicted and verified. This includes, for example, the different mortality submodels.
8. Code reviews. The code was peer-reviewed, i.e., it was thoroughly compared with the written formulation of the model by one other scientist and with published DEB-IBMs.

6 Model output verification

This TRACE element provides supporting information on: (1) how well model output matches observations and (2) how much calibration and effects of environmental drivers were involved in obtaining good fits of model output and data.

Summary:

Here we summarize the how well the model recreates the input data. This includes data on length, biomass, individual body growth at different temperatures and food conditions, the resulting number of eggs per reproductive event and the adult number in populations.

To test if the GUTS implementations reproduced the data, we first analyzed the GUTS model outputs. Figure 5 shows the results of both the GUTS-SD and GUTS-IT parametrizations for juvenile and adult mortality. The GUTS-IT model gives overall better results, as already indicated by the AIK criterion. This

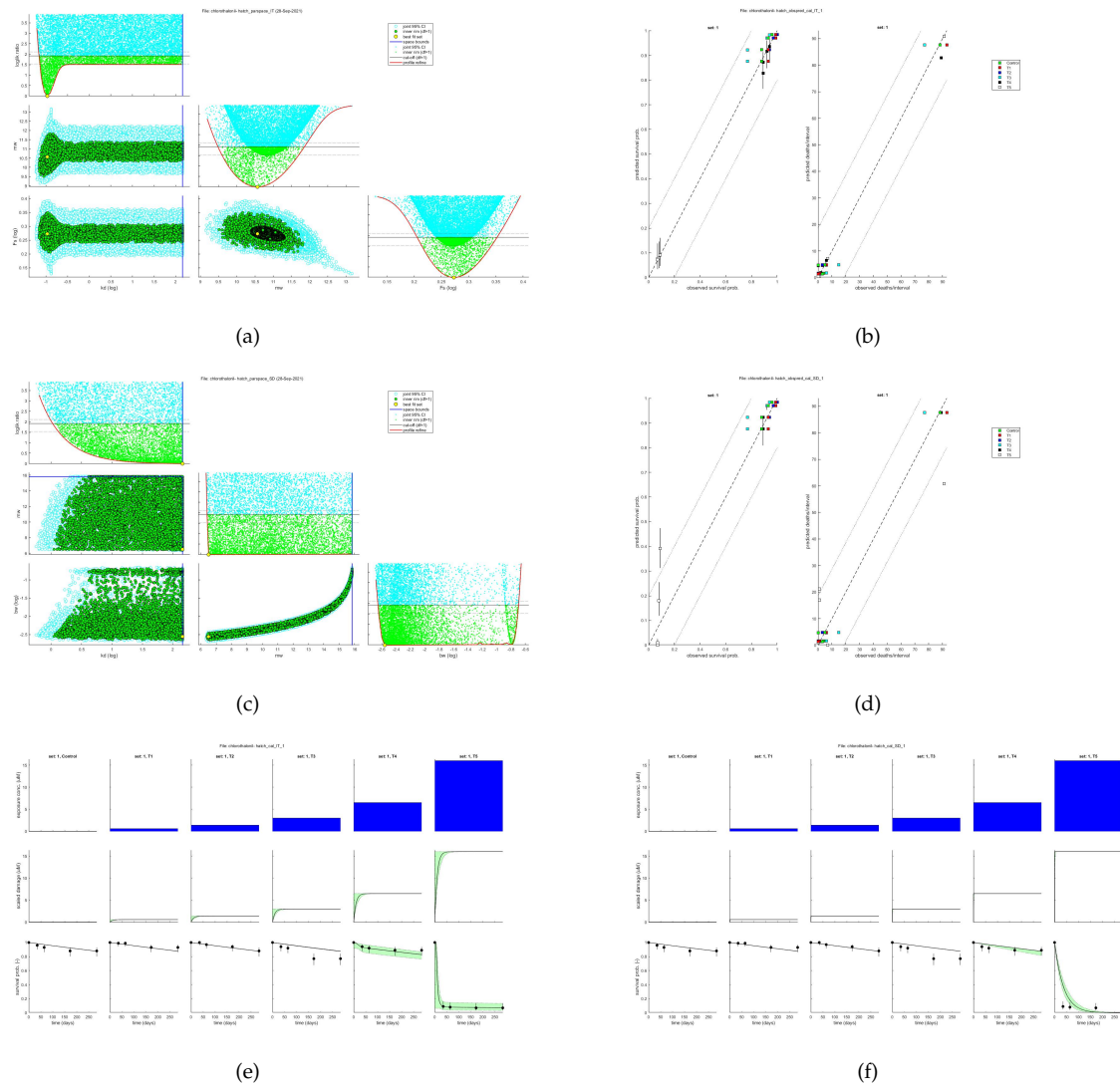


Figure 5: Results of the GUTS-IT model ((a), (b) and (e)) and of the GUTS-SD model ((c), (d) and (f)). (a-c) Likelihood plot of the parameters. The sample provides a coverage of parameter sets that are within the joint 95% confidence region (all symbols). The green symbols indicate those sets that are within the cut-off for $df = 1$, the yellow symbol provides the best fit. (b-d) Predicted and observed survival probabilities for the different treatments. (e-f) Model fit for GUTS-IT (e) and GUTS-SD (f). Top row: exposure scenario, middle row: modeled damage with 95% CI, lower row: modeled survival probability (with 95% CI) and survival observations (with Wilson score interval).

is shown by the trend of the predicted vs. observed survival probabilities (figure 5(b)) and by the model fit (figure 5(e)), where we can see a better overlap between the Wilson score bars on the data and at the CIs on model curves. Both the SD and the IT models judge that all mortality is background mortality for low exposure scenarios (up to the exposure of $3 \mu\text{g/L}$). This is a common result because observation intervals with high mortality carry more weight in the likelihood function used by the GUTS algorithm than observation intervals with low mortality.

Figure 6 shows the results of the GUTS calibration on hatching-success data. Both the GUTS-IT and GUTS-SD calibrations show that there is a non-identifiability problem. The plots do not clearly indicate which model to choose, and the AIC criterion is slightly smaller for the SD (432.71 for SD versus 447.1 for IT). However, since both calibrations are not satisfying and we have a GUTS-IT model for juvenile and adult survival, we decided not to add to model complexity and use the GUTS-IT model for hatching success.

To further test the GUTS and TKTD sub-models, we implemented the NetLogo code for FHM at

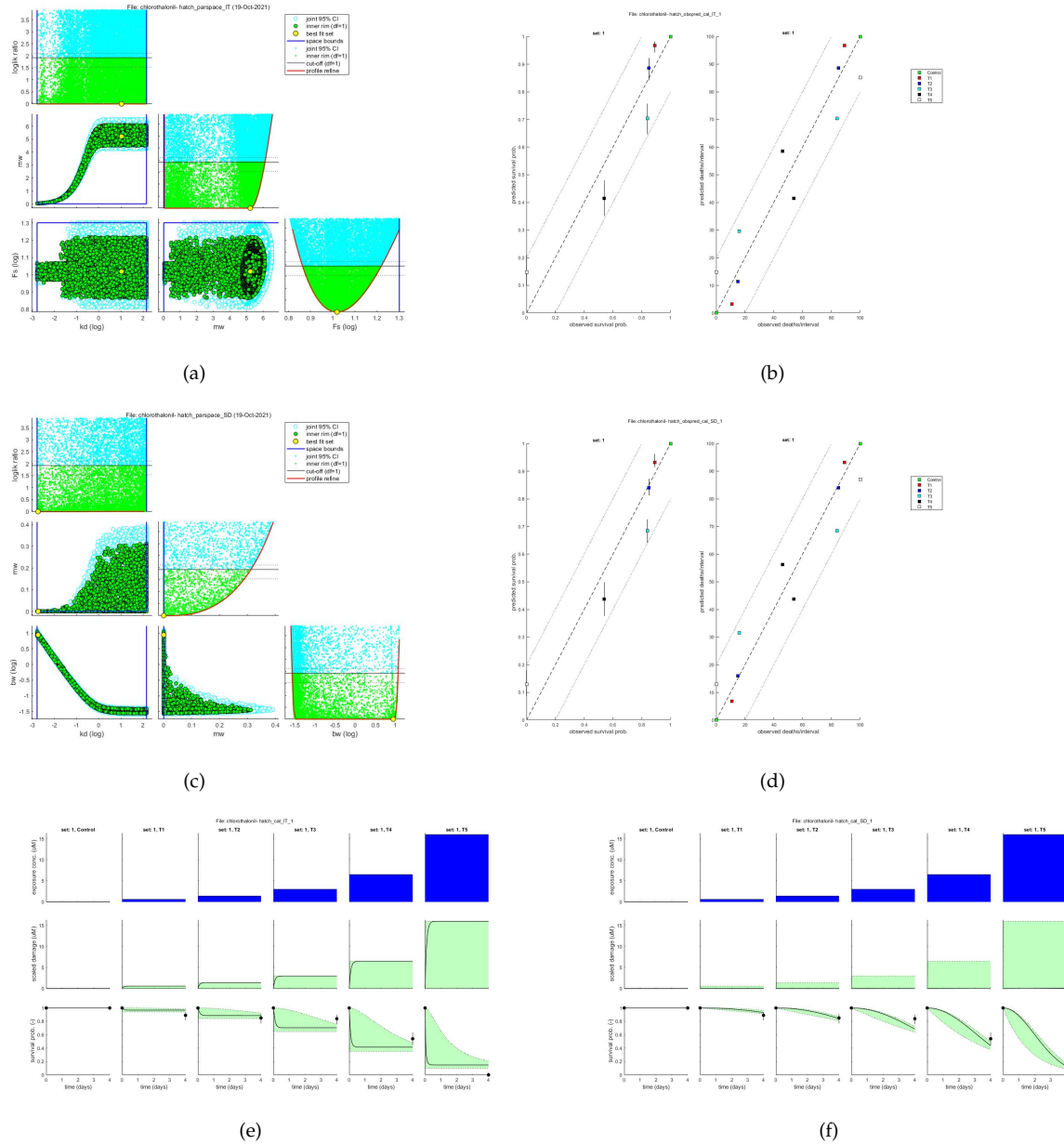


Figure 6: Results of the GUTS-IT model ((a), (b) and (e)) and of the GUTS-SD model ((c), (d) and (f)) for hatching. (a-c) Likelihood plot of the parameters. The sample provides a coverage of parameter sets that are within the joint 95% confidence region (all symbols). The green symbols indicate those sets that are within the cut-off for $df = 1$, the yellow symbol provides the best fit. (b-d) Predicted and observed survival probabilities for the different treatments. (e-f) Model fit for GUTS-IT (e) and GUTS-SD (f). Top row: exposure scenario, middle row: modeled damage with 95% CI, lower row: modeled survival probability (with 95% CI) and survival observations (with Wilson score interval).

constant temperature (25 ° C) and unlimited food (as in the lab experiment) and compared the outputs to the data. The DEB-parametrization for FHM can be found in Vaugeois, Venturelli, and Forbes, 2020. Tables 13 and 14 show survival of juveniles and adults of FHM when exposed to five different concentrations of chlorothalonil (lab data and simulation results, respectively). Table 15 shows the simulation results when verifying the GUTS model on hatching. In this latter case, we noticed that multiple runs of the GUTS model for hatching on the same data set gave different parameter values. The best result of the GUTS calibration gave the parameter values shown on table 10.

The GUTS calibrations we performed, even if not wholly satisfying, were the best we could have given the available data. First, we only had few time-data points. Moreover, survival records were not

consistent. For example, survival at 35 days post-hatch is higher at a concentration of $1.4 \mu\text{g/L}$ than $0.6 \mu\text{g/L}$. Similarly, survival at 172 days post-hatch is lower at $3 \mu\text{g/L}$ than $6.5 \mu\text{g/L}$. Some accidents occurred during the experiment (e.g., all fish in one control died between days 16 and 33). Moreover, on day 64, only some fish were selected to continue the exposure, and the same was done on day 172, creating some confusion on actual survival rates. Finally, the available data on hatching did not include the temporal resolution necessary for GUTS fitting (only hatching success was reported, not egg survival at intermediate time points). Meanwhile, we ran the GUTS sub-models anyway because our work aims to create a tool that can be later adapted to new problems and integrate new datasets. Our procedure allows to replicate, even if not perfectly, the data available. The poorness of fit is probably due to the lack of data, both tests performed and replicates.

To set up the TKTD model, we assumed that c_0 is equal to the reported NOEC ($1.4 \mu\text{g/L}$), and that the internal concentration D_i corresponds to the values of the external concentration C_{ext} , because the organisms are exposed since their egg stage to constant chemical concentrations. As an output, we have the reduction in egg production at the nominal constant concentrations tested in the lab experiment. Since the simulations were not reproducing the data accurately, we tried different values of c_T by dividing by 2, 4, 8 the values found with the optimization. The best value is $c_T = 2 \cdot 10^{-6} \text{ g/L}$, as shown by table 16. Higher and lower values give respectively too high or low reproduction efficiency at concentrations of $3 \mu\text{g/L}$.

Table 13: Lab test results on juvenile and adult mortality.

Nominal concentration [$\mu\text{g/L}$]	35-days survival (%)	64-days survival(%)	172-days survival(%)	283-days survival(%)
0	95	93	88	88
0.6	99	99	92	92
1.4	100	97	93	87
3.0	94	92	76	76
6.5	94	92	88	88
16	9	8	7	7

Table 14: Model results on juvenile and adult mortality for FHM (GUTS-IT model).

Nominal concentration [$\mu\text{g/L}$]	35-days survival(%)	64-days survival(%)	172-days survival(%)	283-days survival(%)
0	100	100	100	100
0.6	100	100	100	100
1.4	100	100	100	100
3.0	100	100	100	100
6.5	94	93	93	93
16	7	6	6	6

Table 15: Results of the lethal module describing the decrease on hatching success (F_1) for FHM.

Nominal concentration [$\mu\text{g/L}$]	Hatching success (lab experiment)	Hatching success (no bkg mortality)	Hatching success (simulation)
0	93%	100%	100%
0.6	83%	89%	100%
1.4	79%	85%	100%
3.0	78.5%	84%	70%
6.5	50%	54%	41%
16	0%	0%	0%

Table 16: Results of the sub-lethal module describing the decrease on reproduction efficiency for FHM. $c_T = 2 \cdot 10^{-6}$ g/L

Nominal concentration [$\mu\text{g/L}$]	% of eggs produced in the lab experiment	% of eggs produced in the simulation
1.4	95%	100%
3.0	20%	20%
6.5	11%	0%
16	2%	0%

7 Model analysis

This TRACE element provides supporting information on: (1) how sensitive model output is to changes in model parameters (sensitivity analysis), and (2) how well the emergence of model output has been understood.

Summary: In this section, the results of sensitivity analysis are presented. The analysis was conducted by simultaneously varying 20 parameters. and testing the effects on total and adult abundance of Humpback chub and Topeka shiner.

We performed a sensitivity analysis to check how changes in parameter values affected the total and the adult population abundances of Humpback chub and Topeka shiner. Performing the analysis on at least two species allows exploring if the model behaves similarly. We simultaneously varied 20 parameters: some of the DEB parameters (12 core DEB parameters), survival rates, density-dependence parameters, and reproductive periods. All the non-DEB parameter values have been changed in a continuum interval between $\pm 50\%$ of their original value. DEB parameters varied in a range of $\pm 25\%$, to avoid dramatic changes of the energetic cycle. The only exception is κ that changed in an interval of $\pm 2\%$ because it cannot be higher than 1. Reproduction starting and ending dates are changed to cover the more extensive time interval found in the literature. All the modified parameters are listed in table 17. The number of simulations N had to satisfy an empirical inequality: $N > 4/3 * K$, where K is the number of parameters (Blower and Dowlatabadi, 1994). In our case, $K = 20$, therefore N had to be bigger than 27. We repeated each simulation 20 times to account for model stochasticity and performed a total number of runs of 6400 for each species. The results from the simulation runs were analyzed using a partial rank correlation. This method is applied to assess the association between two random variables (here, the total or adult population abundance and one of the modified parameters) after the elimination of the effect of all other random variables (i.e., all the other modified parameters) (Kim, 2015).

The sensitivity analysis showed that the most influential parameter for the four outputs (i.e., total and adult abundance of Humpback chub and Topeka shiner) is κ , the DEB parameter leading the energy allocation to reproduction/maturation and growth/maintenance (figure 7). Other sensitive parameters were those defining survival rates and density dependence. In particular, Humpback chub population is more affected by changes in density-dependence parameters and Topeka shiner population by changes on survival rates. Furthermore, Topeka shiner was more sensitive to changes in the energy-threshold parameters, \dot{v} and κ_R , and less sensitive to changes in the reproductive dates. Moreover, PRCC values were generally higher (in absolute values) for Topeka shiner (see table 18). Total and adult population abundances were affected almost equally by parameter changes. The only remarkable difference concerned juvenile and adult mortality rates in the case of Humpback chub: the total population was less affected by changes in those parameters than the adult abundance, probably because of density-dependence compensation mechanisms. Finally, some parameters combinations caused the populations to go extinct. Table 18 shows the rank of the parameters by their absolute value of partial rank correlation coefficient (PRCC), from the highest to the lowest.

Table 17: Parameters that have been changed for the sensitivity analysis. The table shows the base values for Humpback chub (HC) and Topeka shiner (TS) and the range of change.

Parameter name	Base value for HC	Base value for TS	Range	
<i>reprod – start</i>	80	135	HC:60	TC: 143
<i>reprod – end</i>	135	212	HC: 212	TC: 218
<i>area</i>	1000	1000	$\pm 25\%$	
<i>lifespan</i>	5	3	$\pm 25\%$	
<i>gamma_dd_egg_survival</i>	0.01	0.25	$\pm 25\%$	
<i>egg – survival</i>	0.1	0.1	$\pm 25\%$	
<i>juvenile – mortality – rate</i>	0.004	0.008	$\pm 25\%$	
<i>adult – mortality – rate</i>	0.003	0.006	$\pm 25\%$	
κ	0.97579	0.96612	$\pm 2\%$	
\dot{v}	0.020708	0.025042	$\pm 10\%$	
$[\dot{p}_M]$	105.9616	295.6485	$\pm 10\%$	
$[E_G]$	5199.9956	5237.4441	$\pm 10\%$	
E_H^b	0.1427	2.49E-02	$\pm 10\%$	
E_H^j	2.743	3.75E-02	$\pm 10\%$	
E_H^p	11990	1.54E+02	$\pm 10\%$	
\dot{k}_J	0.002	0.002	$\pm 10\%$	
κ_R	0.95	0.95	$\pm 10\%$	
κ_X	0.8	0.8	$\pm 10\%$	
\dot{F}_M	6.5	6.5	$\pm 10\%$	
<i>zoom</i>	2.2479	0.85829	$\pm 10\%$	

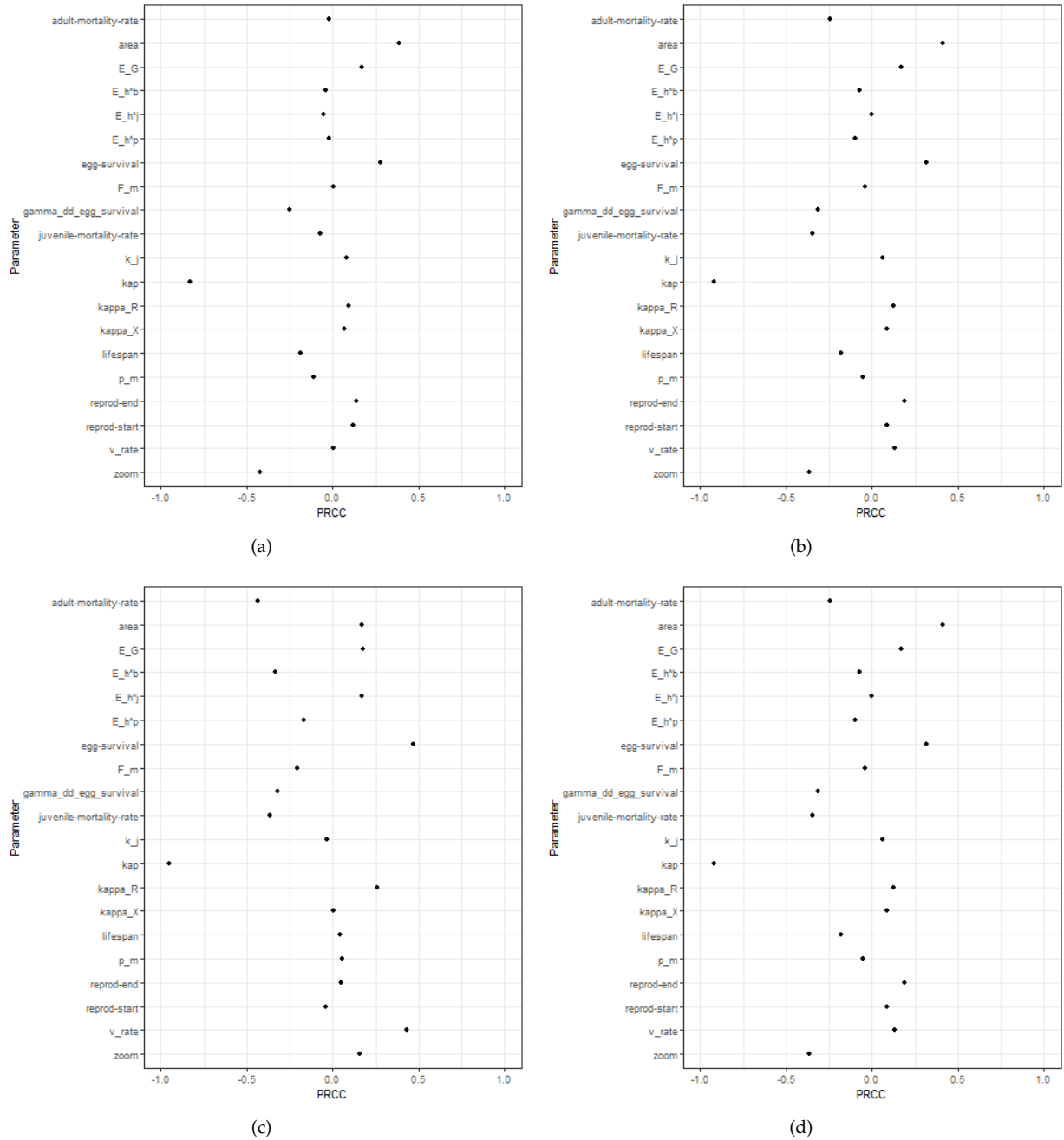


Figure 7: Partial rank correlation coefficients (PRCC) for Humpback chub (top) and Topeka shiner (bottom). The figures on the left show the results when considering the total population, whereas on the right they correspond to the adult population.

Table 18: Ranking of the input parameters by their absolute value of PRCC for the four outputs analyzed. The parameters with the highest influence on model output are listed at the top of the table, the parameters with the least influence at the bottom. Parameters with absolute PRCC < 0.05 are marked in grey. The parameters highlighted in red are those for which the first PRCC values are less than 0.2

Humpback chub		Topeka shiner	
Total population	Adult population	Total population	Adult population
κ	κ	κ	κ
<i>zoom</i>	<i>area</i>	<i>egg – survival</i>	<i>adult – mortality – rate</i>
<i>area</i>	<i>zoom</i>	<i>adult – mortality – rate</i>	\dot{v}
<i>egg – survival</i>	<i>juvenile – mortality – rate</i>	\dot{v}	<i>juvenile – mortality – rate</i>
<i>gamma_dd_egg_survival</i>	<i>egg – survival</i>	<i>juvenile – mortality – rate</i>	<i>egg – survival</i>
<i>lifespan</i>	<i>gamma_dd_egg_survival</i>	E_H^b	E_H^b
$[E_G]$	<i>adult – mortality – rate</i>	<i>gamma_dd_egg_survival</i>	<i>gamma_dd_egg_survival</i>
<i>reprod – end</i>	<i>reprod – end</i>	κ_R	<i>zoom</i>
<i>reprod – start</i>	<i>lifespan</i>	\dot{F}_M	E_H^p
$[\dot{p}_M]$	$[E_G]$	$[E_G]$	κ_R
κ_R	\dot{v}	<i>area</i>	E_H^j
\dot{k}_J	κ_R	E_H^p	\dot{F}_M
<i>juvenile – mortality – rate</i>	E_H^p	E_H^j	<i>area</i>
κ_X	κ_X	<i>zoom</i>	$[E_G]$
E_H^j	<i>reprod – start</i>	$[\dot{p}_M]$	$[\dot{p}_M]$
E_H^b	E_H^b	<i>reprod – end</i>	\dot{k}_J
<i>adult – mortality – rate</i>	\dot{k}_J	<i>lifespan</i>	<i>lifespan</i>
E_H^p	$[\dot{p}_M]$	<i>reprod – start</i>	<i>reprod – start</i>
\dot{v}	\dot{F}_M	\dot{k}_J	<i>reprod – end</i>
\dot{F}_M	E_H^j	κ_X	κ_X

8 Model output corroboration

This TRACE element provides supporting information on: How model predictions compare to independent data and patterns that were not used, and preferably not even known, while the model was developed, parameterized, and verified. By documenting model output corroboration, model users learn about evidence which, in addition to model output verification, indicates that the model is structurally realistic so that its predictions can be trusted to some degree.

Summary:

So far our model has not been compared to independent data. Nevertheless, we summarize some points of strength of our model.

Our model is a theoretical study, based on the strong assumptions of DEB theory and TKTD (including GUTS) theory. The individual metabolism implementation is based on published DEB outputs and DEB models, and the key values of the different species life cycles are well represented.

Stressors effects are based on the only study available, therefore cannot be validated. Data about population dynamics are very few, and since we did not sample any new data for this study, we had to use all the knowledge we had to parametrize the model. Therefore, a comparison with independent data has not been possible so far. However, we studied model behavior when changing some structural assumptions, and we plan to develop further studies to explore more into details the influence of factors such as mortality and density-dependence on the modeled outputs.

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