Applying a hybrid modelling approach to evaluate potential pesticide effects and mitigation effectiveness in simulated oxbow habitats

Supplementary Material

Appendix B

Individual-based population model for the Topeka shiner (*Notropis topeka*) with the representation of lethal and sublethal effects from pesticide exposures

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The documentation of the model (TS-IBM) presented here follows the TRACE (transparent and comprehensive ecological model) documentation (Schmolke et al. 2010; Grimm et al. 2014). The model description (Section 2) is organized according to the ODD (overview, design, and details) protocol (Grimm et al. 2006, 2010).

The TRACE documentation describes the updated model version applied in the current publication. The TRACE documentation of the previous TS-IBM version was published in Schmolke et al. (2019), Appendix B. Changes to the previous TRACE documentation include the description of the extension of the model with the effect representation and additional model outputs. Changes and additions to the TRACE documentation appear in green font.

The model code, input files and scripts linking it with $CASM_{OC}$ are available on GitHub: https://github.com/Waterborne-env/Topeka-shiner-model

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1. MODEL DESCRIPTION

1.1. Overview

1.1.1. Purpose

Persistence of populations depends upon species' ecology, habitat conditions, and stressors that could affect them. Fish populations may experience various stressors in their habitat including stressors mediated by the aquatic food web the fish depend upon for their diet. The endangered Topeka shiner (*Notropis topeka*) serves as example of a fish species of concern. We combined an individual-based population model of the Topeka shiner (TS-IBM) and an aquatic food-web model ($CASM_{OC}$) to explore potential impacts of alterations in the food web on Topeka shiner populations. The purpose of the hybrid model is to estimate the potential impacts of direct and indirect stressors on the species' populations over time. The TS-IBM described below provides the species-specific representation of the Topeka shiner populations. $CASM_{OC}$ is described separately.

The current version of TS-IBM (TS_IBM_Effects_Mar2020.nlogo) was adapted to a) link to the $CASM_{OC}$ which is specific to Topeka shiner oxbow habitats (in Iowa) and b) represent direct effects of a pesticide (benzovindiflupyr), including lethal and sublethal effects on Topeka shiners.

1.1.2. Entities, state variables and scales

Topeka shiners are represented individually in the model and characterized by one of five life stages: egg, larva, juvenile, subadult or adult. In addition, each fish is characterized by its sex, age (in days), biomass (g wet weight), standard length (mm SL), condition and minimal condition leading to death, spawn date (if the fish is an adult female) and bioenergetics parameters. The model is not spatially explicit and the resource distribution is assumed to be homogeneous within the waterbody. Daily time steps are simulated. The environmental conditions are represented by the temperature and depth of the waterbody. Biomasses of guilds in the food web making up the diet of juvenile (copepods, cladocerans, microzooplankton, rotifers, detritus) and adult Topeka shiners (copepods, cladocerans, chironomids, mayflies, caddisflies, periphyton and detritus) are exchanged with the aquatic food web model $CASM_{OC}$ on a daily time step or read in from a file produced by $CASM_{OC}$. Predation by largemouth bass on subadult and adult Topeka shiners is also determined in $CASM_{OC}$. Presence and absence of sunfish in the food web impact egg survival of Topeka shiners.

1.1.3. Process overview and scheduling

In each time step, each simulated Topeka shiner grows according to the fish bioenergetics submodel in which consumption, respiration and waste losses are dependent on fish biomass and temperature (Section 1.4.8.). Consumption is additionally dependent on the food availability in the waterbody (submodel Functional response to prey density, Section 1.4.7.). Growth of juveniles, subadults and adults can be impacted due to sublethal effects of pesticide exposure. Sublethal effects on growth are implemented affecting the maximum consumption rate (C_{max}). During spawning time in every year, adult females spawn once, losing the weight of the clutch. Eggs are assumed to remain unchanged in weight for the time they stay in this stage. Larvae hatch from eggs and are unable to eat (resulting in body mass loss during larval stage). After a set number of days in egg and larval stage (5 days each), fish reach the juvenile stage and start feeding (submodel Topeka shiner life history and reproduction, Section 1.4.1.). Fish experience stochastic background mortality with rates dependent on life stage (submodel Mortality, Section 1.4.2.). In addition, subadult and adult fish may die from predation by largemouth bass (submodel Predation, Section 1.4.4.). Fish cannot decrease in their body length but can lose body mass due to starvation or spawning. Lack of biomass growth leads to decline in fish condition. If the condition of a fish drops below an individual threshold, the fish dies (submodel Fish condition, section 1.4.9.). Juveniles, subadults

and adults can experience death due to pesticide exposure (implemented following the GUTS model). An overview of the most important model processes ia given in Figure S1. In Table S1, the submodels in the TS-IBM are listed with a short description.

Table S1. Submodels in the TS-IBM.

Section number	Submodel name	Short description
1.4.1	Topeka shiner life history and reproduction	Topeka shiner life stages, stage transitions and reproduction
1.4.2	Mortality	Background mortalities applied to fish dependent on stage and age
1.4.3.	Density dependence	Survival rates of eggs and larvae dependent on subadult and adult fish density in the population. Density-dependence is optional in the model, i.e. the model can also be run in a density-independent version
1.4.4.	Predation	Mortality of subadult and adult Topeka shiners due to predation by largemouth bass
1.4.5.	Sunfish hosts	Egg survival rates dependent on the assumed presence or absence of sunfish hosts
1.4.6.	Topeka shiner diet	Diet composition of Topeka shiners in the model
1.4.7.	Functional response to prey density	Functional response to densities in diet items, affecting consumption rates by Topeka shiners
1.4.8.	Bioenergetics	Fish bioenergetics (following Hanson et al. 1997; Deslauriers et al. 2017)
1.4.9.	Fish condition	Fish condition dependent on feeding rate, and threshold fish condition for survival
1.4.10	Lethal effects of pesticide exposure	GUTS implementation of mortality rate due to benzovindiflupyr exposure (Ashauer et al. 2013)
1.4.11	Sublethal effects of pesticide exposure	Implementation of effects on C_{max} due to benzovindiflupyr exposure following the approach by Jager and Zimmer (2012)

1.2. Design concepts

1.2.1. Basic principles

Simulated Topeka shiners feed on a range of other species in the waterbody. Food consumption, and thus growth and reproduction, are dependent on water temperature and food availability. Growth of individual fish is modeled according to the fish bioenergetics model (Hanson et al. 1997; Deslauriers et al. 2017). Fish may be predated on by largemouth bass, and egg survival may be affected by sunfish. Direct effects of pesticide exposure affect juvenile, subadult and adult survival using the GUTS model and growth via effects on consumptions (Ashauer et al. 2013; Jager and Zimmer 2012).

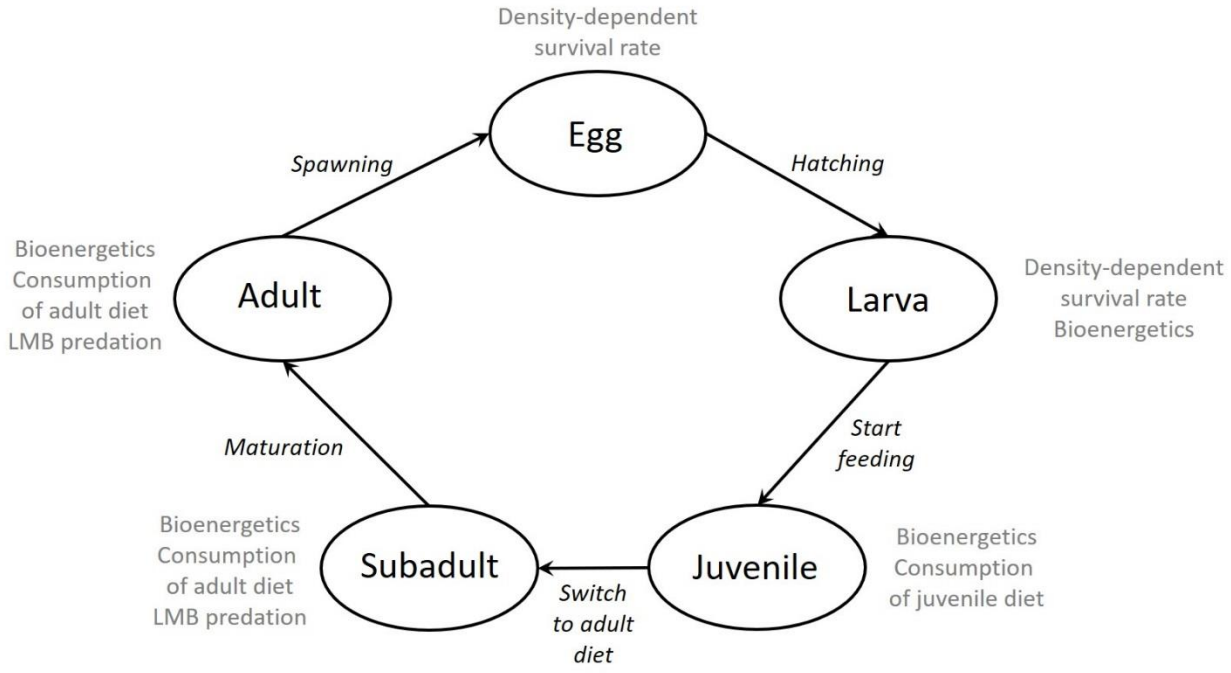


Figure S1. Overview of the Topeka shiner life cycle represented in the model.

1.2.2. Emergence

Individual fish properties such as body size emerge from prey availability and prescribed physiological processes. Population dynamics of fish emerge in the model as functions of food availability, density-dependent survival of eggs/larvae, waterbody conditions and largemouth bass (affecting Topeka shiner subadult and adult survival).

1.2.3. Adaptation

No adaptation is included in the model.

1.2.4. Sensing

No sensing is included in the model.

1.2.5. Interaction

The fish agents may interact with each other indirectly through prey consumption, see submodel Functional response (Section 1.4.7.). Density dependence is imposed as increased mortality of eggs and larvae with increased biomass of subadult and adult Topeka shiner in the waterbody (Section 1.4.3.).

1.2.6. Stochasticity

Several processes are implemented stochastically in the model. For processes occurring with each simulated Topeka shiner in each time step, individual fish are called in random order. Stage-specific survival rates are applied as daily survival probability of each fish. Timing of spawning is chosen stochastically each year. At the start of each simulated year, the start, end and peak date of spawning is

chosen randomly from uniform distributions. Once the spawning start day is reached, each adult female is assigned a spawn date from a triangular distribution defined by the three dates.

Fish condition gives the weight-to-length status of the fish. Topeka shiner are assumed to die if their condition drops below a threshold (K_{min}). This threshold is chosen stochastically from a normal distribution at time of creation of a Topeka shiner (upon model initialization or spawning).

If predation occurs, a subadult or adult fish is chosen randomly. Its chance of being eaten is calculated from the biomass of Topeka shiners eaten that day (defined as input from $CASM_{OC}$) and the biomass of the fish, and determined stochastically. Stochastic processes in the TS-IBM are listed in Table S2.

Table S2. Stochastic processes in the TS-IBM and the submodel in which it occurs.

Stochastic process	Submodel	Description
Spawning timing	Topeka shiner life history and reproduction	Spawning season is determined stochastically each year from a range for start, peak and end of spawning; each adult female is assigned a spawning date by stochastically choosing from a triangular distribution defined by those three dates
Background mortality	Mortality; Density dependence	Daily survival rates represent probability of survival dependent on fish stage and age; in the density-dependent model version, the daily survival rate of eggs and larvae is dependent on subadult and adult density
Predation	Predation	Subadult or adult fish are chosen randomly for predation death; if the chosen fish has a higher biomass than the Topeka shiner biomass to be eaten by largemouth bass, the ratio between the biomass eaten and the fish biomass defines the probability of the fish to die
Fish condition	Fish condition	Each fish agent draws its minimal condition for survival from a normal distribution defined by the average minimal condition (K_{min}); a fish dies if its condition drops below its own threshold.
Lethal effects of pesticide exposure	GUTS	Mortality due to pesticide exposure is drawn from a distribution in each sub-daily time step in GUTS-SD, and for each fish agent upon its creation in GUTS-IT

1.2.7. Collectives

No collectives are included in the model.

1.2.8. Observation

Model outputs are generated on a daily time step. Observations include number of Topeka shiners in each life stage, cumulative Topeka shiner biomass per life stage, biomass of prey guilds (after consumption by Topeka shiner), biomass and number of fish in each life stage eaten by largemouth bass.

1.3. Details

1.3.1. Initialization

Initial Topeka shiner number is derived from Topeka shiner biomass present on the first day (1 January) of the simulation; the sum of biomasses used for Topeka shiner juveniles and adults as used for initialization of $CASM_{OC}$ food web is used as initial biomass of Topeka shiner in the TS-IBM.

Demographic composition of Topeka shiner populations reported for October (Dahle 2001) are applied to initial Topeka shiner biomass. Note that no juveniles are present in winter in TS-IBM. Accordingly, all initial Topeka shiner biomass is distributed across subadults and adults age 0-2 years old including biomass listed for juveniles in the CASM food web input file.

Parameters defining functional response, bioenergetics and other fish parameters are set in a parameter input file.

1.3.2. Input data

Waterbody conditions are inputs to the model and provide daily water temperature and water depth. Input data applied to these abiotic properties are identical to the input data used in corresponding $CASM_{OC}$ simulations. Daily biomasses (in g carbon-equivalent, gC) of each prey guild generated by $CASM_{OC}$ are inputs to the model. Guilds representing Topeka shiner diet are Copepoda, Cladocera (representing Cladocera and Ostracoda), Rotifera, microzooplankton, mayflies (Ephemeroptera), caddisflies (Trichoptera; representing all insect diet other than mayflies and chironomids), Oligochaeta, Chironomida, detritus (Sediment POC) and periphyton. Biomass of Topeka shiner eaten by largemouth bass is also listed in the food web input file generated by $CASM_{OC}$. Benzovindiflupyr daily concentrations (in µg/L or ppb) are read from an input file.

1.4. Submodels

1.4.1. Topeka shiner life history and reproduction

Individual fish are characterized in the model by their age (days), life stage, sex, weight (g wet weight) and standard length (mm). Additional parameters define the fish condition and bioenergetics as well as the spawning dates for adult females. The age counter is started on the day when an egg is laid, and the sex of the individual is determined randomly assuming a 1:1 sex ratio (see Section 2.1.2.).

Sizes of Topeka shiners and other fish species may be reported as weight or lengths in the literature. In order to compare fish sizes of the simulated fish with data in the literature, both measures are assigned to each fish in the model. Biomass and fish length are proportional within a species (Equation (1), see Section 2.1.1. for parameterization for Topeka shiner):

(1) $$log_{10}(W) = \alpha_{LW} log_{10}(SL) + \beta_{LW}$$

where

SL: standard fish length (mm)
W: fish wet weight (g)
α_{LW}: slope (g/mm)
β_{LW}: intercept (g)

The life cycle of fish is characterized by the following life stages: eggs, larvae, juveniles, subadults and adults (Figure S1). Eggs remain unchanged throughout their life stage. Larvae are assumed to use energy

(from yolk), but not consume any food. Once Topeka shiner transition to juvenile stage, they start food consumption. The transition of an individual from one life stage to the next is defined by individual age for egg and larval stage (model input parameters 'EggDevTime' and 'YolkLasting', respectively; Table S4) and by fish size in standard length for the transition from juvenile to subadult and subadult to adult (model input parameters 'MinSizeSubadult' and 'MinSizeMat', respectively; Table S4). Consumption is dependent on fish biomass, temperature and food availability, and respirationon fish biomass and temperature (see submodel Bioenergetics, Section 1.4.8.).

Spawning occurs during the time period defined by a start and end date. The spawning period is assigned stochastically in each simulated year by drawing from three uniform distributions. Each distribution is defined by the earliest and the latest date observed (in literature). The three distributions define the start date, the peak date and the end date of spawning. On the start day of spawning in a given simulated year, each mature female chooses her spawning date of the year by drawing from a triangular distribution defined by the year's start, peak and end date of spawning. A single spawning event per spawning season is assumed. Females that do not reach maturity by the year's start date of spawning will not spawn. The data available about the spawning season in Topeka shiners is described in Section 2.1.3.

The egg laying rate is dependent on the female's wet weight on the spawning date (Equation (2)).

(2) $$\ln(F) = \beta_0 + \beta_1 W$$

where

F: number of eggs
W: spawning female's wet weight (g)
β_0: intercept (unitless); fitted to data (see Section 2.1.3.)
β_1: slope (g^{-1}); fitted to data (see Section 2.1.3.)

Initial egg mass is determined by the input parameter 'EggWeight'. The weight of the eggs spawned ($F \times$ EggWeight) is subtracted from the spawning female's wet weight. The parameters relevant to the life history representation in the model are summarized in the parameter table (Table S4). The data available from the literature, and their use for the model are described in Section 2.1.

1.4.2. Mortality

Fish are assumed to experience background mortality. Background rates of mortality are applied stochastically in the model, and vary according to fish stage and age. Mortality rates of fish in juvenile, subadult and adult stages were derived from demographic rates reported in the literature (Dahle 20001; Kerns and Bonneau 2002). Stage- and age-specific daily survival rates of fish in the model are listed in the Parameter Table (Table S4). In Section 2.2., the data sources and analysis for the background survival rates are described. Daily survival rates were applied stochastically, i.e. the rates reflect the daily probability of a fish agent to survive to the next time step in the model. Based on the oldest fish observed in the field, Topeka shiners in the model cannot live beyond the spawning season after it reaches the age of 3 years. Accordingly, fish agents may reproduce after reaching the age of 3 years, but die after the spawning season.

Because no information for egg and larval survival rates in Topeka shiners were available, the daily survival rates of these life stages were used for calibration of the model (Section 5.1.2.). In the density-dependent version of the model, density dependence was applied to the survival rates of eggs and larvae (Sections 1.4.3. and 5.1.2.). Separate from the background mortality rate, fish agents in the model may die of poor condition (Section 1.4.8.) or predation (Section 1.4.3.).

1.4.3. Density dependence

In the TS-IBM, we assume that Topeka shiner populations are density-regulated. A mechanism of density-dependence in the species is suggested in the literature where egg and larva cannibalism by Topeka shiner is described (Campbell et al. 2016). In the model, we assume that egg and larva survival rates decrease with increasing biomass of subadult and adult Topeka shiner present (Figure S2). Density dependence is implemented as a Ricker function (Morris and Doak 2002; Equation (3)).

(3) $$s_{egg}(B_{TS}) = s_{egg}(0)e^{-\beta B_{TS}}$$

where

$s_{egg}(0)$: daily egg and larva survival rate in the absence of subadult and adult Topeka shiner (unitless)
B_{TS}: combined biomass of all subadult and adult Topeka shiner present in the waterbody on a given day (g wet weight)
β: steepness of function

Density dependence of daily egg and larva survival rate is controlled by the switch 'DD_egg_larva', and the parameters $s_{egg}(0)$ and β are defined as model input parameters (see Table S4).

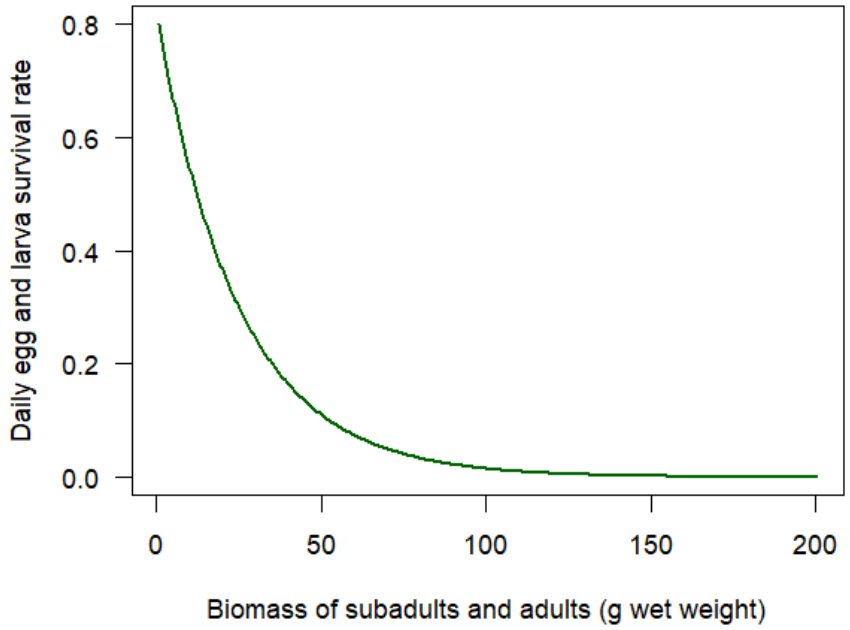


Figure S2. Ricker function applied to daily egg and larva survival rates dependent on combined biomass of subadult and adult Topeka shiner present in the population.

1.4.4. Predation

The presence of largemouth bass in a waterbody with Topeka shiners were identified as an important reason for decline of the populations (Schrank et al. 2001; Campbell et al. 2016). Largemouth bass are included in the aquatic food web in $CASM_{OC}$, and the biomass of Topeka shiners consumed by largemouth bass in every daily time step is estimated in $CASM_{OC}$. It is assumed that largemouth bass only

prey on subadult and adult Topeka shiners (combined as adult Topeka shiner in $CASM_{OC}$; also see Section 2.4.).

Simulations with and without predation by largemouth bass can be run with the TS-IBM by setting a switch ('Predation') in the interface accordingly. If predation is included, an individual is chosen randomly from the simulated Topeka shiner population (with life stage subadult or adult). If the biomass to be eaten by largemouth bass exceeds the biomass of the chosen Topeka shiner, the individual dies. The remaining biomass to be eaten by largemouth bass is used to decide about the fate of the next randomly chosen Topeka shiner. If the remaining biomass to be eaten by largemouth bass is smaller than the biomass of the focal Topeka shiner, the fish's survival probability is calculated as the ratio: remaining biomass to be eaten divided by the biomass of the focal fish. Whether the focal fish dies or not is determined stochastically. No further Topeka shiners are removed afterwards, i.e. no further predation occurs on the given day.

1.4.5. Sunfish hosts

Topeka shiner males defend small territories at the edges of sunfish nests to attract females. After spawning, the parental fish do not guard their clutch but benefit from the nest guarding by the host sunfish. Topeka shiner were reported to be brood parasites of orange spotted sunfish, *Lepomis humilis*, and green sunfish, *Lepomis cyanellus*. The egg development time of host and Topeka shiner were reported to be similar (Dahle 2001; Kerns and Bonneau 2002; Stark et al. 2002; Campbell et al. 2016). The egg development time for Topeka shiner is derived from reported egg development times of the host sunfish (Campbell et al. 2016; also see Section 2.5.).

No quantitative data on the effect of presence or absence of sunfish on Topeka shiner reproductive behavior, egg and larva survival are available from the literature. In the model, we assume that the absence of sunfish in the waterbody leads to decreased survival rates in eggs (larval survival rates are independent of sunfish presence or absence). If sunfish hosts are assumed to be absent from the waterbody, 'Sunfish' can be switched 'Off', resulting in the multiplication of daily egg survival rate by 'SunfishFactor' (input parameter set between 0 and 1). Including this factor makes it possible to test potential impacts on Topeka shiner populations due to the absence of sunfish hosts. The baseline assumption in the model is that sunfish are present and daily eggs survival rate is multiplied by 1.

1.4.6. Topeka shiner diet

In the model, we assume that juvenile and subadult/adult Topeka shiners rely on different food compositions. Guilds (organism groups or detritus) in the food web used by Topeka shiners as diet in the model were aligned with qualitative gut content data reported in the literature for adult Topeka shiner (see Section 2.6.). No data were available for juvenile Topeka shiner. Assumptions about guilds making up the diet of juvenile and subadult/adult Topeka shiner in the model were applied in both, the TS-IBM and the $CASM_{OC}$. Diet guilds as applied in the model are listed in Table S3.

For the transfer of data of Topeka shiner and prey biomasses between $CASM_{OC}$ and the TS-IBM, conversions have to be applied. $CASM_{OC}$ uses the carbon equivalent (gC) of biomasses for all guilds while the TS-IBM uses g wet weight. The conversion factors from gC to g wet weight for each relevant guild (gC_ww_<guild name>) are listed in the parameter table along with the functional response parameters for each prey guild.

Table S3. Prey guilds consumed by juvenile and subadult/adult Topeka shiner in the model. Periphyton summarizes 10 guilds simulated separately in $CASM_{OC}$. Note that Cladocera and Ostracoda simulated as separate guilds in $CASM_{OC}$ are combined in the TS-IBM diet guild Cladocera. The TS-IBM diet guild Trichoptera combines all insect diet other than Ephemeroptera and Chironomids. Accordingly, the $CASM_{OC}$ guilds 'Trichoptera', 'Corixids', 'Coleopterans' are added up for input to TS-IBM.

Diet guild	Juvenile TS	Subadult/adult TS	Remarks
Microzooplankton	+		
Rotifera	+		
Copepoda	+	+	
Cladocera	+	+	Combine the CASM diet guilds 'Cladocerans' and 'Ostracods'
Chironomidae		+	Diet guild (from CASM) representative of all Diptera eaten by TS
Ephemeroptera (mayflies)		+	
Trichoptera (caddisflies)		+	Combines the diet guilds (from CASM) representative of all insects other than Diptera and Ephmeroptera, and Hydrocarina eaten by TS $CASM_{OC}$ diet guilds combined: 'Trichoptera', 'Corixids', 'Coleopterans'
Periphyton		+	Guild from CASM included in Periphyton: Diatom 3-5; Chlorophyte 5-7; Crytophyte 1; Cyanophyte 5-6; Euglenoid 1; Elodea; Potamogeton
Detritus	+	+	Sediment POC in CASM

1.4.7. Functional response to prey density

Consumption rate by Topeka shiner is dependent on food availability (density) in the waterbody. If a fish has food available *ad libitum*, its consumption rate is limited by a maximum consumption C_{max} dependent on temperature (f_C(T)), i.e. p=1 (see Equation (7)). For the model, we are interested in the effects of food limitation on fish growth and reproduction. We apply a functional response function that scales daily consumption of each fish to the density of the prey available that day, i.e. the functional response calculates the value of the factor p from Equation (4).

Applying a functional response assumes that rather than all prey biomass being readily available for consumption by all Topeka shiner in the model until complete depletion, decreasing densities of prey (biomass in the water body) result in reduced encounter rates with prey, and accordingly, reduced consumption rates.

For the functional response, we apply a Holling Type II function also implemented in CASM (Bartell et al. 2013; Equation (4)).

(4) $$C_i = C_{max}(T,\ W_{TS})\, W_{TS} \frac{pref_i\, ass_i\, h_i\, W_i}{\sum pref_i\, ass_i\, h_i\, W_i}$$

where

C_i: consumption rate by Topeka shiner of prey type i (J g^{-1} d^{-1})
$C_{max}(T, W_{TS})$: maximum consumption rate per day (J g^{-1} d^{-1}) dependent on water temperature T (see equation (8))
W_{TS}: biomass of Topeka shiner (g wet weight)
$pref_i$: preference of Topeka shiner for prey type i (unitless)
ass_i: assimilation efficiency for prey i (unitless)
h_i: handling efficiency for prey i (set to 1 for all prey guilds; unitless)
W_i: biomass of prey i (g wet weight)

and

$$\mathrm{C}(d) = \sum C_i$$

The parameter values as applied in $CASM_{OC}$ for the Topeka shiner are used in the TS-IBM and are listed in the model parameter table (Table S4). For the estimation of preferences for different prey types by Topeka shiner, see Section 2.7.

For the calculation of the functional response, daily biomass values from $CASM_{OC}$ (provided in carbon equivalent of the biomass per m^2 of the waterbody, gC/m^2) are converted to biomasses in wet weight in the whole water body using guild-specific factors (gC_ww parameters, see Table S4) and the pond area, resulting in prey guild biomasses in g wet weight. Because consumption by Topeka shiner is given in J, $C_{max}(T,\ W_{TS})$ is divided by the average energy density of the prey guilds to estimate consumption in g per fish.

The consumed biomass from each prey guild by each Topeka shiner is subtracted from the guild's daily biomass pool available. The biomass (in g wet weight) of each prey guild is converted to energy (by multiplying with the guild-specific energy density, *ED* in J/g). The sum of the energies consumed from each prey guild is the daily consumption (J/d) per fish, and is used to calculate the growth of the fish.

The biomass of each prey guild available for consumption by an individual Topeka shiner in the model is scaled to the fish's size. This is based on the assumption that smaller fish have a smaller range of daily foraging than larger fish. We apply a scaling of the search area according to the ¾ power (Accolla et al. 2015). The biomass within the search area is calculated according to Equation (5). For free-swimming prey (Copepoda, Cladocera, Rotifera, microzooplankton, periphyton), a volume is assumed (i.e. scaling the biomass in the simulated waterbody to the search volume). For bottom-dwelling prey (Ephemeroptera, Trichoptera, Oligochaeta, Chironomids, detritus) the biomass is scaled according to waterbody area.

(5) $$\mathrm{S} = \mathrm{z}\left(\frac{SL}{1000}\right)^{\frac{3}{4}}$$

where

S: search area (m^2) or search volume (m^3)
z: scaling factor (default: $z = 1$; unitless)

SL: standard length of fish (mm)

1.4.8. Bioenergetics

For the implementation of the bioenergetics submodel, we use the Wisconsin fish bioenergetics model (Hanson et al. 1997, Deslauriers et al. 2017). Fish in all stages are represented by their biomass (g wet weight). Biomass in eggs is assumed to be constant between time of spawning and hatching, and newly hatched larvae are assumed to have the same biomass as eggs.

In the initial phase after hatching, larvae do not feed and lose biomass as they deplete their yolk sacs. Growth is represented as change in existing weight according to the fish bioenergetics model. Investment in gonadal growth is assumed in adult fish, but not represented explicitly in the model (outside of growth). Females lose biomass when they spawn according to the weight of the produced clutch.

Growth

Growth is simulated as the gain in weight due to energy from food consumption *C* (J/g) that is not lost to excretion and egestion (*E*(*C*); J/g) or used for metabolism (*M*(*T*); J/g) results in fish growth.

(6) $$\Delta W = \big(C(p,T) - M(T) - E(C)\big) ED_{TS}^{-1}$$
$$= (C(p,T) - (c_{oc}R(T) + A + S) - \big(F(C) + U(C)\big)\, ED_{TS}^{-1}$$

where

ΔW: weight gain (g/g wet weight)
p: factor accounting for food availability; see submodel Functional response (Section 1.4.7.)
T: water temperature (in °C)
C: consumption (J/g)
M: metabolic losses (J/g)
E: waste losses (J/g)
ED_{TS}: Energy density of Topeka shiner, J/g wet weight
c_{oc}: oxycalorific coefficient
R: respiration (g O_2/g)
A: active metabolism (J/g; assumed 0 for TS, see below)
S: special dynamics action (J/g)
F: egestion (J/g)
U: excretion (J/g)

The parameter values applied in the model are listed in the parameter table (Table S4). The literature sources for energy densities of Topeka shiner and its prey are reported in Section 2.8.1.

Consumption

The daily energy consumption *C* by a fish depends on food availability (*p*), water temperature (*T*) and the maximum consumption rate C_{max} (J/(g d)) as observed in *ad libitum* feeding studies at optimum temperature for the fish.

(7) $$C(p,T) = C_{max}\, p\, f_c(T)$$

The maximum consumption rate C_{max} is assumed to be dependent on fish weight, calculated according to Equation (8):

(8) $$C_{max} = \alpha_{cmax} W^{\beta_{cmax}}$$

where
C_{max}: maximum consumption rate in J/g fish wet weight
α_{cmax}: slope (J g^{-2}; calibrated parameter: see Section 5.1.1.)
W: fish wet weight (g)
β_{cmax}: unitless; calibrated parameter: see Section 5.1.1.

For the relationship between consumption and temperature, we apply the equation from Fish Bioenergetics cool- and cold-water species (Thornton and Lessem 1978; Equation (9) for consumption in Fish Bioenergetics; also applied in $CASM_{OC}$).

(9) $$f_c(T) = K_A K_B$$

where

$$K_A = \frac{CK1 \cdot L1}{1 + CK1(L1 - 1)}$$

$$K_B = \frac{CK4 \cdot L2}{1 + CK4(L2 - 1)}$$

$$\mathrm{L1} = e^{G1(T - CQ)}$$

$$\mathrm{G1} = \frac{1}{CTO - CQ} \cdot log\left(\frac{0.98(1 - CK1)}{0.02CK1}\right)$$

$$\mathrm{L2} = e^{G2(CTL - T)}$$

$$\mathrm{G2} = \frac{1}{CTL - CTM} \cdot log\left(\frac{0.98(1 - CK4)}{0.02CK4}\right)$$

In these equations $f_c(T)$ is essentially the product of two sigmoid curves: one curve fit to the increasing part of the consumption-at-temperature curve (K_A), and one curve fit to the decreasing part of the consumption-at-temperature curve (K_B). In K_A, *CQ* is the lower water temperature at which the temperature dependence is a small fraction (*CK1*) of C_{max} and *CTO* is the water temperature at which $\mathrm{C} = 0.98\, C_{max}$. In K_B, *CTM* is the water temperature ($\geq$ *CTO*) at which $\mathrm{C} = 0.98\, C_{max}$ and *CTL* is the temperature at which consumption is a small fraction (*CK4*) of C_{max}.

Data from fathead minnow as surrogate species are applied to Topeka shiner populations in $CASM_{OC}$ and individual Topeka shiner in TS-IBM. The variable *p* is calculated in the model in each time step dependent on food availability, see submodel Functional response (Section 1.4.7.). The maximum consumption rate, $C_{max}(T,\ W_{TS})$, is handed to the functional response where the actual daily consumption is calculated dependent on prey densities in the waterbody. Note that 'day_consumption' is the actual consumption by each Topeka shiner on a given day in J per fish. In the calculation of fish growth, it is scaled to the fish's biomass (J/g wet weight) to match the units of metabolic rates (see Section Metabolism below).

Metabolism

The fish are assumed to use energy for metabolism including respiration *R* and specific dynamic action *S*. Active metabolism from sustained swimming is assumed to be negligible, i.e. *A* = 0. Specific dynamic action is a constant fraction of consumption (not temperature dependent).

Accordingly, metabolic expenses can be calculated applying Equation (10).

(10) $$\mathrm{M(T)} = \mathrm{R(T)} + \mathrm{SDA(C - F)}$$

where

SDA: specific dynamic action (unitless)
C: consumption; see Equation (7); J/(g d)
F: egestion rate J/(g d); see Equation (13)

Respiration *R(T)* is defined as follows:

(11) $\mathrm{R}(T) = \mathrm{RA}\, W^{RB}\, f_R(T)$

where

R(*T*): specific rate of respiration ($g(O_2)/(g\ d)$)
W: fish wet weight (g)
RA: intercept of the allometric mass function ($g(O_2)/g^2$)
RB: slope of the allometric mass function (unitless)
$f_R(T)$: temperature dependence function for respiration (see Equation (12); unitless)
T: water temperature (°C)

In the fish bioenergetics equations (Hanson et al. 1997; Deslauriers et al. 2017), respiration is multiplied by an additional factor, ACTIVITY. For the TS-IBM, no additional respiration dependent on swimming speed is assumed, i.e. ACTIVITY = 1.

For the temperature dependence function for respiration, we used respiration model 2 from Fish Bioenergetics 4.0 (Kitchell et al. 1977).

(12) $f_R(T) = V^X\, e^{X(1-V)}$

where

$\mathrm{V} = (\mathrm{RTM} - \mathrm{T})/(\mathrm{RTM} - \mathrm{RTO})$

$\mathrm{X} = (\mathrm{Z}^2(1 + (1 + 40/\mathrm{Y})^{0.5})^2)/400$

$\mathrm{Z} = \ln(\mathrm{RQ})(\mathrm{RTM} - \mathrm{RTO})$

$\mathrm{Y} = \ln(\mathrm{RQ})(\mathrm{RTM} - \mathrm{RTO} + 2)$

In these equations, *RTO* is the optimal respiration temperature (°C); *RTM* is the maximal lethal water temperature; *RQ* approximates the Q_{10} (the rate at which the function increases over relatively low water temperatures).

Consumption and metabolism peak at different temperature which has important impacts on fish bioenergetics.

Waste losses (egestion and excretion)

Waste losses, excretion and egestion, are modeled as constant proportions of consumed energy (*C*; J/g). Here egestion (*F*; J/g) represents fecal loss (i.e., energy in undigested food) and excretion (*U*; J/g) represents energy lost in nitrogenous waste (i.e., urination).

(13) $E(C) = F(C) + U(C)$

where

$\mathrm{F} = \mathrm{FA} \times \mathrm{C}$
$\mathrm{U} = \mathrm{UA}(\mathrm{C} - \mathrm{F})$
FA: constant proportion of consumption (unitless)
UA: constant proportion of assimilated energy (unitless)

1.4.9. Fish condition

If fish consume less food than is lost due to metabolism and waste losses combined, the condition of the fish declines (Van Winkle et al. 1998). The fish loses biomass while the length is assumed to be maintained. Fish condition, *K*, is implemented as the ratio between the actual wet weight of the fish and its expected weight according to its length. The expected weight is calculated from its length according to Equation (1). If *K*>1, fish length is recalculated from its weight, i.e. the fish is growing. Fish condition can drop below 1 either because of food limitation or due to spawning by adult female Topeka shiner. If $K < K_{min}$, the fish dies. When a new Topeka shiner is created in the model (upon model initialization or at time of spawning), it draws a value for K_{min} from a normal distribution around the model input parameter 'AverageKmin'. The standard deviation of the normal distribution is defined by 10% of the average.

1.4.10. Lethal effects of pesticide exposure

If pesticide exposure and effects are simulated, the GUTS submodel results in additional mortality of juveniles, subadults and adults dependent on the daily exposure pattern (provided as input to the model). The general unified threshold model of survival (GUTS) was calibrated using raw data from standard fish acute toxicity tests performed with fathead minnows and carp by Ashauer et al. (2013). The lethal effects of benzovindiflupyr are implemented in the TS-IBM using the model and parameterization described by Ashauer et al. The GUTS model is a simplified toxicokinetic-toxicodynamic (TKTD) model. Because internal concentrations within the organism (determined by uptake and elimination) were not measured in the available toxicity studies, the time course of the scaled internal concentration *Ci* is dependent on the external (water) concentration *Cw* using a dominant rate constant *ke* (Equation 14).

$$\frac{dCi(t)}{dt} = ke \times \left(Cw(t) - Ci(t)\right) \quad (14)$$

The scaled internal concentration determines the survival probability of the fish. Two models for the probability of death dependent on the internal concentration have been proposed: a) assuming all individuals in a population have the same threshold leading to mortality from exposure whereby likelihood of survival until time *t* can be described by a normal distribution (stochastic deaths, GUTS-SD); b) assuming that individuals in the population vary in their internal concentration thresholds that cause death (individual tolerance, GUTS-IT). In the TS-IBM, we implemented both versions of GUTS.

For GUTS-SD, the hazard rate *H* is the instantaneous probability for an organism to die (Equation 15).

$$\frac{dH(t)}{dt} = kk \times \max(Ci(t) - z, 0) \quad (15)$$

Where *kk* is the killing rate, *Ci* is the scaled internal concentration, and *z* is the concentration threshold. Note that no 'control' mortality is applied because the TS-IBM assumes background mortality in the absence of pesticide exposure which is applied prior to the GUTS submodel. The probability of survival *S* is then defined as:

$$S(t) = e^{-H(t)} \quad (16)$$

The dominant rate constant *ke*, the killing rate *kk* and the concentration threshold *z* were fit to data from the toxicity study (Ashauer et al. 2013), and are inputs to the TS-IBM using GUTS-SD.

For GUTS-IT, each fish in the TS-IBM draws a threshold concentration for survival from a distribution. The concentration distribution is pre-calculated using Equation (17).

$$F(t) = \frac{1}{1+\left(\frac{Ci}{\alpha}\right)^{-\beta}} \quad (17)$$

Where α and β are shape parameters of the distribution (unitless) which were fit to the benzovindiflupyr study data along with the dominant rate constant *ke* (Ashauer et al. 2013). The GUTS-IT thresholds are calculated upon setup of the model, and stored in a look-up table.

Each simulated fish is assigned with its threshold at the start of the simulation run or when it is spawned as egg during the simulation. The individual threshold of a fish does not change until its death. If the internal concentration of the fish exceeds its threshold, it dies.

Whether GUTS-SD or GUTS-IT is applied in a simulation is determined by a switch. The parameters for GUTS are defined as model parameters (listed in Table S4). Parameters reported by Ashauer et al. (2013) for fathead minnow were applied.

The GUTS submodel is applied in sub-daily time steps to achieve a monotonous function $\frac{dCi(t)}{dt}$.

1.4.11. Sublethal effects of pesticide exposure

If sublethal effects of pesticide exposures are simulated, the simulated growth of Topeka shiners is affected by a reduction in their maximum consumption rate, C_{max}. The implementation follows a toxicokinetic-toxicodynamic (TKTD) model that simulated the uptake and elimination of the chemical from the water and the effects of the internal concentration. The TKTD model was implemented following Jager and Zimmer (2012).

The internal concentration of simulated fish is dependent on the daily external (water) concentration (read in from an input file). The internal concentration c_v is simulated according to a one-dimensional kinetics model (Jager and Zimmer 2012; Equation 18).

$$\frac{dc_v}{dt} = k_E \frac{L_m}{L}(c_d - c_v) - c_v \frac{3}{L}\frac{dL}{dt} \quad (18)$$

In this expression, k_E is the elimination rate; L_m is the average maximal length of Topeka shiner (mm); L is the current body length of the simulated fish (mm); and c_d is external concentration in µg/L (ppb).

If the internal concentration cv exceeds the threshold for sublethal effects c0, the Topeka shiner is assumed to experience stress. Stress is implemented as a proportional stress term that can take values between 0 (no stress/effect) and 1 (highest stress level). The stress term, *s*, is calculated according to Equation 19.

$$s := \begin{cases} \frac{1}{c_T}(c_v - c_0) & \text{if } c_v > c_0, \\ 0 & \text{otherwise} \end{cases} \quad (19)$$

Where c_v is the scaled internal concentration of the chemical (µg/L); c_0 is the greatest concentration at which the chemical has no effect on individual fish, or NOEC (µg/L), and c_T is the tolerance gradient (µg/L), i.e. the sensitivity to the toxicant at concentrations above c_0. Stress *s* is required to be in the interval [0, 1]; values calculated to be >1 are set to 1.

The stress term is then applied to the maximum consumption by Topeka shiner in the functional response submodel (section 1.4.7) according to Equation 20.

$$C_{maxS} = C_{max}(1 - s) \quad (20)$$

The sublethal effects model is implemented using sub-daily time steps to achieve a monotonous function for Equation 18. The same temporal resolution for the sub-daily time steps is applied as for the lethal effects model (defined by an interface model parameter, guts_n). To allow the simulation of the sublethal effects on a sub-daily time step, the functional response (section 1.4.7) and growth according to the bioenergetics model (section 1.4.8) are re-implemented for the sublethal TKTD model to simulate the sub-daily (guts_n) time steps.

1.5. Model parameters

Table S4. Model parameters and their values applied in the TS-IBM are listed.

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
Submodel: Topeka shiner life history and reproduction							
α_{LW}	F	l2w_a	g	3.3798	(1)	Dahle 2001; Kearns and Bonneau 2002	Calculation of Topeka shiner weight (g) from fish length (mm SL); parameters fit to data presented in the two studies (Section 2.1.1.)
β_{LW}	F	l2w_b	-	-5.3722			
Earliest start date of spawning	F	StartSpawning_early	Day of year	135		Dahle 2001; Kerns and Bonneau 2002	Spawning period reported late May through early August, dependent on study (Section 2.1.3.)
Latest start date of spawning	F	StartSpawning_late	Day of year	143			
Earliest peak date of spawning	F	PeakSpawning_early	Day of year	162			
Latest peak date of spawning	F	PeakSpawning_late	Day of year	197			
Earliest end date of spawning	F	StopSpawning_early	Day of year	212			

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
Latest end date of spawning	F	StopSpawning_late	Day of year	218			
β_0	F	beta_0	g^{-1}	5.6671	(2)	Dahle 2001; Kerns and Bonneau 2002	Function fit to fecundity data from the two studies (Section 2.1.3.)
β_1	F	beta_1	-	0.3695			
EggWeight	F	EggWeight	g	0.00054		Dahle 2001	Initial wet weight of eggs; derived from average diameter of ova (0.835 +/- 0.046 mm; range: 0.726 – 0.972 mm)
EggDevTime	F	EggDevTime	d	5		Campbell et al. 2016	Assumption that egg development time is similar to Orangespotted and green sunfish
YolkLasting	F	YolkLasting	d	5			Estimated duration of larval stage
MinSizeSubadult	F	MinSizeSubadult	mm	15		Kerns and Bonneau 2002	Standard length (SL); Topeka shiner reported to reach subadult pigmentation at this length
MinSizeMat	F	MinSizeMat	mm	30		Kerns and Bonneau 2002	Smallest mature female SL reported; note that males seem to be bigger when reaching maturity (≥36 mm SL)
DailySurvival_Egg_Larva	F	DailySurvival_Egg_Larva	-	0.76			Calibrated to achieve +/- stable populations (Section 5.1.2.)
DailySurvivalRate_Juv	F	DailySurvivalRate_Juv	-	0.9955		Dahle 2001; Kerns and Bonneau 2002	Derived from demography in Topeka shiner field survey reported in study (Section 2.2.)
DailySurvivalRate_Subadult	F	DailySurvivalRate_Subadult	-	0.9955			

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
DailySurvivalRate_Yr2	F	DailySurvivalRate_Yr2	-	0.9981			
DailySurvivalRate_Yr3	F	DailySurvivalRate_Yr3	-	0.9925			
Submodel: Bioenergetics							
c_{oc} (oxycalorific coefficient)	F	OxycalCoeff	J/g O_2	13560	(6)	Deslauriers et al. 2017	
α_{cmax}	F	a_cmax	-	0.1	(8)		Calibrated to match Topeka shiner growth data (see Calibration to $CASM_{OC}$ food web)
β_{cmax}	F	b_cmax	-	-0.27			
CQ	F	te1	˚C	10.8	(9)	Equation: Thornton and Lessem (1978)	Temperature parameters fit to data from Koehle (2006), see Section 2.9.
CTO	F	te2	˚C	26.6			
CTM	F	te3	˚C	27.8			Temperature parameters fit to data from Koehle (2006), see Section 2.9.
CTL	F	te4	˚C	34.9			
CK1	F	xk1		0.01		Equation: Thornton and Lessem (1978)	Values from $CASM_{OC}$; Input file: casm_TS_bio_parms_RSK_WithTS_08Oct2018.txt
xk2	F	xk2		1			
xk3	F	xk3		1			
CK4	F	xk4		0.01			
SDA	F	SDA		0.172	(10)		Values for fathead minnow from fish bioenergetics 4.0 (Deslauriers et al. 2017)
RA	F	RA	-	0.0096	(11)	Hartman (2017)	

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
RB	F	RB	-	-0.041			Values for fathead minnow from fish bioenergetics 4.0 (Deslauriers et al. 2017)
RTO	F		°C	26.7	(12)	Equation: Kitchell et al. 1977	Temperature parameters fit to data from Koehle (2006), see Section 2.9.
RTM	F		°C	39.5			
RQ	F		$°C^{-1}$	4.9	(12)		
FA	F		J/(g d)	0.1	(13)		Values for fathead minnow from fish bioenergetics 4.0 (Deslauriers et al. 2017)
UA	F		J/(g d)	0.1	(13)		
Submodel: Functional response, juvenile TS							
$pref_{cladocerans}$	F	juv_pref_cladocerans		0.25	(4)		Preferences assumed equal due to lack of diet data for Topeka shiner juveniles; assimilation rates from $CASM_{OC}$ used, see Appendix A, section 2.2.7; input file: web_casmTS_HRM_20Jun2018.dat
$pref_{copepods}$	F	juv_pref_copepods		0.25			
$pref_{microzoo}$	F	juv_pref_microzoo		0.25			
$pref_{rotifers}$	F	juv_pref_rotifers		0.25			
$pref_{detritus}$	F	juv_pref_detritus		0.25			
$ass_{cladocerans}$	F	juv_ass_cladocerans		0.75			
$ass_{copepods}$	F	juv_ass_copepods		0.75			
$ass_{microzoo}$	F	juv_ass_microzoo		0.75			
$ass_{rotifers}$	F	juv_ass_rotifers		0.75			
$ass_{detritus}$	F	juv_ass_detritus		0.35			
$h_{cladocerans}$	F	juv_h_cladocerans		1			
$h_{copepods}$	F	juv_h_copepods		1			

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
$h_{microzoo}$	F	juv_h_microzoo		1			
$h_{rotifers}$	F	juv_h_rotifers		1			
$h_{detritus}$	F	juv_h_detritus		1			
Submodel: Functional response, subadult and adult TS							
$pref_{cladocerans}$	F	adt_pref_cladocerans		0.26	(4)		Preferences derived from Topeka shiner diet studies (Section 2.6.)
$pref_{copepods}$	F	adt_pref_copepods		0.04			
$pref_{chironomids}$	F	adt_pref_chironomids		0.28			
$pref_{maflies}$	F	adt_pref_mayflies		0.01			
$pref_{caddisflies}$	F	adt_pref_caddisflies		0.06			
$pref_{oligochaetes}$	F	adt_pref_oligochaetes		0.02			
$pref_{periphyton}$	F	adt_pref_periphyton		0.16			
$pref_{detritus}$	F	adt_pref_detritus		0.17			
$ass_{cladocerans}$	F	adt_ass_cladocerans		0.75			Assimilation rates from $CASM_{OC}$ used, see Schmolke et al. (2019), Appendix A, section 2.2.7; input file: web_casmTS_HRM_20Jun2018.dat
$ass_{copepods}$	F	adt_ass_copepods		0.75			
$ass_{chironomids}$	F	adt_ass_chironomids		0.75			
$ass_{maflies}$	F	adt_ass_mayflies		0.75			
$ass_{caddisflies}$	F	adt_ass_caddisflies		0.75			
$ass_{oligochaetes}$	F	adt_ass_oligochaetes		0.75			
$ass_{benthicalgae}$	F	adt_ass_periphyton		0.45			
$ass_{detritus}$	F	adt_ass_detritus		0.35			

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
$h_{cladocerans}$	F	adt_h_cladocerans		1			
$h_{copepods}$	F	adt_h_copepods		1			
$h_{chironomids}$	F	adt_h_chironomids		1			
$h_{maflies}$	F	adt_h_mayflies		1			
$h_{caddisflies}$	F	adt_h_caddisflies		1			
$h_{oligochaetes}$	F	adt_h_oligochaetes		1			
$h_{benthicalgae}$	F	adt_h_periphyton		1			
$h_{detritus}$	F	adt_h_detritus		1			
z	I	ScalingSearchArea		1	(5)	Accolla et al. 2015	Section 1.4.7.
Detritus depth	I	MaxDetritusDepth	cm	1.5			Depth of detritus accessible for consumption by Topeka shiner (detritus depth derived from Sediment POC from $CASM_{OC}$)
Conversion factors to calculate g wet weight from gC							
	F	gC_ww_cladocerans	g wet weight/gC	28.6		Wiebe et al. 1975	
	F	gC_ww_copepods		28.6		Wiebe et al. 1975	
	F	gC_ww_microzoo		28.6		Wiebe et al. 1975	
	F	gC_ww_rotifers		28.6		Wiebe et al. 1975	

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
	F	gC_ww_chironomids		13.2		Evans-White et al. 2005, Waters 1977 (cited in Benke and Huryn 2017)	
	F	gC_ww_mayflies		13.2			
	F	gC_ww_caddisflies		13.2			
	F	gC_ww_oligochaetes		13.2			
	F	gC_ww_periphyton		31.3			
	F	gC_ww_detritus		31.3		Sladecek and Sladeckova 1963	
	F	gC_ww_fish		8.75			
Energy densities of prey guilds and TS							
Cladocera	F	ED_cladocerans	J/g wet weight	2837			See section 2.8.1. in this document
Copepoda	F	ED_copepods		3461.2			
Rotifera	F	ED_rotifers		3442.5			
Microzooplankton	F	ED_microzoo		3467.2			
Chironomidae	F	ED_chironomids		3044.7			
Ephemeroptera	F	ED_mayflies		4444.8			
Trichoptera	F	ED_caddisflies		4334.2			
Oligocheata	F	ED_oligochaetes		2654.8			

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
Total periphyton (sum of 10 algae guilds represented in $CASM_{OC}$)	F	ED_periphyton		2300.4			
Detritus (sediment POC)	F	ED_detritus		3331.8			
Juvenile Topeka shiners	F	ED_TS_juv		2553.2			
Adults Topeka shiners	F	ED_TS_adt		4864.1			
Submodel: Density dependence							
Density dependence mode	I	DD_egg_larva	-	On			Switch: if 'Off', egg and larva survival rate is density independent (Section 1.4.3.)
$s_{egg}(0)$	F	DailySurvival_Egg_Larva_0	-	0.8	(3)		Calibrated to achieve +/- stable populations (see Calibration to CASMOC food web)
β	F	beta_dd_egg_survival	-	0.06			
Submodel: Fish condition							
Average K_{min}	I	AverageKmin	-	0.68			Section 1.4.9.
Submodel: Predation							

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
Predation	I	Predation	-	Off			Switch: if 'On', Topeka shiner biomass eaten by largemouth bass leads to mortality (Section 1.4.4.)
Submodel: Sunfish hosts							
Sunfish presence	I	Sunfish	-	On			Switch: if 'Off', egg survival is reduced (Section 1.4.5.)
Submodel: Lethal effects of pesticide exposure							
GUTS-SD dominant rate constant, *ke*	I	GUTS-SD-ke	1/d	1.28	(14)	Ashauer et al. (2013)	GUTS-SD fit to benzovindiflupyr toxicity study data conducted with fathead minnow
GUTS-SD killing rate, *kk*	I	GUTS-SD-kk	L/(µg × d)	0.42	(15)	Ashauer et al. (2013)	GUTS-SD fit to benzovindiflupyr toxicity study data conducted with fathead minnow
GUTS-SD concentration threshold, *z*	I	GUTS-SD-z	µg/L	3.85	(15)	Ashauer et al. (2013)	GUTS-SD fit to benzovindiflupyr toxicity study data conducted with fathead minnow
GUTS-IT dominant rate constant, *ke*	I	GUTS-IT-ke	1/d	0.47	(14)	Ashauer et al. (2013)	GUTS-IT fit to benzovindiflupyr toxicity study data conducted with fathead minnow
GUTS-IT threshold distribution shape parameter, α	I	GUTS-IT-a	-	3.97	(17)	Ashauer et al. (2013)	GUTS-IT fit to benzovindiflupyr toxicity study data conducted with fathead minnow

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
GUTS-IT threshold distribution shape parameter, β	I	GUTS-IT-b	-	5.54	(17)	Ashauer et al. (2013)	GUTS-IT fit to benzovindiflupyr toxicity study data conducted with fathead minnow
Number of sub-daily time steps in GUTS and sublethal effects model	I	guts_n	1/d	1440			
Submodel: Sublethal effects of pesticide exposure							
Elimination rate, k_E	I	TKTD-sl-ke	-	0.00061	(18)	York (2010)	Fit to data from York (2010), see Section 2.10.
Average maximal length of Topeka shiner, L_m	I	TS_max_SL	mm	53.2	(18)	Kerns and Bonneau 2002	Average length of Topeka shiner at maximum age (≥36 months) observed in the field
Tolerance gradient, c_T	I	TKTD-sl-cT	µg/L	8.8389	(19)	York (2010)	Fit to data from York (2010), see Section 2.10.
Greatest concentration without effects, c_0	I	TKTD-NOEC	µg/L	0.95	(19)	York (2010)	NOEC for benzovindiflupyr reported by York (2010)
Other interface parameters							

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
Waterbody area (TS-IBM)	I	pondArea	m^2	100			Waterbody area simulated in TS-IBM: needed for calculation of per-area biomasses
Waterbody area ($CASM_{OC}$)	I	CASM_pool_area	m^2	1125			Waterbody area simulated in $CASM_{OC}$: needed for calculation of per-area biomasses
Hybrid version	I	DailyIO	-				Switch: if 'On', daily transfer files are read in and written out (models linked on daily basis; Section 3.)
Random number seed	I	RandomNumberSeed	-				Using the same random number seed leads to identical model outputs if all parameters are equal
Output file	I	BiomassOutput	-				Output file with daily biomass values of Topeka shiner and its diet (Tables S5, S6)
Input parameters	I	InputParameters	-	InputParameters_20Jun2018.txt			Input file with parameter value definitions listed in this table; separate parameter files produced for SA and alternative detritus preferences
Temperature and water depth	I	WaterConditionInput	-	env_casmTS_2010_08May2018.prn			Input file with daily water temperatures and depths; identical input file is used by $CASM_{OC}$

Parameter name	**Input method** F: from file I: set on interface	**Name in TS-IBM**	**Parameter unit**	**Value**	**Equation**	**Reference**	**Remarks**
Biomass input	I	DailyPreyBiomass	-	IBM_TS_master_ref_LMB_yr6_28Jun2018.txt			$CASM_{OC}$-generated input file with Topeka shiner diet guild biomasses (Tables S5, S6)
Model run time	I	YearsToRun	years				Number of years TS-IBM is run (simulation stops automatically at the end of the defined year; yearly inputs are repeated for every simulated year)
Simulation of effects	I	EffectsModule	-	On/off			Switches simulation of effects on or off
Effects type	I	Effects	-	Multiple options			Options allow to choose between the simulation of lethal effects (GUTS-SD or GUTS-IT), sublethal effects or their combination
Exposure input	I	ExposureProfile	-				Input file: list with 365 concentration values (µg/L), file format as used for $CASM_{OC}$
Pesticide name	I	PesticideName	-	Benzovindiflupyr			Pesticide name must match the name in the Exposure input (line 7, entry 2): only used for verification of the correct match between exposure input and effects settings

2. DATA EVALUATION FOR MODEL CONCEPTUALIZATION AND PARAMETERIZATION

2.1. Topeka shiner life history and reproduction

2.1.1. Fish size measures

Length-at-age

Growth of individual Topeka shiner is determined by the bioenergetics model. Fish sizes were used for the calibration of individual growth in the TS-IBM (see Section 5.1.1.). Data were collected from literature; primarily Dahle (2001) and Kerns and Bonneau (2002). Overall means and variances were estimated for each age class. The results are shown in Table S5.

Table S5. Means and partitioned variances for length-at-age of *Notropis topeka*. Mean is in mm; variances are in mm^2.

Age	$\mu_{overall}$	σ^2_{total}	$\sigma^2_{sampling}$	$\sigma^2_{temporal}$
0	23.4	21.0	12.8	8.2
1	32.0	23.3	8.9	14.4
2	43.3	11.0	8.5	2.5
3	50.6	21.0	2.0	18.9

Length-weight relationship

In fish, length and weight of a fish are generally proportional whereby the relationship varies between species (Schneider et al. 2000). Weight-at-length data for Topeka shiners were reported by Dahle (2001) and Kerns and Bonneau (2002) (Table S6), and the relationship was expressed by applying Equation (14):

$$\log_{10} W = \alpha_{LW} + \beta_{LW\log_{10}} SL \quad (14)$$

In this model, W is mass in g, and SL is standard length in mm.

For the application in the TS-IBM, we fit Equation (14) to all three data sets available. For each length, the mean weight was calculated. This mean weight was weighted by the sample size of each estimate of intercept of slope. Finally, a log-log linear model was fit for the mean weights-at-length to generate a composite weight-at-length model (Table S6; Figure S3).

Table S6. Parameters for three weight-at-length models

Source	Sex	N	Intercept (α_{LW})	Slope (β_{LW})
Dahle (2001)	Female	373	-5.309	3.288
Dahle (2001)	Male	293	-5.657	3.529
Kerns and Bonneau (2002)	Both	300	-5.2439	3.3742
Composite (used in model)	Both		-5.3722	3.3798

In the model, therefore, weight can be calculated from length as:

(15) $$W = 10^{3.3875 \log_{10}(SL) - 12.3848}$$

And length can be calculated from weight as:

(16) $$SL = 10^{\left(\frac{\log_{10}(W) + 5.3722}{3.3798}\right)}$$

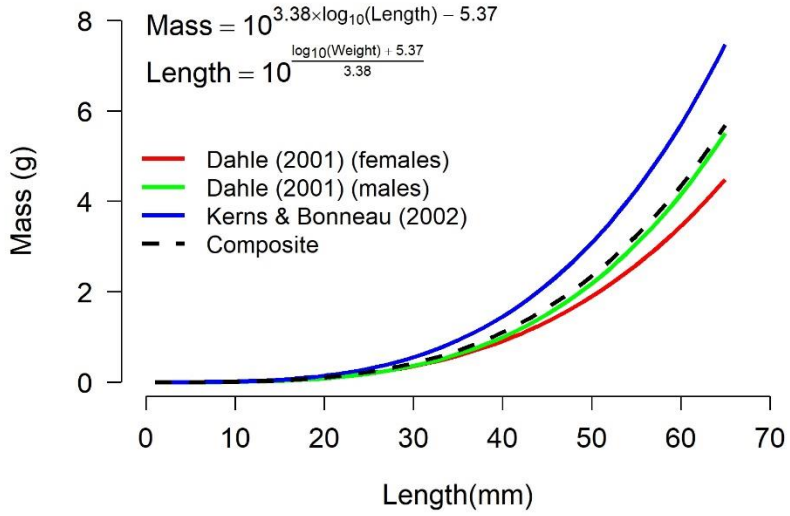


Figure S3. Mass as a function of length in Topeka shiner.

2.1.2. Sex ratio

The sex ratio is defined as a proportion of animals that is female. For Topeka shiner, Kerns and Bonneau (2002) report sex ratios for 3 age classes within a population over two years in Kansas. Dahle (2001) reported sex ratios for 3 age classes in 3 populations. Sex ratio for each was calculated as the proportion of individuals that were female (Table S7). Variance of this ratio was estimated by assuming that the proportion female was the probability of a binomial distribution (p) and the number of individuals was the sample size (N). The variance of a binomial distribution X is:

(17) $$\widehat{\sigma^2}(X) = np(1-p)$$

Table S7. Sex ratios and sample sizes reported by Kerns and Bonneau (2002) and Dahle (2001) for Topeka shiner.

Source	Site	Age	N	# females	p(female)	$\widehat{\sigma^2}$
Kerns and Bonneau (2002)		0	672	352	0.5238	6.8594×10^{-4}
Kerns and Bonneau (2002)		1	304	162	0.5329	7.0994×10^{-4}
Kerns and Bonneau (2002)		2	26	6	0.2308	1.3314×10^{-4}
Dahle (2001)	BC	1	106	65	0.6132	9.4006×10^{-4}
Dahle (2001)	BC	2	38	23	0.6053	9.1586×10^{-4}
Dahle (2001)	BC	3	1	1	1.0000	2.5000×10^{-3}
Dahle (2001)	LP	1	155	90	0.5806	8.4287×10^{-4}
Dahle (2001)	LP	2	36	29	0.8056	1.6223×10^{-3}
Dahle (2001)	LP	3	7	7	1.0000	2.5000×10^{-3}
Dahle (2001)	MC	1	58	43	0.7414	1.3741×10^{-3}
Dahle (2001)	MC	2	91	49	0.5385	7.2485×10^{-4}
Dahle (2001)	MC	3	6	0	0.0000	0.0000

Using the formulae reported by Gould and Nichols (1998), the following parameters for sex ratio were estimated. Note that because there is only one report of age-0 sex ratio, temporal variance cannot be estimated.

Table S8. Estimated means and variances for age-specific sex ratios (proportion female).

Parameter	Mean	Total σ^2	Sampling σ^2	Temporal σ^2
SR_{age-0}	0.5238	6.8594×10^{-4}	6.8594×10^{-4}	
SR_{age-1}	0.6170	7.9628×10^{-3}	9.6674×10^{-4}	6.9960×10^{-3}
SR_{age-2}	0.5450	0.5678	8.4904×10^{-4}	0.5593
SR_{age-3}	0.6666	0.3333	1.6667×10^{-3}	0.3317

In the model, sex is assigned to each individual upon egg production. Because the sex ratio in the first year (age 0) is not considerably different from 1:1, we use the 1:1 ratio in the model. The sex ratio changing with fish age would point to differing mortality rates in females and males. Given the variances in the age-dependent sex ratios and the variability between the two studies and sites, we do not apply sex-dependent survival rates in the model based on the data. Note that sex ratio is not implemented as model variable (i.e. it cannot be changed upon initialization).

2.1.3. Reproduction

Spawning date

Spawning in Topeka shiner occurs during a limited time of the year and is characterized by earliest possible spawn date, latest possible spawn date, and peak spawning time. The day on which an individual spawns varies across this range, with probability greatest at peak spawning time.

Dahle (2001) reported female Topeka shiner in spawning condition as early as 15 May and as late as 6 August. Kerns and Bonneau (2002) report females in spawning condition as early as 23 May and as late as 31 July. Dahle (2001) reports the peak of spawning being approximately 16 July; Kerns and Bonneau (2002) report the peak as closer to 11 June. These data are summarized in Table S9.

Table S9. Reported dates for the onset, end, and peak of spawning. Day of year is given in parentheses.

Source	Onset	Peak	End
Dahle (2001)	15 May (135)	16 July (197)	6 August (218)
Kerns and Bonneau (2002)	23 May (143)	11 June (162)	31 July (212)

Because of the range of spawning season reported, we implement the spawning time stochastically in the model. Spawn dates are drawn in a two-step process:

1. For each year, the starting, ending, and peak spawning dates are chosen by drawing from uniform distributions defined by the dates found by Dahle (2001) and Kerns and Bonneau (2002). E.g., earliest spawn date is chosen from a uniform distribution in [135, 143].
2. For each fish within the year, the date of spawning is drawn from a triangular distribution defined by that year's randomly-selected earliest, latest, and peak dates.

Spawning probability

The spawning probability is the probability that an individual will spawn in a season. Note that in the model, females spawn if they reached the minimum size of maturity at the beginning of the spawning season. The data presented here can be used for model verification, i.e. spawning rates of females in the model can be compared to spawning rates reported in the literature.

Dahle (2001) and Kerns and Bonneau (2002) reported proportions of females spawning (Table S10).

Table S10. Proportions of individuals spawning.

Age	Proportion spawning	Source
1	0.52	Dahle (2001)
1	0.62	Kerns and Bonneau (2002)
2	0.93	Dahle (2001)
2	1.0	Kerns and Bonneau (2002)
3	1.0	Dahle (2001)
3	1.0	Kerns and Bonneau (2002)

Sample sizes from the two studies could not be extracted. In the summary statistics presented in Table S11, the mean proportion spawning for each age is the mean of the two age-specific estimates. For each age class, the variance of the proportion spawning was estimated by first using the two estimates and their mean as the parameters of a triangular distribution, then calculating the variance using the definition of the triangular distribution. The resulting parameters for spawning probability for ages 1 and 2 are shown in Table S11. Because all age 3 individuals in both studies were spawners, we assume that all age-3 individuals spawn during the season.

Table S11. Mean, SD, and beta distribution parameters for spawning probability by Topeka shiner age class. Terms α and β are the shape and scale parameters of a β distribution, which is a more natural way of describing the variability of a proportion. Spawning probability of age-3 individuals is assumed 1.

Age	Mean	SD	α	β
1	0.57	0.0204	334.7268	252.5132
2	0.965	0.0143	158.6736	5.7550

Fecundity

Fecundity, i.e. egg numbers spawned per season, is related to the biomass of the female fish. Dahle (2001) reported raw fecundity at length data for Topeka shiner (Figure S4).

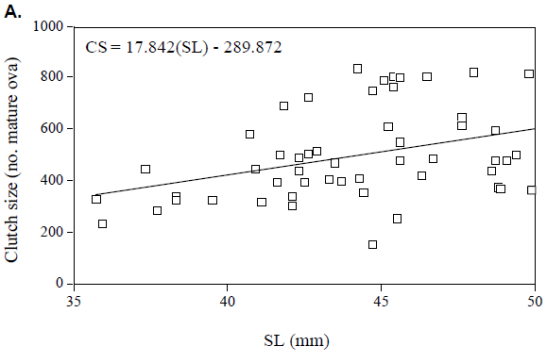


Figure S4. Fecundity at length for Topeka shiner. Figure reproduced from Dahle (2001), p. 50, Figure 2.6 panel A.

To express the relationship between female length (SL in mm) and number of eggs produced, the author fit a linear regression to these data following Equation (18) where F is the fecundity and W is the fish biomass in g. The parameters β_0 (g^{-1}) and β_1 (unitless) are the fitted slope and intercept, respectively.

(18) $$F = \beta_0 W - \beta_1$$

Kerns and Bonneau (2002) report data for fecundity at weight rather than at length. Similar to Dahle (2001), they fit a linear model to the data (Figure S5).

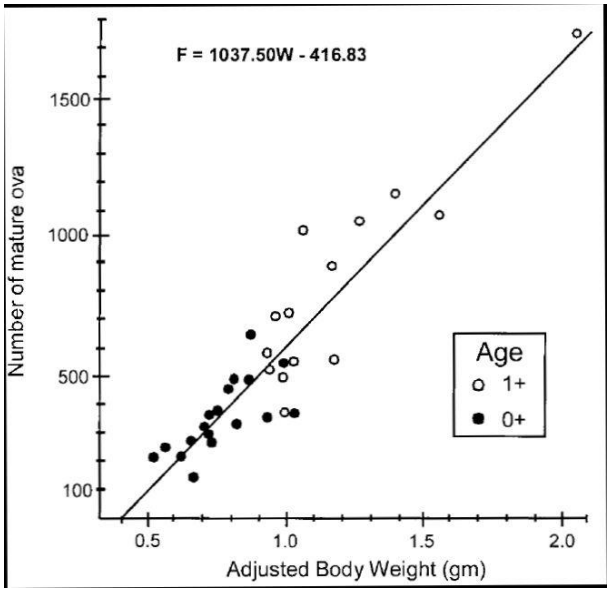


Figure S5. Fecundity at weight for Topeka shiner. Figure reproduced from Kerns and Bonneau (2002), Figure 1.

The lengths in the fecundity data from Dahle (2001) were converted to weights using the length-weight relationship (Section 2.1.1) so that both datasets could be used to fit a model for size-dependent fecundity. The resulting linear fit to the combined data sets is presented in Table S12.

Table S12. Parameters of the model of fecundity at weight.

Term	Estimate	SE	Z	P
β_0	275.7756	76.9645	3.5832	0.0006
β_1	186.1864	54.3279	3.4271	0.0010

2.2. Mortality

Mortality rates of Topeka shiners after larval stage were derived from demographic data reported by Dahle (2001) and Kerns and Bonneau (2002). Fish numbers per age class were reported in both studies whereby fish age was determined from scales. Due to different times of the year that surveys were conducted, age classes did not align between the studies. Age classes and observed % fish in each age class are listed in Table S13 for the data from Dahle (2001) and Table S14 for the data from Kerns and Bonneau (2002).

Table S13. Age classes and percentage of Topeka shiners observed in surveys conducted by Dahle (2001). Across the 2-year survey, 927 fish were caught (544 females, 383 males). Age-0 fish are potentially under-represented because they were too small to catch reliably.

Age class	Age range	Number of TS	Percentage of TS
Age-0	3-4 months	158	17%
Age-1	10-16 months	510	55%
Age-2	22-27 months	241	26%
Age-3	34-37 months	19	2%

Table S14. Age classes and percentage of Topeka shiners observed in surveys conducted by Kerns and Bonneau (2002). Across the 2-year survey, 1002 fish were caught (544 females, 383 males). Age-0 fish are potentially under-represented because they were too small to catch reliably.

Age class	Age range	Number of TS	Percentage of TS
Age-0	0-12 months	672	67%
Age-1	13-24 months	304	30%
Age-2	25-36 months	26	3%

Survival rates in the first year cannot be derived from these data sets. In the model, the daily survival rates of eggs and larvae are assumed to be identical and are calibrated in the model to reach stable population sizes in the density-independent model. Alternatively, density-dependent egg and larval survival rates are applied (Section 2.3.).

A default background survival rate of Topeka shiner in their first year (10-355 days old, including juvenile and subadult stage) is applied (20% survival rate; no data available from literature). Survival

rates of adults (12-36 months old) are assumed to depend on age of the fish, and are derived from the demographic data listed in Tables S13 and S14 (Ross 2013). Thereby, the number of fish per age class are treated as if they represent numbers of the same fish in consecutive years. For instance, if 510 fish with the age of ~1 year old are present and 241 fish with age ~2 year, it is assumed that 241 out of 510 fish (or 47.3%) survive their second year. The survival rates used in the model are listed in Table S15.

Table S15. Survival rates of Topeka shiner by age. Survival rates for juveniles and subadults are not based on Topeka shiner data.

Topeka shiner age	Life stage in IBM	Survival rates across whole period derived from demographic data	Default survival rates across whole period applied in the model	Default daily survival rate applied in the model
0 – 10 days	Egg, larva	n/a	0.06	0.76
<12 months	Juvenile, subadult	n/a	0.22	0.9955
12 – 24 months	Adult	0.45 – 0.5	0.50	0.9981
24 – 36 months	Adult	0.05 – 0.1	0.06	0.9925

2.3. Density dependence

Data on the potential density dependence of Topeka shiner populations are not available, but density dependence has been identified as an important population-level process (Morris and Doak 2002). The TS-IBM can be run in a density-independent (see Section 2.2. for details) and a density-dependent version. Whether density dependence is applied or not is defined via input to the model (see Table S4). Simulations presented in the current document and the main manuscript all apply density dependence unless otherwise stated. Density dependence is simulated as effect on egg and larval survival rates. In the density-dependent mode, maximum egg and larva daily survival rate is defined, and a Ricker function is applied that reduces this survival rate dependent on biomass of subadult and adult Topeka shiners (Section 1.4.3.). The steepness of the Ricker function is calibrated to achieve stable population abundances across years (Section 5.1.2.).

2.4. Predation

The presence of largemouth bass in a waterbody was suggested to lead to declines and possible extirpation of Topeka shiner populations (Campbell et al. 2016). Quantitative data on the predator-prey relationship of the two species are not available. To simulate predation by largemouth bass on Topeka shiner, we simulated food web relationships simulated by $CASM_{OC}$ as inputs to the TS-IBM. In $CASM_{OC}$, largemouth bass feed on multiple other fish guilds represented in the food web including Topeka shiner. For every simulated day, the biomass of Topeka shiner consumed by largemouth bass is calculated and provided as output in the $CASM_{OC}$-generated daily biomass file. From the biomass eaten, the number of Topeka shiner to be killed due to predation is determined in the TS-IBM (Section 1.4.4.).

2.5. Sunfish hosts

Topeka shiner were observed to spawn in sunfish nests. No brood care by Topeka shiner occurs, but sunfish defend their nests until their eggs are hatched and larvae disperse (Campbell et al. 2016). Topeka shiner brood benefits from the guarding behavior of the sunfish hosts. Though spawning by Topeka shiner occurs in the absence of sunfish, the recruitment success is reduced (Campbell et al. 2016). No quantitative data on the importance of sunfish hosts for Topeka shiner recruitment success are available. For the model, we assume that sunfish hosts are present, and calibrate the model to population stability. Sunfish hosts can be removed in the model which results in the reduction of egg and larva survival by a defined factor. This makes it possible to test different hypothetical efficiencies of brood guarding by the host sunfish and their population-level impacts. Reductions in egg and larva survival due to absence of sunfish hosts were not applied in the simulations presented in the current document and the main manuscript.

2.6. Topeka shiner diet

Topeka shiners are reported to be omnivorous. In analyses of Topeka shiner gut content, insects from multiple families were found along with microcrustaceans, fish eggs, other animal groups, plant matter and detritus (Dahle 2001; Hatch and Besaw 2001; Kerns and Bonneau 2002). Gut content from adult fish were analyzed in the studies. Chironomid larvae and pupae were observed most frequently across seasons and sites, but varied considerably in percent volume of gut content. Other diet items were also highly variable in occurrence, frequency and volume. Qualitative findings on gut content from the literature are summarized in Table S16.

Table S16. Qualitative summary of gut content analysis of adult Topeka shiners from three studies. Diet items included if reported at more than one site and number per gut >0.1. Note that gut content categories combining several taxonomic groups were not applied across all three studies, but were aligned for this table.

Diet organism	**Hatch and Besaw 2001 (sampling conducted May – Aug)**	**Kerns and Bonneau 2002 (sampling conducted Mar and Jul)**	**Dahle 2001 (sampling conducted Apr – Sep)**
Chironomidae	High frequency at most sites and times (May – Aug)	Both dates; much higher frequency in March	Diptera (in text: mainly chironomidae); high frequency at all sites
Simuliidae	At 2 sites (June); low frequency	--	
Ephemeroptera	2 sites	Low in March, somewhat higher in July	
Corixidae	3 sites	--	
Cladocera	3 sites	Low in March, none in July	Daphnia: most dates Bosmia: site 1: most dates, variable; more frequent at site 2

Diet organism	**Hatch and Besaw 2001 (sampling conducted May – Aug)**	**Kerns and Bonneau 2002 (sampling conducted Mar and Jul)**	**Dahle 2001 (sampling conducted Apr – Sep)**
			Chydorus: common at site 3
Copepoda	2 sites, low frequency	Low in March, none in July	All dates, medium frequency at site 1, lower frequ. At site 2
Ectoprocta	4 sites, low frequency	--	
Other (all kinds of stuff incl. fish larvae)	4 sites	Fish eggs low in March	Eggs, Some dates at all sites, very variable
Plants matter	At all sites; frequency variable		Very variable, at all sites
Detritus	At all sites; frequency variable	High frequency; combined detritus, algae, sand, etc.	All dates, medium frequency (incl. sand)
Sand	Most sites, very variable		
Other insects (unidentified)		Fairly high frequency on both dates	Medium frequency at site 3
Annelida			At site 3 with low frequency, pooled in other category in other studies

In $CASM_{OC}$, a set of guilds represents the food web. From the represented guilds, we chose a subset that is assumed to constitute the diet of the Topeka shiners in the model. Ontogenetic shifts to larger prey have been demonstrated in many fish species (Werner and Gilliam 1984; Graeb et al. 2006; Tabor et al. 2007; Linzmaier et al. 2018). Accordingly, we assumed that juvenile Topeka shiners rely on smaller food items than adults for the purpose of the model. Their diet in the model is composed of microzooplankton, rotifers, cladocerans, copepods and detritus. Subadult and adult Topeka shiner are assumed to consume cladocerans, copepods, chironomids, mayflies (Ephemeroptera), caddisflies (Trichoptera), oligochaetes, periphyton (total periphyton in CASM) and detritus (sediment POC in $CASM_{OC}$).

2.7. Functional response to prey density

For the parameterization of the functional response to prey density by Topeka shiner, diet preferences were derived from reported gut contents. Hatch and Besaw (2001) report gut contents, but they do not report abundances within guts. They report percentage of guts in which a prey type was found; and mean number per gut of countable items. However, they do not report the latter information for every food type. Their data were not used because it was impossible to calculate volume percentages. Kerns and Bonneau (2002) and Dahle (2001) reported diet composition in percentage of volume gut contents, and we used their data for the estimation of food preferences in Topeka shiner.

Diet items were combined into the eight adult diet categories also represented in $CASM_{OC}$ (Table S17). Prey categories with low volumes in the gut contents and lacking match with the eight identified adult

diet categories were excluded (Ostracoda, Amphipoda, Nematoda, Nematodomorpha, Bryozoa, Porifera, eggs, fish scales). The percentage of the diet comprised of the remaining prey types by volume in gut contents was calculated.

Table S17. Prey categories included in the TS-IBM and $CASM_{OC}$ and their alignment with reported adult Topeka shiner gut content items.

$CASM_{OC}$ guild	Topeka shiner diet items included
Cladocerans	All cladocerans
Copepods	All copepods
Chironomids	All Diptera with Chironomida reported as most common dipteran.
Ephemeroptera	All mayflies
Trichoptera	All other insects (other than flies or mayflies) and hydracarina mites
Oligochaetes	Annelids and molluscs
Total periphyton	All algae and plant matter
Sediment POC	Sand/detritus

Diet compositions in 26 samples are shown in Figure S6. Each sample represents the mean of several fish (mean = 22.3, range = [5, 37]). Each panel shows the same 26 samples, ordered by a different dominant prey category (clockwise from top-left: diptera, cladocera, detritus, and periphyton).

The average diet is defined by the mean percentages of each prey type across all samples (Table S18). We apply the assumption that the average diet composition reflects the diet preferences of Topeka shiner.

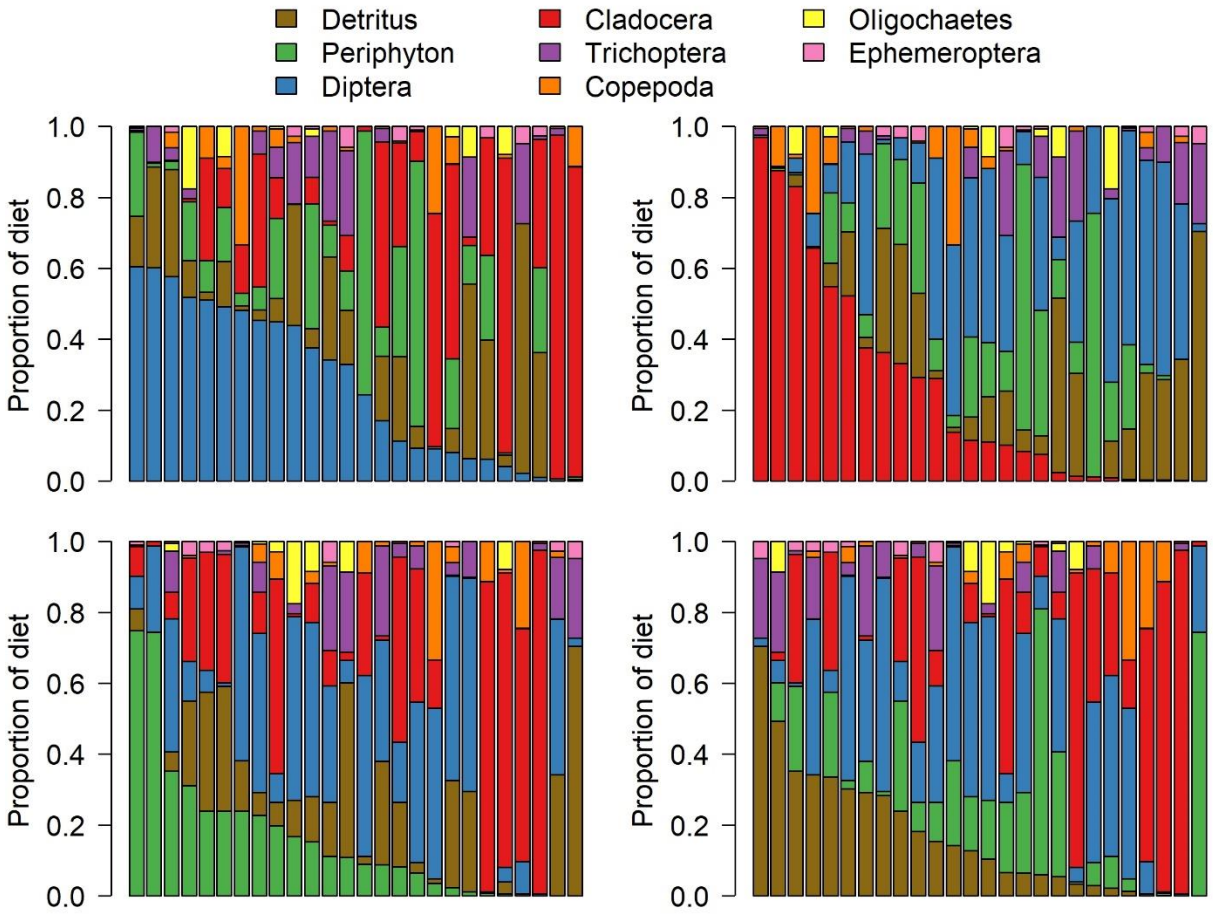


Figure S6. Observed diet compositions in 26 samples of 8 categories of food. Each sample represents the mean %-volume in 5 to 37 fish. The four plots show the same data sorted by the four most prevalent diet groups, respectively; clockwise from top left: Diptera, Cladocera, detritus, and periphyton (representing all plant material).

Table S18. Potential diet compositions for Topeka shiner by percentage mass.

Prey item	Average % of diet
Diptera	27.59
Cladocera	25.93
Detritus	16.92
Periphyton	16.32
Trichoptera	6.25
Copepoda	4.14
Oligochaetes	1.85
Ephemeroptera	1.00

2.8. Bioenergetics

Fish bioenergetics (Hanson et al. 1997; Deslauriers et al. 2017) was applied to link food consumption of Topeka shiner to their growth in a mechanistic way. However, bioenergetics parameters for Topeka shiner are not available. A complete set of parameters is available from FB4 (Deslauriers et al. 2017) for the fathead minnow (*Pimephales promelas*), a small-bodied fish species from the same family as *Notropis* (Cyprinidae). The bioenergetics parameters applied in the model are listed in the Parameter Table (Table S4).

2.8.1. Energy densities of Topeka Shiner and its prey

Topeka shiner

For the calculations of consumption, respiration and waste losses, and their translation into Topeka shiner growth, the energy densities of the fish and its diet items need to be estimated. No measurement of energy density for *Notropis topeka* could be located. Energy density measurements for three closely-related species were found (Table S19).

We have no information on variation in energy density between life stages of *N. topeka*. However, the increase in energy density of *N. hudsonius* over the course of the year observed by Bryan et al. 1996 is congruent with the greater energy density in adult *Macrhybopsis* chubs (personal communication, N. Green) because presumably a greater proportion of individuals are juveniles earlier in the year. So, it is reasonable to assume that adult *N. topeka* have greater energy density than juvenile or young-of-year *N. topeka*. In the absence of more data, we can assume that the ratio of juvenile *N. topeka* energy density to adult *N. topeka* energy density is the same as for juvenile *Macrhybopsis* to adult *Macrhybopsis* (0.5249).

Bryan et al. (1996) report three values of energy density for adult *N. hudsonius*. The mean was applied as final energy density for Topeka shiner in the model (Table S20). The SD of ED_{adult} was calculated as the square-root of the mean of the variances of those intra-annual measurements. The mean for juvenile energy density was calculated as $ED_{juvenile} = 0.5249 ED_{adult} = 2553.2$. The SD for juvenile energy density was calculated so that $ED_{juvenile}$ would have the same coefficient of variation (CV) as ED_{adult}.

Table S19. Energy density (J/g wet weight) measurements for 3 species of cyprinid minnows.

Species	Stage	DOY	Mean	SD	Min	Max	Mode	Variance
Macrhybopsis spp. [a]	Juv.		3418.2	402.7				
Macrhybopsis spp. [a]	Adult		6511.7	767.1				
Pimephales promelas[b]	All		4165.6[d]	119.9[d]	3907.9	4485.2	4103.7	14370.2[d]
Notropis hudsonius[c]	All	121	4486.6[d]	206.5[d]	3933.0	4924.6	4602.4	42645.2[d]
Notropis hudsonius[c]	All	182	4931.5[d]	302.2[d]	4297.0	5744.6	4753.0	91305.7[d]
Notropis hudsonius[c]	All	244	5174.2[d]	277.4[d]	4468.5	5824.1	5230.0	76959.6[d]
Notropis hudsonius[c]	All		4864.1[e]	265.1[e]				70303.5[e]

[a]personal communication (N. Green)

[b]Duffy 1998

[c]Bryan et al. 1996

[d]Estimated from reported minimum, maximum, and mean

[e]Mean of three intra-annual estimates

Table S20. Final *N. topeka* energy density values (in J/g wet weight).

Topeka shiner life stage	**Mean**	**SD**
Notropis topeka (juvenile)	2553.2	139.1
Notropis topeka (adult)	4864.1	265.1

Prey energy densities

Estimates of energy densities of the taxonomic groups included in the Topeka shiner diet were compiled from the literature (Table S21). From the data, averages across studies were calculated and applied as energy densities in the model (Table S22).

No energy density estimate for stream detritus could be located. Instead, the energy density of detritus was calculated as the mean energy density of all other prey categories. Variability of detritus energy density is estimated from the mean coefficient of variation of the energy densities of all other prey categories (Table S22).

Table S21. Energy density data compiled for taxonomic groups included in the Topeka shiner diet

Topeka shiner diet: taxonomic category	**Species**	**Mean energy density (J/g wet weight)**	**Source**
Chironimidae	*Chironomus* spp.	3044.7	Personal communication (N. Green)
Cladocera	Cladocerans and copepods	2850	Laurence (1976); Vijverberg and Frank (1976)
Cladocera	*Daphnia* spp.	3770	Luecke and Brandt (2011)
Cladocera	*Daphnia* spp.	1891	Snow (1972)
Copepoda	*Cyclops vernalis*	4430.5	Cummins and Wuycheck (1971)
Copepoda	*Mesocyclops edax*	3857.2	Cummins and Wuycheck (1971)
Copepoda	*Acartia tonsa*	1945.0	Durbin and Durbin (1981)
Copepoda	*Calanus helgolandicus*	3801.7	Slobodkin and Richman (1961)
Copepoda	*Trigriopus californicus*	3882.4	Slobodkin and Richman (1961)
Ephemeroptera	Ephemeroptera	4444.8	Brey (2001)
Microzooplankton	Zooplankton	2512.0	Cummins and Wuycheck (1971)
Microzooplankton	Numerous	3000.0	Hunt et al. (1981)
Microzooplankton	Numerous	3000.0	Hunt et al. (2000)
Microzooplankton	Invertebrates	4000.0	Hunt et al. (2000)
Microzooplankton	*Paramecium caudatum*	3202.0	Klekowski and Shuskina (1966)
Microzooplankton	*Colpidium campylum*	4030.0	Laybourn and Stewart (1975)
Microzooplankton	Amoeba	3500.0	Rogerson (1979)
Microzooplankton	Ciliates	4000.0	Rogerson (1979)
Microzooplankton	*Tetrahymena*	4968.0	Slobodkin and Richman (1961)
Microzooplankton	*Anisogammarus*	2460.0	Smith et al. (1986)
Oligochaeta	Oligochaeta	3935.4	Brey et al. (1988)
Oligochaeta	Annelida	2717.1	Jangaard (1974); Bigg (1981); Brey (2001)
Oligochaeta	Oligochaeta	1311.9	Jangaard (1974); Bigg (1981); Brey (2001)
Periphyton	*Ditylum brightwellii*	1646.4	Durbin and Durbin (1981)
Periphyton	Cyanobacteria	2150.6	Ling (1966); Reynolds (1984)
Periphyton	Bacillariophyceae	2401.7	Ling (1966); Reynolds (1984)
Periphyton	Chlorophyta	2753.1	Ling (1966); Reynolds (1984)
Periphyton	Cryptophyta	2615.1	Ling (1966); Reynolds (1984)
Periphyton	Peridinium spp.	3966.5	Brody (1945); Berman (1978); Wynne et al. (1982)
Periphyton	Phytoplankton	5299.9	Platt and Irwin (1973)
Periphyton	Algae	4184.0	Schneider (1992)
Periphyton	*Egeria* (formerly *Elodea)*	1212.9	Spencer et al. (1997)
Periphyton	*Eichhornia*	1094.9	Spencer et al. (1997)
Periphyton	*Hydrilla*	1237.1	Spencer et al. (1997)

Topeka shiner diet: taxonomic category	**Species**	**Mean energy density (J/g wet weight)**	**Source**
Periphyton	*Myriophyllum*	1129.3	Spencer et al. (1997)
Periphyton	*Potamogeton*	1279.4	Spencer et al. (1997)
Periphyton	*Zannichellia*	1235.2	Spencer et al. (1997)
Rotifera	*Brachionus plicatilis*	3503.9	Fernandez-Reiriz et al. (1993)
Rotifera	*Brachionus plicatilis*	3141.5	Jeeja et al. (2011)
Rotifera	*Brachionus plicatilis*	3682.0	Theilacker and Kimball (1971)
Trichoptera	Trichoptera	4334.1	Brey (2001)

Table S22. Final composite energy densities and their standard deviations (where available). Units are J/g wet weight.

Diet category	**Mean**	**SD**
Chironimidae	3044.7	157.1
Cladocera	2837.0	939.6
Copepoda	3461.2	901.4
Ephemeroptera	4444.8	229.3
Microzooplankton	3467.2	786.8
Oligochaeta	2654.8	1312.8
Periphyton	2300.4	1341.6
Rotifera	3442.5	275.4
Trichoptera	4334.1	223.6
Detritus	3331.8	788.9

2.9. Fitting the fish bioenergetics model to temperature-dependent Topeka shiner growth data

In the previous application of the hybrid model for the Topeka shiner (Bartell et al. 2019; Schmolke et al. 2019), we applied parameters from fathead minnow (*Pimephalis promelas*) to the fish bioenergetics model included in the TS-IBM (Hanson et al. 1997; Deslauriers et al. 2017). In the absence of bioenergetics parameters for Topeka shiner, we had chosen fathead minnow as surrogate because bioenergetics parameters are available for the species. Fathead minnow may serve as a surrogate for bioenergetics because a) the species is commonly observed as part of the species community including Topeka shiner, suggesting generally similar climatic and habitat preferences (Bakevich et al. 2013); b) fathead minnow and Topeka shiner are related species, belonging to the Cyprinidae and are comparable in size.

In the current application of the hybrid model, we are interested in assessing the effects of environmental factors on the simulated Topeka shiner populations. Assumed Topeka shiner temperature preferences are important in this context because they impact the timing of feeding during the year. The available parameters for fathead minnow (Duffy 1998; Deslauriers et al. 2017) suggest that the species has a broad temperature range for consumption and respiration. Applying this broad range to Topeka shiners, particularly the onset of consumption at very low water temperatures, may interact with the simulation of different temperature profiles in the waterbody.

To achieve a more realistic representation of temperature preferences by Topeka shiner in the model, we fit the fish bioenergetics model to experimental data reported by Koehle (2006). The author assessed the optimum temperature for growth in Topeka shiner in a series of laboratory experiments. Fitting the fish bioenergetics model to the presented data is used to determine the temperature parameters in the fish bioenergetics model for Topeka shiner. Parameters in the fish bioenergetics model other than temperature parameters remain unchanged, i.e. fathead minnow parameters continue to be used.

2.9.1 Experiments and data from Koehle (2006)

Summary of methods in temperature experiments

From the study by Koehle (2006), we extracted data from the reported experiments assessing optimal temperatures for growth in Topeka shiners. Experiments assessing impacts on growth from dissolved oxygen in the water were not used. Three experiments (T1-T3) were reported in which water temperature was varied. In the second experiment (T2), all Topeka shiner were infected with the Asian tapeworm, potentially shifting the fish's optimal temperature for growth. In T3, a subset of Topeka shiner with tapeworm infection were included to assess the impact of the infection on fish growth. For the fitting on temperature parameters, we excluded data from Topeka shiner infected with the tapeworm, using only data from T1 and uninfected fish from T3.

In Table S23, we provide an overview of the experiments T1 and T3 from Koehle (2006). The experiment design and the origin of the Topeka shiner included in the experiments differed, impacting the robustness of the data for the temperature fit. Notably, fish spawned during experiment T1. The spawning activity was likely caused by the simulated light-dark cycle in the laboratory. During spawning, particularly female fish loose considerable amounts of body mass, interfering with the assessment of growth based on fish weight and length which were only measured at the beginning and end of the experiments. Accordingly, the growth observed in T1 cannot be separated from the spawning activity, not allowing a robust estimation of growth dependent on temperature.

The specific growth rate (SGR) of the fish in the experiments was reported by the author. In the method description, the author states that the SGR was calculated as SGR = [ln (final measure – initial measure)] / [number of days elapsed between measurements]. However, in the result figures, SGR is shown as % growth per day, i.e. $\%SGR = 100 \times \delta W/W$; where δW is the daily weight change and W is the fish weight (in g). Note that the absolute weights of the fish at the start and end of the experiment are not provided by the author.

In three additional experiments, the critical thermal maximum (CTM) was assessed by the author. Fish from the two highest temperature treatments in experiments T1 and T3 were entered into the CTM1 and CTM3 experiments, respectively. Data from experiment CTM2 and Topeka shiner infected with Asian tapeworm in CTM3 were not used in the context of the temperature parameter fitting. In CTM1, a total of 50 Topeka shiner were used, and 6 Topeka shiner in CTM3. During the experiments, the temperature in the aquarium was raised by 0.3°C per minute. The CTM for each individual fish was determined as the temperature when the fish could no longer regain equilibrium.

Table S23. Experiment design of the temperature-dependent growth in Topeka shiner reported by Koehle (2006).

Experiment design characteristic	**Experiment T1**	**Experiment T3**	**Remarks**
Topeka shiner origin	Minnesota fish hatchery (originally collected from breeding population from Creek at Pillsbury Crossing (T11S, R9E, Sec 5), Riley County, Kansas)	Kansas fish hatchery (originally collected from breeding population from Creek at Pillsbury Crossing (T11S, R9E, Sec 5), Riley County, Kansas)	
Tapeworm infection status	Fish from MN hatchery were never infected with Asian tapeworm	Fish from KS hatchery were previously infected with Asian tapeworm; part of the cohort had been treated prior to the experiment	T3: only data used from fish that had been treated and were free of tapeworm during the experiment
Fish age (since hatching) at start of the experiment	13 months	12 months	
Light:dark cycle applied	16 h light : 8 h dark	15 h light : 9 h dark	Daylength was reduced in T3 to prevent spawning activity
Feeding	Feeding with brine shrimp 3x a day (to satiation)	Feeding with brine shrimp 3x a day (to satiation)	
Acclimation temperature	22°C	20°C	
Experiment duration	30 days	28 days	
Experimental temperatures (mean of two repeat experiments each)	12.7; 18.1; 23.4; 27.8; 33°C (experimental target temperature reached over the first 10 days of the experiment)	14.6; 19.7; 24.5; 29.6; 34.6°C (experimental target temperature reached over the first 13 days of the experiment)	T1: spawning activity was observed in the 3 highest temperatures, with increasing activity with increasing temperature
Number of fish per temperature treatment	14 fish per replicate treatment, 2 replicates per temperature	14 fish per replicate treatment, 2 replicates per temperature	

Summary of results from temperature experiments

The results from experiments T1 and T3 are summarized in Figures 1 and 4 in the thesis, respectively. In T1, the tested temperature with the highest mean %SGR was determined to be 18.1°C for both Topeka shiner weight and length. Note that the higher tested temperatures (23.4°C and higher) all resulted in spawning activity of the fish). In experiment T3, fish without tapeworm infections had the highest %SGR in 24.4°C temperature treatment.

We extracted the data on %SGR across tested temperatures from Figures 1 and 4 (using WebPlotDigitizer: https://apps.automeris.io/wpd/). The extracted data are presented in Tables S24 and S25, respectively.

Critical thermal maxima of 38.9°C and 39.6°C were observed in experiment CTM1, and 38.7°C and 39.8°C in CTM3 (without tapeworm infection).

Table S24. Data extracted from Figure 1 in Koehle (2006) showing the results from experiment T1. Two experiments per temperature were conducted, leading to two data points per temperature treatment (with slight deviation from the target temperature in the two repetitions). %SGR based on length and weight, respectively, are listed.

Experimental temperature (°C)	%SGR based on Topeka shiner length	%SGR based on Topeka shiner weight
12.8	0.010101	0.116981
12.7	0.020202	0.320755
17.9	0.151515	0.788679
18.3	0.141414	0.818868
23.4	0.050505	0.588679
23.3	0.191919	0.275472
27.8	-0.0404	-0.06038
27.8	-0.05051	-0.26038
32.9	-0.0404	-0.68679
32.9	-0.10101	-0.50566

Table S25. Data extracted from Figure 4 in Koehle (2006) showing the results from experiment T3 in fish without tapeworm infection. Two experiments per temperature were conducted, leading to two data points per temperature treatment (with slight deviation from the target temperature in the two repetitions). %SGR based on length and weight, respectively, are listed.

Experimental temperature (°C)	%SGR based on Topeka shiner length	%SGR based on Topeka shiner weight
14.5	0	0.008541
14.8	0.1125	0.099041
19.8	0.33	0.661078
19.8	0.2175	0.79212
24.5	0.69	2.330759
24.5	0.675	2.290438
29.7	0.675	2.520273
29.6	0.3975	1.211575
34.4	0	-0.02834
34.4	-0.045	-0.09883

2.9.2 Methods for fitting the fish bioenergetics model to the Koehle (2006) data

The Wisconsin Fish Bioenergetics model (FB4; Hanson et al. 1997; Deslauriers et al. 2017) was used to simulate growth resulting from consumption, respiration, and waste losses in Topeka shiner individuals in the Topeka shiner population model (TS-IBM; Schmolke et al. 2019). The fish bioenergetics model consists of multiple equations, and requires several parameters based on observations in fish. Because detailed experiments on the bioenergetics of Topeka shiners are not available from the literature, we are using parameters from fathead minnow as surrogate (Duffy 1998; Deslauriers et al. 2017). The parameters in the fish bioenergetics model that are not related to temperature, and their values applied are listed in Table S26. These parameter values were held constant, i.e. they were not included in the fit to the Koehle (2006) data sets.

The temperature parameters included in the fish bioenergetics model are listed in Table S27. We determined ranges for the fit in these parameters to the Koehle data. Parameters te1-te4 defining the temperature-dependence of consumption (Hanson et al. 1997; Thornton and Lessem 1978) applied to the fish bioenergetics model have to fulfill the following condition: te1 < te2 < te3 < te4. Correspondingly, the parameters in the function defining the temperature-dependence of respiration have to fulfill the condition RTO < RTM.

For the fitting of the bioenergetics model to the data presented by Koehle, we conducted simulations of the fish bioenergetics model (implemented in R). The parameter space defined in Table 27 was explored by using latin hypercube (LHC) simulations. The LHC allows to sample the parameter space evenly, and is a variation of the Monte Carlo approach (Blower and Dowlatabadi 1994). The LHC was setup for 8000 samples from the temperature parameter space, corresponding to 8000 simulations with different parameter combinations.

The following LHC simulation sets were conducted for fitting of the fish bioenergetics model to the reported Topeka shiner % SGR:

A. Based on weight, data sets from both experiments combined
B. Based on length, data sets from both experiments combined
C. Based on weight, data set from T3 only
D. Based on length, data set from T3 only

A fit to data from experiment T1 only was not applied because the fish SGR at higher temperatures was confounded by spawning activity. Fish bioenergetics were simulated for a single day. The initial size of Topeka shiners was derived from the literature for 12 months old fish (Kerns and Bonneau 2002): 34.6 mm SL corresponding to 0.675 g wet weight. Absolute fish lengths of weights were not reported by Koehle (2006). The results from the LHC simulations were compared to the experiment data (see Tables S24 and S25). The goodness of fit was assessed by calculating mean absolute error (MAE), and the parameter combination with the lowest MAE was considered the best fit.

Table S26. Parameters in the fish bioenergetics model not related to temperature. These parameters were not included in the fit (held constant). The fish bioenergetics model as applied in the TS-IBM is described in Schmolke et al. (2019), Appendix B.

Parameter	Value	Unit	Process in the fish bioenergetics model	Remarks
RA	0.0096	$g(O2)/g^2$	Respiration	Values from fathead minnow (Duffy 1998; Deslauriers et al. 2017)
RB	0.041	-		
SDA	0.172	-	Specific dynamic action	Value from fathead minnow (Duffy 1998; Deslauriers et al. 2017
FA	0.1	-	Waste losses	Values from fathead minnow (Duffy 1998; Deslauriers et al. 2017
UA	0.1	-		
α_{cmax}	0.09	J/g^2	Consumption	Parameter values used from calibrated in TS-IBM (Schmolke et al. 2019)
β_{cmax}	-0.25			
xk1	0.01	-	Consumption	Equation from Thornton and Lessem (1978) used; generic parameters applied (Hanson et al. 1997; Deslauriers et al. 2017)
xk2	1	-		
xk3	1	-		
xk4	0.01	-		
OxycalCoeff	13560	$J/g\ O_2$	Calculation between energy (J) and wet weight (g)	Deslauriers et al. (2017)
ED_TS_adt	4864.1	J/g wet weight	Energy density of adult Topeka shiner	Schmolke et al. (2019)
ED_prey	3500	J/g wet weight	Average energy density of Topeka shiner prey	Schmolke et al. (2019)

Table S27. Parameters defining the temperature-dependence of consumption and respiration in the fish bioenergetics model. The range of values (defined by the minimum and maximum) applied in the fit to the Koehle (2006) data are listed.

Parameter name in TS-IBM / CASM	**Parameter name in FB4**	**Minimum value**	**Maximum value**	**Unit**	**Parameter description**	**Rationale for range** (derived from Koehle data unless stated otherwise)
te1	CQ	2	15	°C	Minimum temperature for occurrence of consumption	Lowest temperatures tested: 12.7°C (T1), 14.5°C (T3)
te2	CTO	15.1	27	°C	Lower temperature for maximum consumption	Based on reported optimum temperature from T1 (18°C)
te3	CTM	27.1	32	°C	Higher temperature for maximum consumption	Based on reported optimum temperature from T3 (27.1°C)
te4	CTL	32.1	38	°C	Maximum temperature for occurrence of consumption	Assumption of range beyond reported maxima, below mortality temperature (CTM)
RTO	RTO	24	37	°C	Temperature of peak respiration rate	Assumption of RTO higher than optimal temperature for consumption, but below mortality temperature (CTM)
RTM	RTM	38	40	°C	Maximum temperature for respiration (threshold for mortality)	Based on reported range of critical thermal maximum (CTM)
RQ	RQ	0.01	5	$°C^{-1}$	Approximates the Q10 (the rate at which the respiration function increases over relatively low water temperatures)	RQ range derived from range of values across all fish species listed in the FB4 parameter compilation (Deslauriers et al. 2017)

2.9.3 Results of temperature parameter fitting

In Figure S7, we present the data from Koehle's experiments T1 and T3 (from fish without tapeworms) and the %SGR (per day) simulated with the fish bioenergetics model using the best fits to weight data (fits A and C). For comparison, the %SGR using the fathead minnow parameters is also included in the plot. In Figure S8, we present the corresponding data and fits based on fish length.

The parameter values for the best fits to the Koehle data are listed in Table S28. For comparison, we also list the parameters for fathead minnow (that were used in the TS-IBM in the prior model version: Bartell et al. 2019; Schmolke et al. 2019) and the ranges of values across fish species in the fish bioenergetics parameter compilation (FB4; Deslauriers et al. 2017). Note that there are not many values available for maximum temperature for the occurrence of consumption, te4 (CTL) from FB4. In addition, the median and maximum value for te3 (CTM) in FB4 is larger than the median and maximum listed te4 (CTL) temperature (see Table S28), suggesting that te4 (CTL) values are not representative in the FB4 compilation, particularly for fish tolerant of higher temperatures.

Fitted temperature parameters correspond closely between fitting to %SGR based on weight and length. This verifies that the fit of the fish bioenergetics model is robust to the two endpoints measured in the Koehle study. As expected, the temperature parameters fit only to data from T3 are shifted to higher temperatures compared to the fit to the combined data from T1 and T3 because growth was confounded with weight loss due to spawning activity in T1.

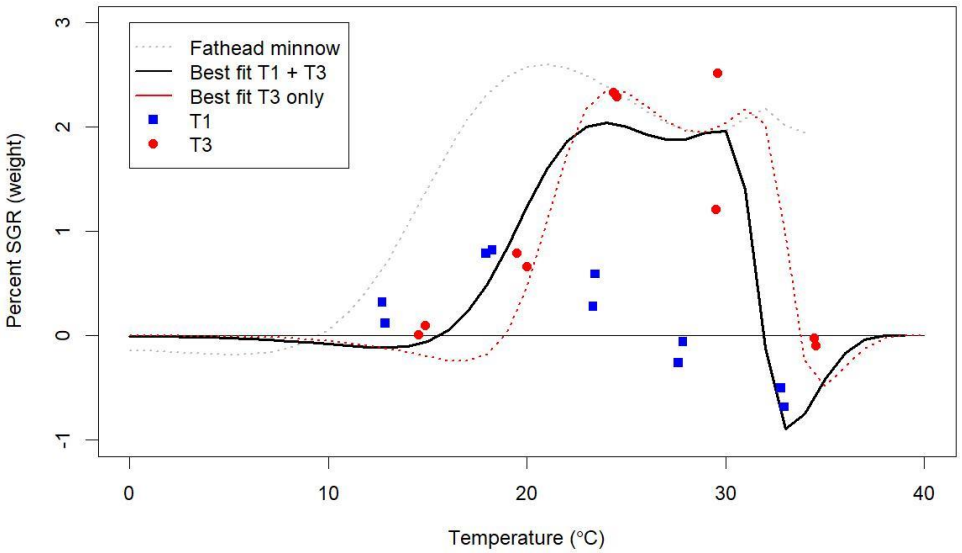


Figure S7. Weight-based % SGR observed by Koehle (2006) in experiments T1 and T3 along with best fits of the fish bioenergetics model. The best fits are shown for the combined data set (data from T1 and T3 combined, fit A) and the T3 data set only (fit C). The %SGR dependent on temperature for fathead minnow was simulated with the fish bioenergetics model for comparison.

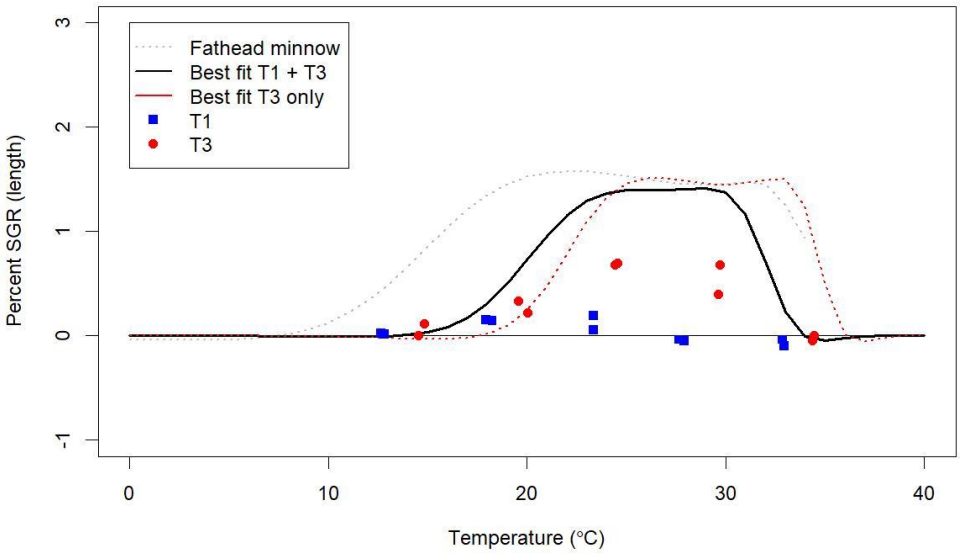


Figure S8. Length-based % SGR observed by Koehle (2006) in experiments T1 and T3 along with best fits of the fish bioenergetics model. The best fits are shown for the combined data set (data from T1 and T3 combined, fit B) and the T3 data set only (fit D). The %SGR dependent on temperature for fathead minnow was simulated with the fish bioenergetics model for comparison.

Compared to the fathead minnow parameters, the fitted Topeka shiner temperature parameters suggest a smaller temperature range for consumption. From the Koehle data, consumption only starts at much higher water temperatures than assumed for fathead minnow. The lowest temperature for consumption (te1) is also in the upper range across fish species listed in FB4. The temperatures of maximum consumption, te3 and te4 are comparable to the values in fathead minnow and well within the range of values compiled in FB4. As mentioned previously, the fitted highest temperature of occurrence of consumption (te4) is above the range of FB4 value for this parameter, but this is likely due to under-reporting of the value in FB4. Note that for fathead minnow, the listed parameter for te4 was based on an estimate.

For respiration, the critical thermal maximum or temperature causing mortality due to the cessation of respiration (RTM) is higher in the fit for Topeka shiner than in the fathead minnow. However, the value falls well within the range of FB4 values for this parameter. The fitted value for RQ falls on the high end of the range in FB4.

Table S28. Best fits of the temperature parameters in the fish bioenergetics model to the data reported by Koehle (2006). For comparison, the temperature parameters for fathead minnow and the parameter ranges across all fish species listed in FB4 are given (Deslauriers et al. 2017).

Parame-ter name (TS-IBM / CASM)	A. Best fit: weight, T1 and T3 data combined	B. Best fit: length, T1 and T3 data combined	C. Best fit: weight, T3 data only	D. Best fit: length, T3 data only	Fathead minnow	FB4: min[1]	FB4: median[1]	FB4: max[1]
te1	9.96	10.81	14.27	14.32	2.4	-0.024	2.565	15
te2	26.51	26.57	24.24	26.98	24	8	22.5	35
te3	28.46	27.82	29.78	31.44	30	11	28	43
te4	33.21	34.88	34.86	36.39	36	16	25	32
RTO	26.88	26.71	27.69	29.21	28	0.0196	23	43
RTM	38.14	39.52	39.76	39.24	33	16	35	46
RQ	4.22	4.92	4.80	4.65	2.6	0.02	1.8	4.6

[1] Values of 0 removed from FB4 table if all 4 values were 0 (for te1) or if te2-4 values were 0; for respiration parameters, values of 0 were removed for RTO and RTM (all values of RQ > 0).

2.9.4 Conclusions

The fish bioenergetics model for Topeka shiner could be fit to the data reported by Koehle (2006) using the temperature parameters. We conducted the fit using %SGR based on weight and length. The parameter fits to weight and length are comparable (compare pairs of fits A and B, and fits C and D in Table S28). We decided to use the temperature parameter fits based on %SGR for length as inputs to the Topeka shiner hybrid model.

Experiment T1 conducted by Koehle comes with the caveat that fish were spawning in the higher temperatures tested, resulting in confounding of growth and weight loss due to spawning. However, lower temperatures were tested in this experiment compared to experiment T3, providing a more robust model fit to the lower temperature range.

For the application to the Topeka shiner hybrid model ($CASM_{OC}$ linked with TS-IBM), we are using the fitted temperature parameters from fit B (fit to length based on T1 and T3 data combined). The parameters are listed in Table S29. In the TS-IBM, these parameters are included in the parameter input file (InputParameters_casmOC_27Feb2020.txt).

Table S29. Temperature parameters in the fish bioenergetics model applied to the Topeka shiner hybrid model for oxbow habitats ($CASM_{OC}$ linked with TS-IBM).

Parameter name (TS-IBM / CASM)	Unit	Parameters applied in TS-IBM / $CASM_{OC}$ (from fit B)
te1	°C	10.8
te2	°C	26.6
te3	°C	27.8
te4	°C	34.9
RTO	°C	26.7
RTM	°C	39.5
RQ	$°C^{-1}$	4.9

2.10. Fitting a TKTD model to sublethal effects of benzovindiflupyr

In the Topeka shiner hybrid model, direct lethal and sublethal effects from exposures to benzovindiflupyr should be represented as well as indirect effects mediated by the food web. In this section, the fitting of sublethal effects on growth observed in two toxicity studies conducted with fathead minnows are used to fit a toxicokinetic toxicodynamic (TKTD) model (Jager and Zimmer 2012). For the fitting, it was assumed that reduction in growth observed in the studies was caused by consumption inhibition. The TK part of the model estimated the internal concentration of benzovindiflupyr within individual fish. The TD part of the model reduced the maximum consumption in response to increasing benzovindiflupyr concentration. This in turn reduced the amount of energy acquired by fish, and thus, their growth. We assumed that Topeka shiner responses to benzovindiflupyr exposure are equal to those of fathead minnows.

2.10.1. Toxicity study data

Data on sublethal effects of benzovindiflupyr on fathead minnow (*Pimephales promelas*) were obtained from a standard toxicity test (York 2010; Fig. 1). The test measured minnow larva survival and growth over a 32-day exposure trial at 7 different exposure levels (including control). A preliminary exposure trial lasting 18 days used nominal exposure levels of 0 (i.e., control), 0.13, 0.25, 0.50, 1.0, and 2.0 µg/L benzovindiflupyr. The primary trial lasting 32 days (4 days pre-hatch, 28 days post-hatch) used nominal exposure levels of 0, 0.25, 0.50, 1.0, 2.0 and 4.0 µg/L. Each treatment within each trial consisted of four replicate samples of 30 eggs each. We used the mean length (in mm) of larvae in each replicate as an input to the analysis. Thus, the dataset consisted of mean lengths for 7 exposure levels and 2 time points post hatch. Each mean length was the mean of ≤30 larvae because not all larvae survived for the length of the trial.

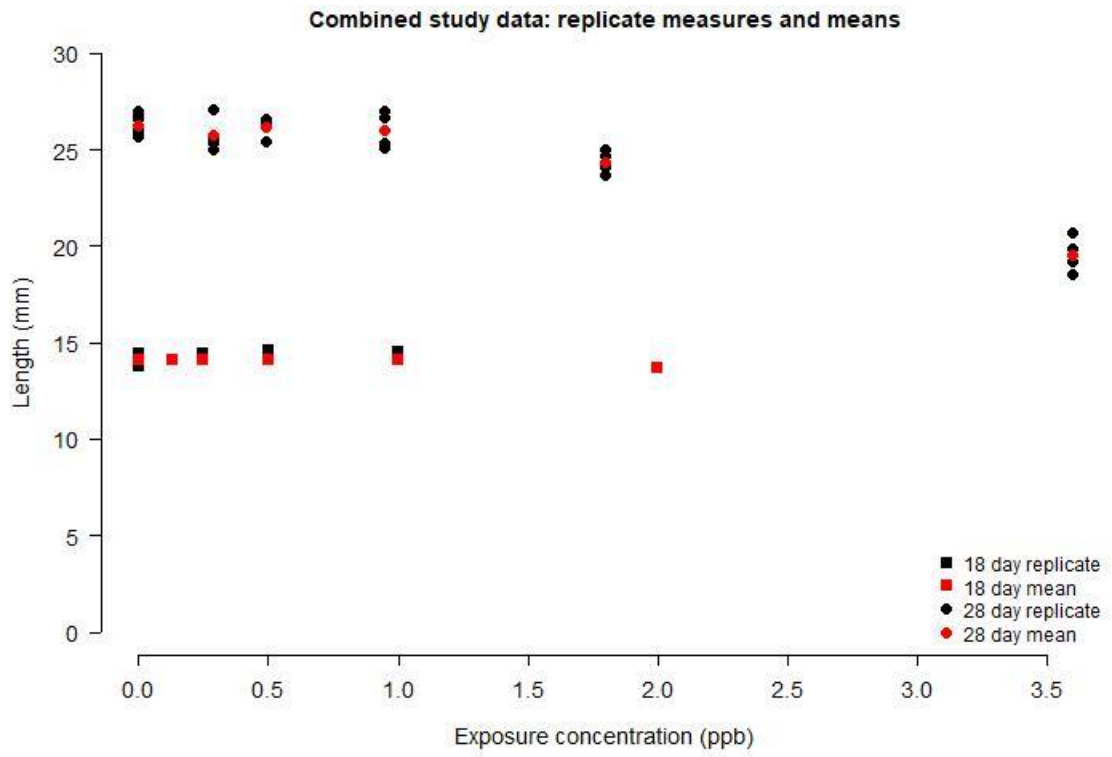


Figure S9. Data from benzovindiflupyr 28-day toxicity test with fathead minnow. Replicates are shown along with the averages. The NOEC was determined as 0.95 µg/L (ppb). Average fish lengths were assumed 100% of controls for concentrations < 0.95 µg/L (ppb).

2.10.2. Representation of growth

We used the Wisconsin fish bioenergetics model to predict growth in fathead minnows (Hanson et al. 1997, Deslauriers et al. 2017). Bioenergetics parameters for fathead minnow were used according to the parameters listed for the species in the available compilation for the fish bioenergetics model, FB4. These parameters were also used in the Topkea shiner hybrid model ($CASM_{OC}$) for the parameterization of fathead minnows. In addition, we use parameters for the conversion between mass (in g) to energy (in J) as well as the oxycalorific coefficient according the TS-IBM. The parameters applied to the bioenergetics model for fathead minnow are listed in Table S30.

Table S30. Parameters for fathead minnow (*Pimephales promelas*) used for the Wisconsin fish bioenergetics model and conversion parameters.

Parameter name	Value	Source/Remarks
CA	0.149	Deslauriers et al. 2017 (FB4 data base)
CB	-0.242	
f_C(T=25 °C)	0.9867	Equation from Thornton and Lessem (1978) using parameters from Deslauriers et al. 2017 (FB4 data base)
RA	0.0096	Deslauriers et al. 2017 (FB4 data base)
RB	-0.041	

Parameter name	Value	Source/Remarks
f_R(T=25 °C)	0.9062913	Equation from Kitchell et al. (1977) using parameters from Deslauriers et al. 2017 (FB4 data base)
FA	0.1 J/(g x day)	Deslauriers et al. 2017 (FB4 data base)
UA	0.1 J/(g x day)	
SDA	0.172	
Oxycalorific coefficient	13560 J/g O_2	Deslauriers et al. 2017
Energy density of brine shrimp (*Artemia salina*, provided as food in the studies)	2935 J/g wet weight	Caudell and Conover 2006
Energy density of fathead minnows (adults)	4165.6 J/g	Duffy 1998; ED for larvae/juveniles not found
Average length of adult fathead minnows at their maximum growth, L_m	73 mm	https://www.fishbase.de/Summary/SpeciesSummary.php?ID=4785&AT=fathead+minnow; https://animaldiversity.org/accounts/Pimephales_promelas/
Initial length of fathead minnows (protolarvae after hatching)	4.6 mm	https://animaldiversity.org/accounts/Pimephales_promelas/
Relation between weight and length for fathead minnow, α	-5.03343	Schneider et al. (2000, Table 17.1)
Relation between weight and length for fathead minnow, β	3.0765	

2.10.3. Estimation of sublethal effects

We assumed that fathead minnows are impacted in their growth due to impairment of feeding. Accordingly, the stress from the exposure to benzovindiflupyr affects consumption in the bioenergetics model. We assume that the fish in the toxicity study were fed ad libitum, i.e. their consumption rate was not impacted by the limitation of food availability. The maximum consumption is defined by C_{max}(T). The temperature T was kept constant in the study (at 25 °C).

We introduce a stress term, s, in the bioenergetics model to reflect the impact of benzovindiflupyr exposures on consumption:

$$C_{maxS} = C_{max}(1 - s)$$

The stress is a proportion calculated as:

$$s := \begin{cases} \frac{1}{c_T}(c_v - c_0) & \text{if } c_v > c_0, \\ 0 & \text{otherwise} \end{cases}$$

Where c_v is the scaled internal concentration of benzovindiflupyr; c_0 is the greatest concentration at which benzovindiflupyr has no effect on individual fish, and c_T is the tolerance gradient, i.e. the sensitivity to the toxicant at concentrations above c_0. Stress is required to be in the interval [0, 1]; values calculated to be >1 are set to 1. All concentrations are given in µg/L (ppb).

The internal concentration c_v was estimated according to the following one-dimensional kinetics model (Jager and Zimmer 2012):

$$\frac{dc_v}{dt} = k_E \frac{L_m}{L}(c_d - c_v) - c_v \frac{3}{L}\frac{dL}{dt}$$

In this expression, k_E is the elimination rate; L_m is maximal length (mm); L is current body length (mm); and c_d is external concentration in µg/L (ppb).

For the fitting of the TKTD model to the available effects data, we assumed that c_0 to be the same as the NOEC estimated from the toxicity study, 0.95 µg/L. We also assumed that L_m was 73 mm, which was reported as typical adult length of fathead minnows (see Table S30).

For the bioenergetics model, an initial size of the newly hatched fish is needed to calculate subsequent growth. We assumed an initial length of fathead minnows of 4.6 mm (length of protolarvae; see Table S23).

The toxicity study reports fish lengths. The bioenergetics model simulates fish growth based on mass. For the calculation between fish length and mass, we used the equation by Schneider et al. (2000):

$$\log_{10}(W) = \alpha + \beta \log_{10}(L)$$

Where W is the fish weight in g, and L is the fish length in mm. The parameters for fathead minnow for this equation are used (see Table S30).

The parameters in the TKTD model that were included in the sublethal effect fitting to estimate the concentration-dependent stress level were accordingly c_T and k_E.

2.10.4. Sublethal effect fitting

Fits were conducted using the average reported lengths for each treatment level. If average lengths in treatments exceeded the average length of the controls, lengths in those treatment levels were forced to the lengths reported for controls. This was applied to avoid fitting to size increases that were insignificant and not the objective of the fit.

Because fish lengths simulated by the bioenergetics model did not exactly match the fish lengths reported in the toxicity studies, the sublethal effects fit was conducted using the proportion of the controls.

The model for internal concentration was evaluated in time steps of 5 minutes to produce smooth dynamics (i.e., 24 hours/day × 12 intervals/hour = 288 intervals/day). For the optimization, the function 'optim' from the 'stats' package in R was used.

We assumed that Topeka shiner responses to benzovindiflupyr exposure are equal to those of fathead minnows.

Because initial optimization runs reached the maximum number of runs, we ran the optimization repeatedly, using best fits for k_E and c_T as starting values for the subsequent optimization until initial and optimized values were identical.

The optimization procedure resulted in the following values:

k_E = 0.00061

c_T = 8.8389

The simulated fathead minnow lengths are plotted against the study data in Figure S10. The bioenergetics model underestimates the fish sizes at 28 days of age. In Figure S11, the relative fish lengths are plotted which was also used for the fitting. The mean absolute error of the fit equals 0.71 % in length reduction.

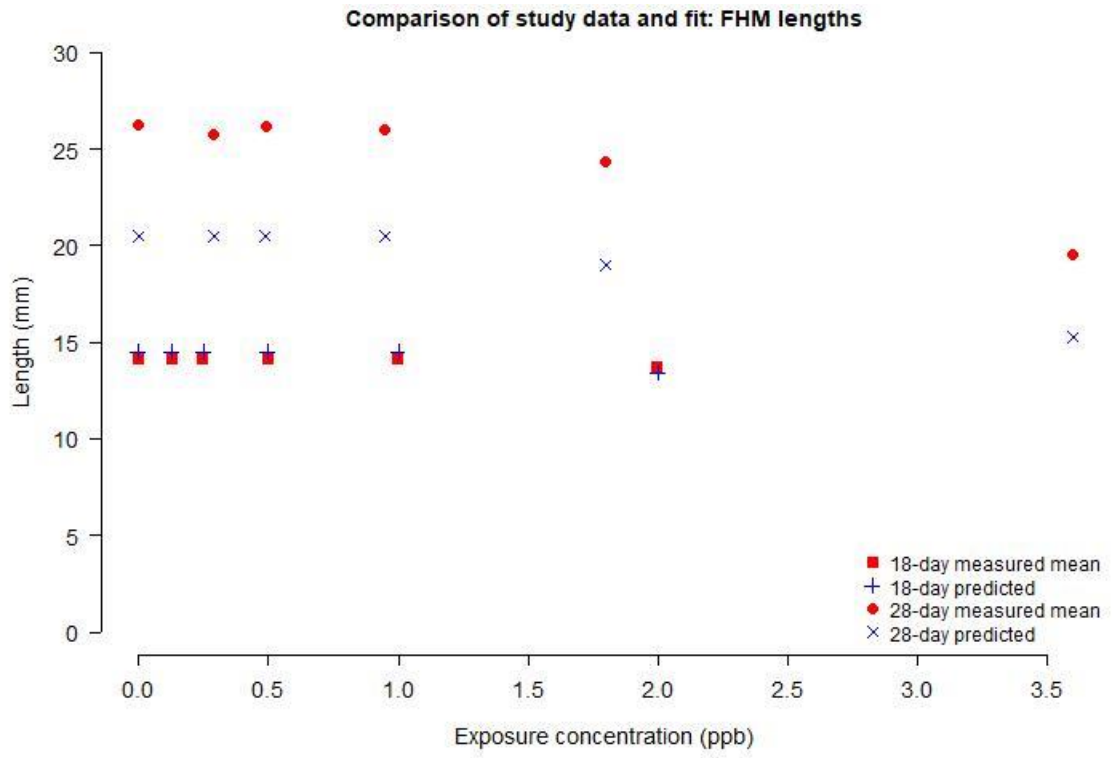


Figure S10. Measured average lengths (red) and predicted average lengths by the bioenergetics model combined with the sublethal TKTD model using the values for k_E and c_T (blue).

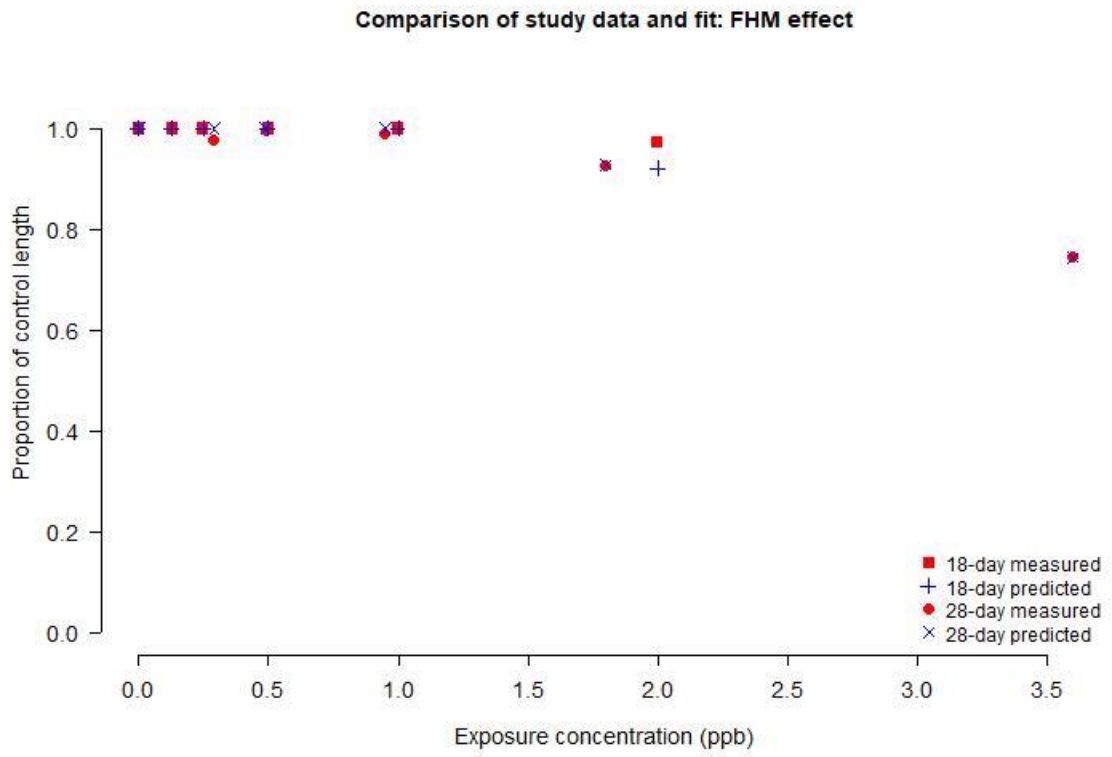


Figure S11. Fish lengths relative to control in the toxicity study (red) and predicted by the bioenergetics model combined with the sublethal TKTD model using the values for k_E and c_T (blue).

3. MODEL LINKING BETWEEN TS-IBM AND CASM$_{OC}$

The hybrid model for Topeka shiner was developed as two stand-alone models (CASM and TS-IBM). For the CASM$_{OC}$ adapted to Topeka shiner oxbow habitats, the species groups represented in the aquatic food web were changed compared to the previous version (CASM$_{OC}$). The following food web guilds representing likely Topeka shiner diet items were added to CASM$_{OC}$: Ostracoda, Corixida and Coleoptera. Ostracoda were found in the gut content of Topeka shiner in a subset of samples (and sites) in the studies conducted by Hatch and Besaw (2001) and Dahle (2001), but not by Kerns and Bonneau (2002). For the TS-IBM, we assume that Topeka shiner consume Ostracoda with the same preference as Cladocera, and that the two diet species correspond in their energy density. Accordingly, the biomasses of Cladocera and Ostracoda from CASM$_{OC}$ are combined to one biomass pool (see Table S3). Insects other than Ephemeroptera and Chironomida were found in Topeka shiner guts at low frequency. Dependent on study, they were typed to insect group or combined as 'other insects' (Dahle 2001; Hatch and Besaw 2001; Kerns and Bonneau 2002). The TS-IBM includes Trichoptera as a diet item that represents all insect (and Hydrocarina) diet except Ephemeroptera and Chironomida. The newly added CASM$_{OC}$ guilds representing Corixida and Coleoptera fall into this pool, and their biomasses are combined with the Trichoptera biomass for input to the TS-IBM.

In Table S31, we list the alignment between CASM$_{OC}$ biomass outputs and TS-IBM diet for the yearly CASM$_{OC}$ output. The current version of the hybrid model was not used with the daily linking between CASM$_{OC}$ and TS-IBM (Bartell et al. 2019; Schmolke et al. 2019). In Table S231, the mapping of the CASM$_{OC}$ (stand-alone) biomass output file (yearly output) to TS-IBM inputs files are listed.

Table S31. Listing of Topeka shiner and Topeka shiner prey biomasses in the $CASM_{OC}$ (stand-alone) biomass output file (yearly output), and the alignment with TS-IBM output file and internal model variables.

$CASM_{OC}$ output column name	**$CASM_{OC}$ output column number**	**$CASM_{OC}$ output unit**	**TS-IBM output column name**	**TS-IBM output column number**	**TS-IBM output unit**	**TS-IBM variable name**	**TS-IBM variable unit**
Day	3	d	"Day"	1	d	ticks	d
Copepods	14	gC m^{-2}	"Copepods"	2	gC m^{-2}	w_copepods	g wet weight (in pond)
Cladocerans	15		"Cladocerans"	3		w_cladocerans	
Rotifers	16		"Rotifers"	4		w_rotifers	
MicroZplankton	17		"MicroZplankton"	5		w_microzoo	
Ostracods	18		"Ostracods"	6		Combined with cladocerans for consumption calculation	
Corixids	28		"Corixids"	7		Combined with caddisflies for consumption calculation	
Ephemeroptera	30		"Ephemeroptera"	8		w_mayflies	
Trichoptera	31		"Trichoptera"	9		w_caddisflies	
Oligochaetes	32		"Oligochaetes"	10		w_oligochaetes	
Chironomids	33		"Chironomids"	11		w_chironomids	
Coleopterans	34		"Coleopterans"	12		Combined with caddisflies for consumption calculation	
SedimentPOC	48		"SedimentPOC"	13		w_detritus	
TotalPeriphyt	50		"TotalPeriphyt"	14		w_periphyton	
TopShiner(juv)	22	gC m^{-2}	"TopShiner(juv)"	15	gC m^{-2}	sum [W] of turtles with [stage = "juvenile"]	g wet weight (in pond)
TopShiner(adt)	23		"TopShiner(adt)"	16		sum [W] of turtles with [stage = "subadult" or stage = "adult"]	
n/a	n/a	n/a	"TopShiner(all)"	17		sum [W] of turtles	
TopShiner(juv)	61	# ind. m^{-3}	"numTopShiner(juv)"	18	# ind. m^{-3}	count turtles with [stage = "juvenile"]	# ind. (in pond)
TopShiner(adt)	62		"numTopShiner(adt)"	19		count turtles with [stage = "subadult" or stage = "adult"]	
n/a	n/a	n/a	"numTopShiner(all)"	20		count turtles	

$CASM_{OC}$ output column name	**$CASM_{OC}$ output column number**	**$CASM_{OC}$ output unit**	**TS-IBM output column name**	**TS-IBM output column number**	**TS-IBM output unit**	**TS-IBM variable name**	**TS-IBM variable unit**
TSnum-eaten (not read from CASM transfer file by TS-IBM)	77	# ind. m^{-3}	"TSnum-eaten"	21	# ind. m^{-3}	TS_eaten_num	# ind. (in pond)
TSgww-eaten	78	g wet weight m^{-3}	"TSgww-eaten"	22	g wet weight m^{-3}	TS_eaten_cumulative	g wet weight (in pond)

4. IMPLEMENTATION VERIFICATION

The model was implemented in NetLogo 6.0.2 (Wilensky 1999). Individual functions or procedures in the model were reimplemented in R (R Project for Statistical Computing) to verify them separately. Procedures verified include the implementation of the equations from the Fish Bioenergetics model, the functional response, relationships between fish length and weight and fish length and fecundity as well as the Ricker function for density dependence.

We also verified that inputs were read correctly from files, including the assignment of data listed in columns to the correct model variables. Biomasses provided as g C (grams of carbon-equivalent of biomass) from $CASM_{OC}$-generated input files were converted to wet weights. We verified that the conversions were applied correctly when data was read in from files and converted back to g C for outputs.

The outputs of the GUTS implementations in the TS-IBM were verified against the implementation of the calibrated models published by Ashauer et al. (2013) using R. In Tables S32 and S33, comparisons of daily survival rates after onset of exposure are listed for the two highest constant concentrations of benzovindiflupyr as tested in the study (4.4 and 9.4 µg/L) and survival rates in the TS-IBM using GUTS-SD and GUTS-IT, respectively. For each exposure, three repeat simulations were conducted with the TS-IBM to qualitatively capture the stochasticity in the TS-IBM. Note that for GUTS-IT, each individual simulated in the TS-IBM gets assigned with a threshold at the time it is 'created' in the model.

Table S32. Expected (from R implementation of GUTS-SD according to Ashauer et al., 2013, for fathead minnow) and simulated survival rates using the TS-IBM with GUTS-SD after onset of the constant exposure.

Day	Benzovindiflupyr concentration (µg/L)	Expected survival rate	Simulated survival rate; run 1	Simulated survival rate; run 2	Simulated survival rate; run 3
1	4.4	100%	100%	100%	100%
2	4.4	98%	97%	97%	98%
3	4.4	84%	85%	80%	83%
4	4.4	68%	68%	64%	66%
5	4.4	55%	54%	52%	54%
6	4.4	43%	42%	41%	44%
7	4.4	35%	33%	31%	34%
8	4.4	27%	27%	25%	27%
9	4.4	22%	21%	21%	21%
10	4.4	17%	17%	17%	16%
1	9.4	66%	70%	66%	66%
2	9.4	12%	15%	10%	14%
3	9.4	1%	1%	1%	1%
4	9.4	<1%	<1%	0%	0%
5	9.4	0%	0%	0%	0%

Table S33. Expected (from R implementation of GUTS-SD according to Ashauer et al., 2013, for fathead minnow) and simulated survival rates using the TS-IBM with GUTS-IT after onset of the constant exposure.

Day	Benzovindiflupyr concentration (µg/L)	Expected survival rate	Simulated survival rate; run 1	Simulated survival rate; run 2	Simulated survival rate; run 3
1	4.4	99%	98%	99%	98%
2	4.4	90%	90%	90%	91%
3	4.4	73%	71%	74%	73%
4	4.4	59%	57%	60%	60%
5	4.4	50%	48%	50%	53%
6	4.4	44%	42%	45%	48%
7	4.4	41%	39%	42%	45%
8	4.4	39%	36%	40%	43%
9	4.4	38%	35%	39%	42%
10	4.4	37%	34%	38%	42%
1	9.4	66%	69%	68%	65%
2	9.4	12%	15%	15%	14%
3	9.4	3%	7%	6%	6%
4	9.4	2%	4%	5%	4%
5	9.4	1%	4%	4%	3%
6	9.4	1%	3%	4%	3%

5. MODEL OUTPUT VERIFICATION

5.1. Calibration

The model was calibrated in two steps: 1) calibration to achieve Topeka shiner sizes (biomass, length) at given ages in the literature, and 2) to achieve population sizes stable across multiple years.

5.1.1. Calibration of Topeka shiner consumption

The parameters of the fish bioenergetics model determine the growth rate of individual Topeka shiner in the model dependent on current fish weight, waterbody temperature, and prey availability (Section 1.4.8.). The parameters applied were estimates for fathead minnow because bioenergetics data for Topeka shiner were not available (Table S4; Section 2.8.). Accordingly, the growth and resulting Topeka shiner sizes may deviate from measured sizes-at-age. To adjust the bioenergetics model to measured Topeka shiner sizes, we calibrated the parameters α_{cmax} and β_{cmax} for the calculation of the maximum consumption rate, C_{max} (Equation (8)).

For this calibration, the hybrid model was run with a single simulated fish from egg stage to three years old (background survival rate set to 1). Yearly food biomass input from $CASM_{OC}$ was used ($CASM_{OC}$ default simulations without Topeka shiner or largemouth bass included; outputs from year 6 were used as repeated yearly inputs to the TS-IBM). A range of combinations of α_{cmax} and β_{cmax} were applied, using the values from fish bioenergetics for fathead minnow as starting point ($\alpha_{cmax} = 0.149$ and $\beta_{cmax} = -0.242$).

Data of Topeka shiner standard length-at-age was reported by Dahle (2001) and Kearns and Bonneau (2002), Table S34. Dahle (2001) reported lengths of female and male fish separately whereby male fish were slightly larger than female fish. In Table S34, the averages across both sexes are listed (also compare to Section 2.1.1.).

Table S34. Measured Topeka shiner lengths dependent on age.

Topeka shiner age (months)	Average Topeka shiner length (SL in mm)	Reference
2	16.5	Kerns & Bonneau 2002
5	25.6	Kerns & Bonneau 2002
11	29.5	Dahle 2001
12	34.6	Kerns & Bonneau 2002
16	43.7	Dahle 2001
17	40.1	Kerns & Bonneau 2002
23	46.5	Dahle 2001
24	42.5	Kerns & Bonneau 2002
36	53.2	Kerns & Bonneau 2002

Growth of Topeka shiner across its life span is depicted in Figure S12 and compared to the growth of fish reported in the literature. The values applied to the parameters in Equation (8) are $\alpha_{cmax} = 0.07$ and $\beta_{cmax} = -0.25$. Females in the simulations remain slightly smaller than the males after they reach

maturity because spawning results in reduced growth. Growth stagnates during the winter months. Fish growth in the simulations with the calibrated model match well with the measured fish lengths.

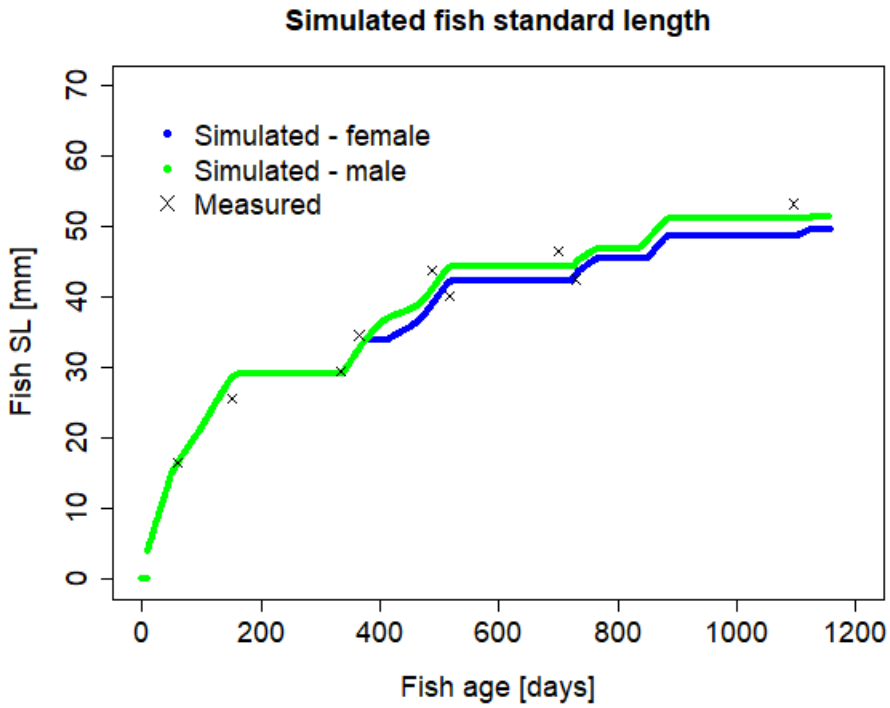


Figure S12. Topeka shiner lengths (in mm SL) by fish age in hybrid model simulations after calibration ($\alpha_{cmax} = 0.07$ and $\beta_{cmax} = -0.25$). Measured lengths reported in the literature (see Table S32) are shown as '×'.

In the main manuscript, simulations were applied in which the detritus preference by Topeka shiners was altered from the default. The simulations were conducted to assess the sensitivity of the modeled populations to reductions in food availability under different assumptions of their diet preferences. However, reducing a single diet preference value results in reduced food uptake by the simulated fish and consequently, their growth. Instead of adjusting all other diet preferences to achieve growth patterns as shown in Figure S12, we recalibrated α_{cmax}. In Table S35, the values for α_{cmax} applied with the reduced detritus preference values are listed.

Table S35. For the simulations with reduced detritus preferences (see main manuscript), TS-IBM was recalibrated to achieve individual fish growth matching field observations (Table S34) in the baseline scenario (no food reductions). Simulations were also tested for stability over 15 years of simulations (population biomass neither increasing nor declining continuously).

Detritus preference ($pref_{detritus}$) of both juveniles and adult Topeka shiners	Calibrated value of α_{cmax} applied
Default: 0.17	Default: 0.0700
0.10	0.0715
0.05	0.0725
0.00	0.0745

5.1.2. Calibration of Topeka shiner egg and larval survival rate

We apply the assumption that Topeka shiner populations do neither continuously increase or decrease over extended time periods, i.e. the populations are approximately stable over time when presented with the default food web, water temperature profile and water depth.

To achieve stable populations, simulations with hybrid model were conducted over 10 years. For the density-independent model, the egg and larval daily survival rate ("DailySurvival_Egg_Larva") was altered. A daily survival rate of 0.76 was identified to result in approximately stable populations. This corresponds to a survival rate across both life stages of 0.064 because Topeka shiner egg and larval life stage are assumed to last 10 days combined. Population sizes do vary within simulated years and between simulated years (Figure S13), but higher daily survival rates of eggs and larvae result in continuing increase in population sizes and lower rates in decreasing populations (eventually leading to population extinction if simulations are run without time limitation).

In the density-dependent model, the egg and larval survival rate is dependent on the biomass of subadult and adult Topeka shiner present. A Ricker function is applied that defines a maximum daily survival rate of 0.8 (or 0.107 across the two life stages), i.e. the hypothetical survival rate in the absence of subadult and adult Topeka shiner (see Section 1.4.3.). A second parameter in the Ricker function, β, defines the slope of the function. This value was calibrated in the density-dependent model to achieve approximate population stability over time with $\beta = 0.04$ applied. The number of Topeka shiner over 10 simulated years with the calibrated density-dependent model are shown in Figure S14.

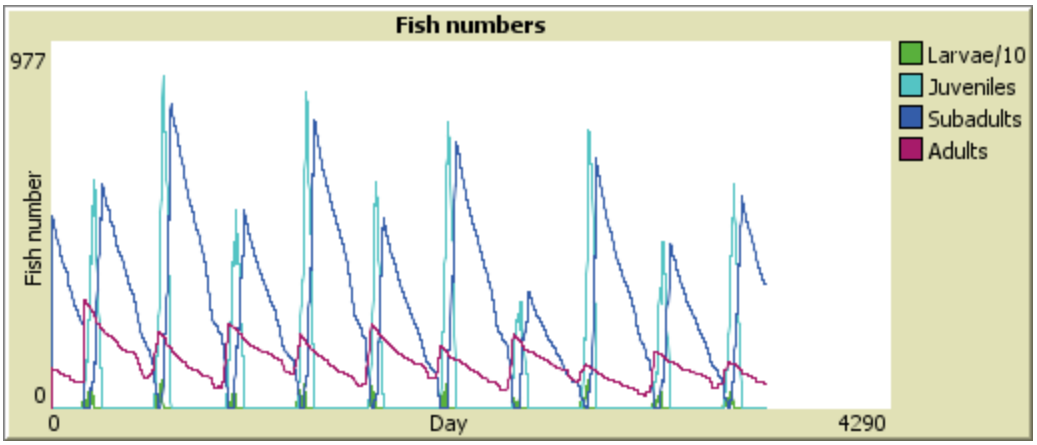


Figure S13. Population sizes in a TS-IBM simulation conducted over 10 years with the density-independent model calibrated for approximate population stability (DailySurvival_Egg_Larva = 0.76). The input files for daily biomasses of prey and environmental conditions were repeated in every simulated year. Population sizes have to be compared at the same time of the year. Although population numbers vary considerably between simulated years, populations are neither growing nor declining continuously over time.

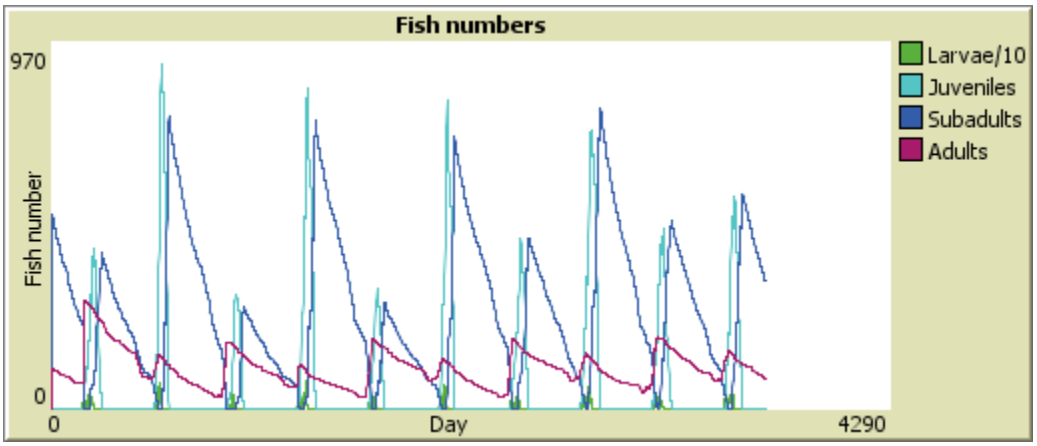


Figure S14. Population sizes in a TS-IBM simulation conducted over 10 years with the density-dependent model calibrated for approximate population stability (beta_dd_egg_survival = 0.04). The input files for daily biomasses of prey and environmental conditions were repeated in every simulated year. Population sizes have to be compared at the same time of the year. Although population numbers vary considerably between simulated years, populations are neither growing nor declining continuously over time.

6. MODEL ANALYSIS

6.1. Sensitivity analysis

We analyzed the sensitivity of hybrid model outputs to changes in a set of identified parameters (Table S36). Figures showing the outcomes of the sensitivity analyses depict single simulation runs with the TS-IBM. The density-dependent model was applied unless stated otherwise. Default values for all other than the tested model parameters were applied, and food biomass inputs from default $CASM_{OC}$ outputs from year 1 were used. The waterbody area simulated in $CASM_{OC}$ was set to 1125 m^2, the waterbody area simulated in TS-IBM was set to 100 m^2 unless stated otherwise.

Single simulation runs were conducted with hybrid model (yearly $CASM_{OC}$ biomass input file) for year 1. Results are shown as combined adult and subadult Topeka shiner biomass across the simulated year. In addition, changes in Topeka shiner biomass at the end of the simulated year (31 December) due to changes in parameter values were calculated. Percent changes in biomass were calculated as the difference between biomass in the simulation with default parameter settings and the simulation using an altered parameter value, and dividing the difference by the biomass from the default simulation. Note that due to stochasticity implemented in the TS-IBM, biomasses vary in default simulations. When repetitions are conducted with identical parameter settings, Topeka shiner biomasses at the of the simulated year range between 0.291 g C/m^2 and 0.402 g C/m^2 with a mean biomass of 0.337 g C/m^2. Accordingly, deviations from the default simulation run of up to 33% can be due to stochasticity in the model. Only applied changes in the parameters a_{cmax} and K_{min} from the select parameters tested in the sensitivity analysis (Table S36) resulted in altered Topeka shiner biomasses when applying this criterion.

Table S36. TS-IBM parameters analyzed in a sensitivity analysis (SA) and the values applied.

Parameter name	Name in model	Default value	Values applied in SA	Explanation of applied range	Reason parameter was included in SA
Waterbody area	pondArea	100 m^2	50, 100, 500, 1125 m^2	Waterbody area of 1125 m^2 identified as representative for Topeka shiner habitat	TS-IBM is not spatially explicit: verification that waterbody area does not affect model outputs (per m^2)
Daily egg and larval survival rate (density-independent model)	DailySurvival_Egg_Larva	0.76	0.743, 0.752, 0.76, 0.767, 0.774	Range of +/- 10%, 20% of default value applied to 10-survival (survival rate across both life stages)	Parameter used for model calibration (see Section 5.1.2); egg and larval survival identified as influential to

Parameter name	**Name in model**	**Default value**	**Values applied in SA**	**Explanation of applied range**	**Reason parameter was included in SA**
					model outcomes
Maximum daily egg and larval survival rate (density-dependent model)	DailySurvival_Egg_Larva_0	0.8	0.782, 0.792, 0.8, 0.808, 0.815	Range of +/- 10%, 20% of default value applied to 10-survival (survival rate across both life stages)	Egg and larval survival identified as influential to model outcomes
Steepness of Ricker function determining egg and larval survival rate (density-dependent model)	beta_dd_egg_survival	0.04	0.032; 0.036; 0.04; 0.044; 0.048	Range of +/- 10%, 20% of default value applied	Parameter used for model calibration (see Section 5.1.2); egg and larval survival identified as influential to model outcomes
α_{cmax}	a_cmax	0.07	0.056, 0.063, 0.07, 0.077, 0.084	Range of +/- 10%, 20% of default value applied	Maximum consumption identified as key parameter for bioenergetics
Topeka shiner assimilation rate of consumed detritus	juv_ass_detritus/ adt_ass_detritus	0.35	0.25, 0.3, 0.35, 0.4, 0.45	Range of values estimated in the literature	Detritus assimilation rate by fish uncertain
Search area scaling factor	ScalingSearchArea	1.0	0.8, 0.9, 1.0, 1.1, 1.2	Range of +/- 10%, 20% of default value applied	Impacts food availability for consumption by individual TS
Average threshold for viable fish condition, K_{min}	Kmin	0.68	0.544, 0.612, 0.68, 0.748, 0.816	Range of +/- 10%, 20% of default value applied	Parameter affects death rate due to starvation

6.1.1. Waterbody area

The TS-IBM is not spatially explicit, but simulates individual Topeka shiners who respond to food density via a functional response. Due to stochastic processes in the model, population-level outcomes may vary considerably for very small populations which would occur in very small water bodies. However, in larger populations occurring in larger waterbodies, the Topeka shiner biomass per area is expected to be similar.

With a sensitivity analysis of waterbody area, we verified the correct model behavior. In Figure S15, we show the biomass (in g C) per m^2 pond for different pond sizes applied (see Table S36). All pond areas resulted in near-identical Topeka shiner biomass dynamics across a simulated year. Changing the pond area results in changes in model output due to stochastic simulations, but no systematic change in the population dynamics occur.

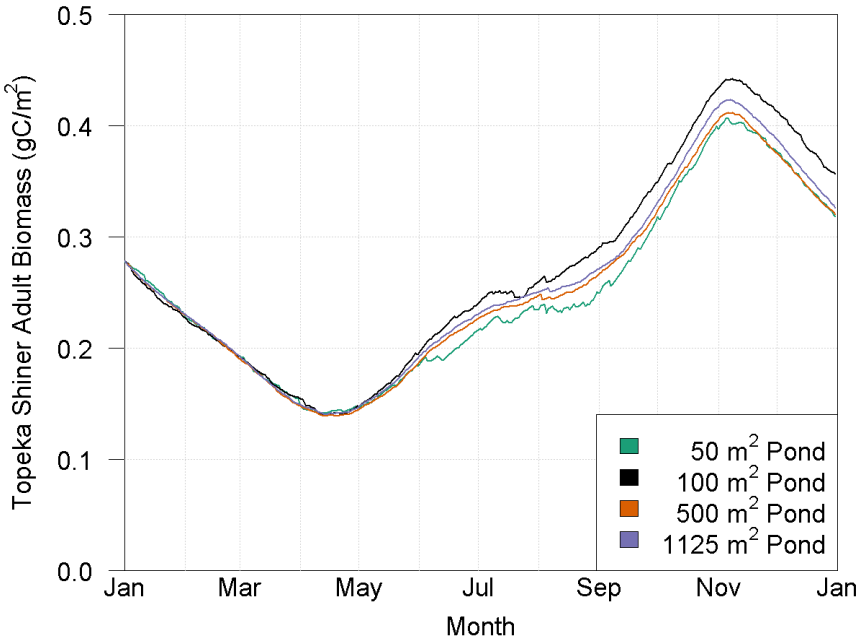


Figure S15. Adult (including subadult) Topeka shiner biomasses (g C/ m^2) across one simulated year. A range of waterbody (pond) areas were simulated in TS-IBM. The waterbody area simulated in the $CASM_{OC}$ simulations that provide the food availability was set to the default of 1125 m^2.

Table S37. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in waterbody (pond) area. Default simulated waterbody area in the TS-IBM is 100 m^2.

Waterbody area (m^2)	% change in adult Topeka shiner biomass
50	-10.6
100	0
500	-10.1
1125	-8.5

6.1.2. Daily egg and larval survival rate (density-independent model)

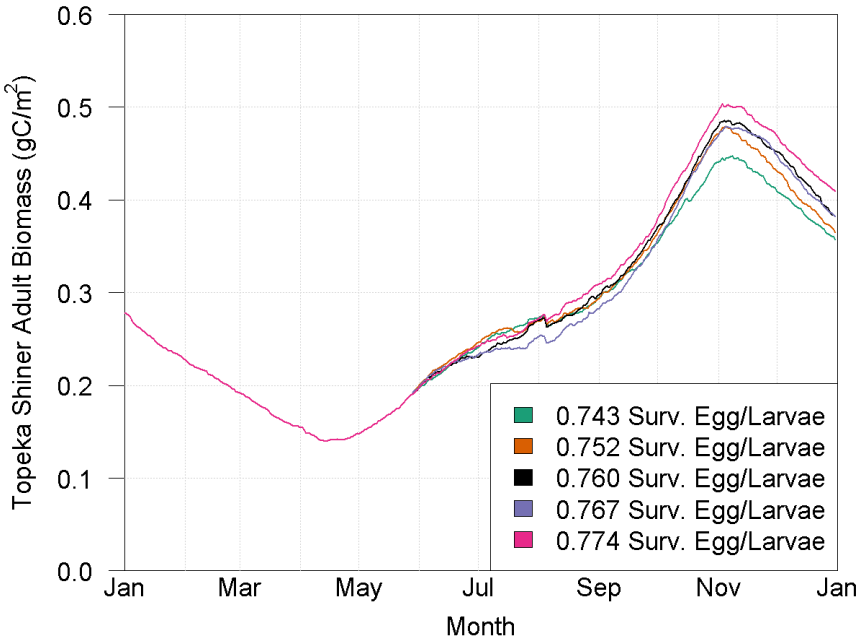


Figure S16. Egg and larval daily survival rate in the density-independent TS-IBM has no clear effect on adult Topeka shiner biomasses. The higher the survival rate, the higher the peak and end-of-year biomass.

Table S38. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in egg and larval daily survival rate. Default simulated egg and larval daily survival rate in the TS-IBM is 0.76.

Egg and larval daily survival rate (density-independent model)	% change egg and larval daily survival rate from default	% change in adult Topeka shiner biomass
0.743	-20	-6.56
0.752	-10	-4.42
0.760	0	0
0.767	10	-0.01
0.774	20	-7.22

6.1.3. Maximum daily egg and larval survival rate (density-dependent model)

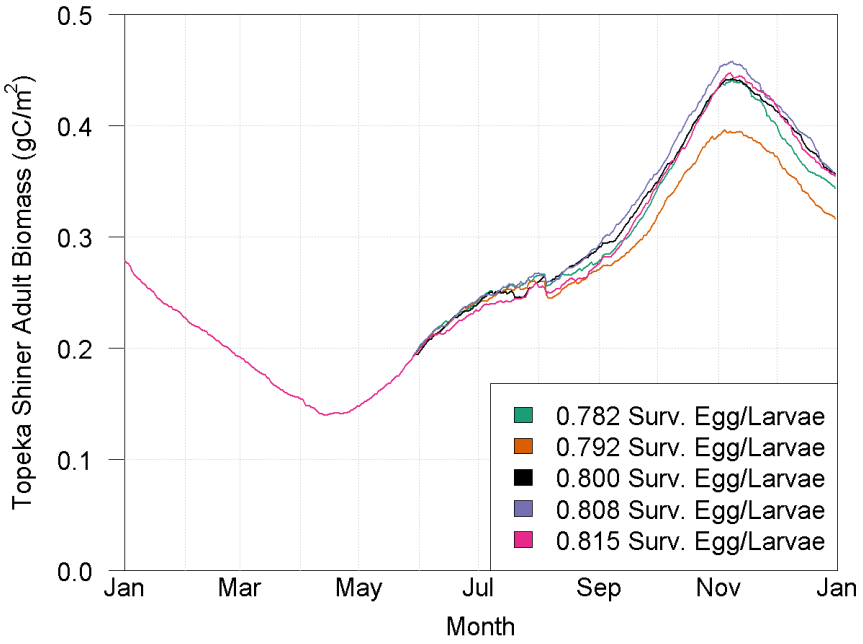


Figure S17. The tested range of maximum egg and larval survival rates in the density-dependent model do not systematically impact Topeka shiner biomass across the year.

Table S39. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in maximum egg and larval daily survival rate in the density-dependent model. Default simulated egg and larval maximum daily survival rate in the TS-IBM is 0.8.

Maximum egg and larval daily survival rate (density-dependent model)	% change in maximum egg and larval daily survival rate from default	% change in adult Topeka shiner biomass
0.782	-20	-3.52
0.792	-10	-11.21
0.8	0	0
0.808	10	-0.4
0.815	20	-0.5

6.1.4. Steepness of Ricker function determining egg and larval survival rate

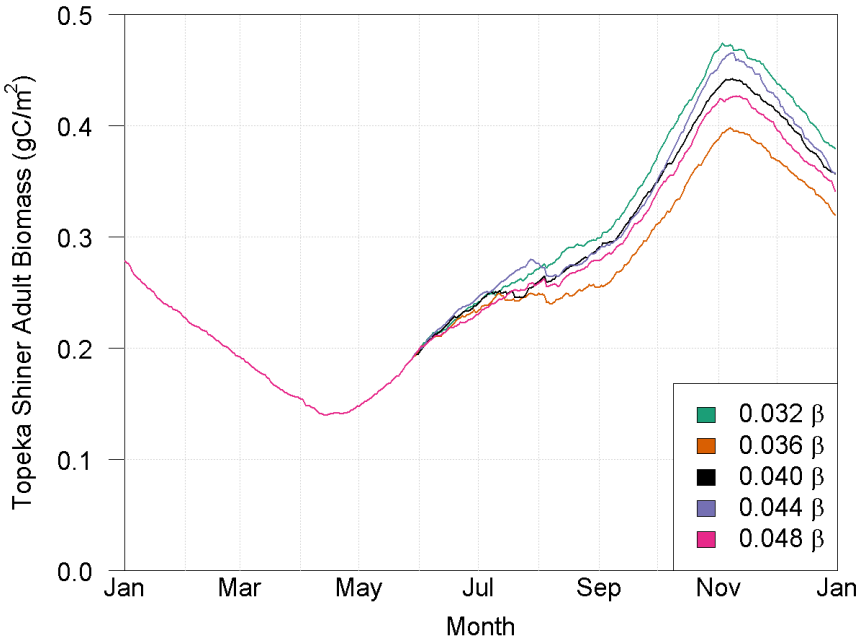


Figure S18. The steepness, β, of the Ricker function in the density-dependent TS-IBM has no clear systematic impact on the Topeka shiner adult biomasses across the year. Egg and larval survival rates are affected by the biomass of subadult and adult Topeka shiners in the density-dependent model.

Table S40. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in slope of the density-dependence (Ricker) function of egg and larval daily survival rate in the density-dependent model. Default steepness of the function in the TS-IBM is 0.04.

Steepness of Ricker function (β) in the density-dependent model	% change steepness of Ricker function (β) for density-dependent egg and larval daily survival rate	% change in adult Topeka shiner biomass
0.032	-20	6.38
0.036	-10	-10.33
0.04	0	0
0.044	10	0.16
0.048	20	-4.39

6.1.5. Factor linking maximum consumption rate C_{max} to fish weight (α_{cmax})

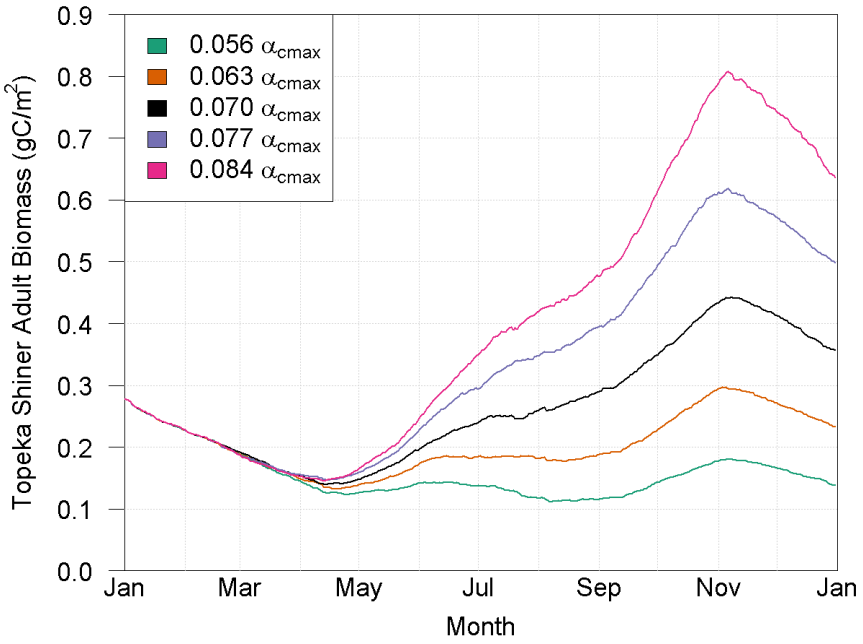


Figure S19. Changes in maximum consumption rates, C_{max}, dependent on fish weight are very important for population-level biomasses of Topeka shiners in the model. C_{max} is a key function for fish consumption, and thus, growth. The default parameters (from fathead minnow values listed by FB4) α_{cmax} and β_{cmax} were calibrated to fit Topeka shiner growth in the model to fish-at-age measures from the literature (Section 5.1.1.).

Table S41. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in α_{cmax} (altering maximum consumption rates). Default α_{cmax} in the TS-IBM is 0.07. Changes due to altered α_{cmax} exceed variability in simulation runs due to stochasticity.

α_{cmax}	% change α_{cmax} from default	% change in adult Topeka shiner biomass
0.056	-20	-61.26
0.063	-10	-34.76
0.070	0	0
0.077	10	39.69
0.084	20	78.5

6.1.6. Topeka shiner assimilation rate of consumed detritus

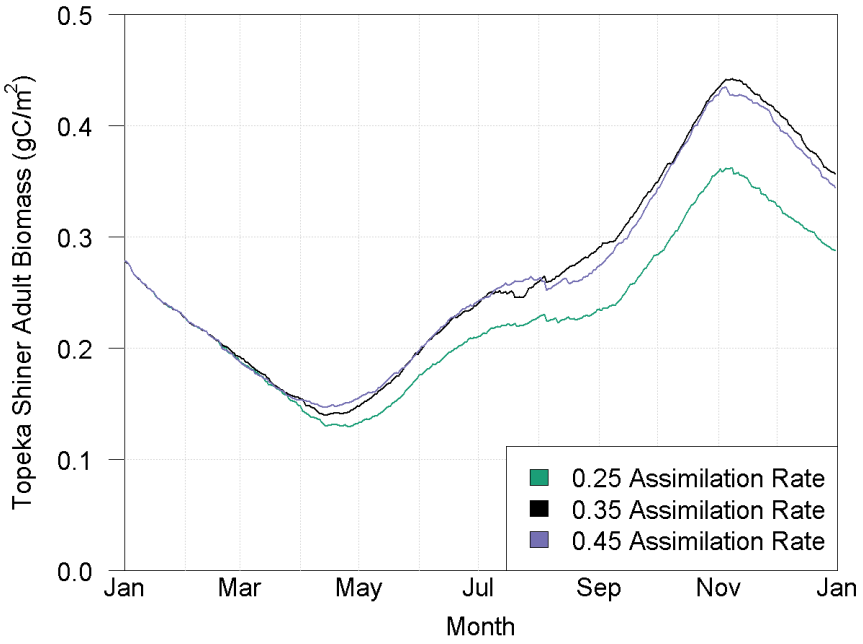


Figure S20. Changes in detritus assimilation rate by Topeka shiners. The default parameter value is 0.35. A reduction in assimilation rate (to 0.25) results in reduced Topeka shiner biomass.

Table S42. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes detritus assimilation rate.

Detritus assimilation rate	% change in detritus assimilation rate from default	% change in adult Topeka shiner biomass
0.25	-28.6	-19.24
0.35	0	0
0.45	28.6	-3.48

6.1.7. Search area scaling factor

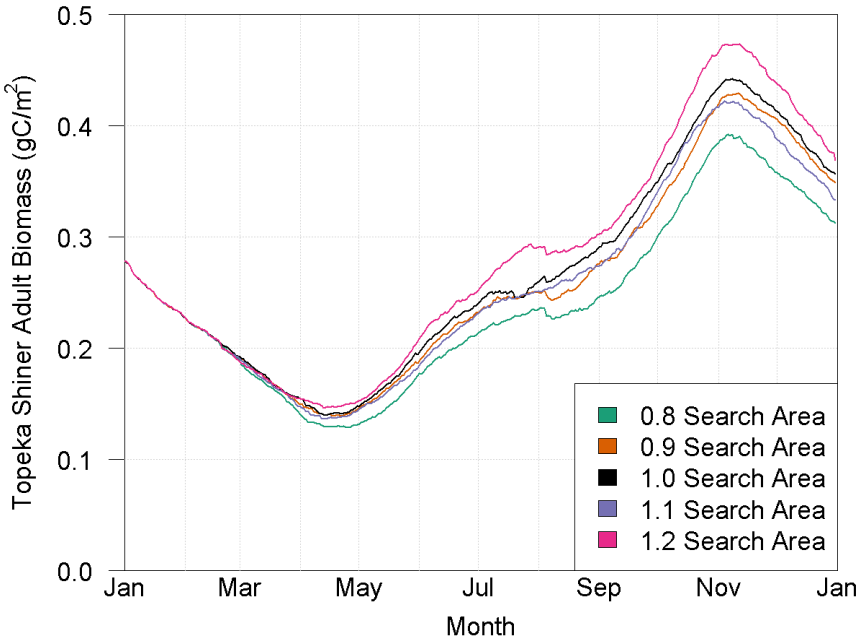


Figure S21. Applying a scaling factor to the search area a fish can consume food from on a daily basis leads to small changes in population-level biomasses across the year. Scaling factor of the search area is not linearly related to Topeka shiner population biomass.

Table S43. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in the scaling factor of the search area (area a fish can search for food per day). Default search area in the TS-IBM is 1.

Scaling factor to the search area	% change scaling factor to the search area from default	% change in adult Topeka shiner biomass
0.8	-20	-12.28
0.9	-10	-2.09
1	0	0
1.1	10	-6.58
1.2	20	3.53

6.1.8. Average threshold for viable fish condition, K_{min}

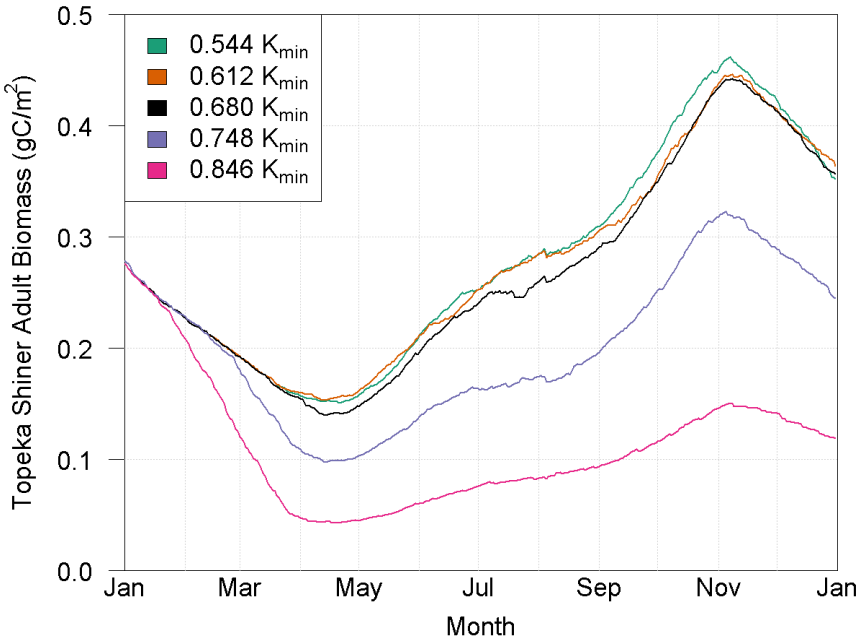


Figure S22. Minimum viable fish condition, K_{min}, has a strong impact on Topeka shiner biomasses across the year. The lower K_{min}, the longer periods of starvation the fish are simulated to survive. Accordingly, higher values of K_{min} lead to lower Topeka shiner population biomasses. Decreasing K_{min} from default does not have clear impacts on simulated Topeka shiner populations but increased K_{min} from default leads to decreased population biomass.

Table S44. Percent changes in adult (including subadult) Topeka shiner biomasses (g C/m^2) at the end of the simulated year (31 December) due to changes in minimum viable fish condition. Default minimum viable fish condition, K_{min}, in the TS-IBM is 0.68. Changes due to increases in K_{min} exceed variability in simulation runs due to stochasticity.

K_{min}	% change K_{min} from default	% change in adult Topeka shiner biomass
0.544	-20	-1.25
0.612	-10	1.99
0.68	0	0
0.748	10	-31.29
0.816	20	-66.54

6.2. Effects on Topeka shiner populations from exposure to benzovindiflupyr

In the main manuscript, the biomasses of the simulated Topeka shiner populations across the year with applied 0VFS and 15VFS oxbow exposure profiles are presented in Figure 3. The effects on population abundances followed a similar pattern (Figure S23). In contrast to biomass, Topeka shiner control abundance peaked in July during the spawning season and declined subsequently due to high background mortality of eggs and larvae assumed in the model. Abundance in exposed populations was unaffected in for both 0VFS and 15VFS exposure profiles. Abundance was considerably reduced due to the peak exposure if a multiplication factor of 2 was applied to the 0VFS exposure profile, and populations collapsed if a multiplication factor of 3 or higher was used. A multiplication factor of 5 applied to the 15VFS profile resulted in considerable effects on Topeka shiner abundance and a factor 10 caused the population to collapse. Accordingly, population abundance represents the less sensitive endpoint for effects compared to population biomass (see main manuscript).

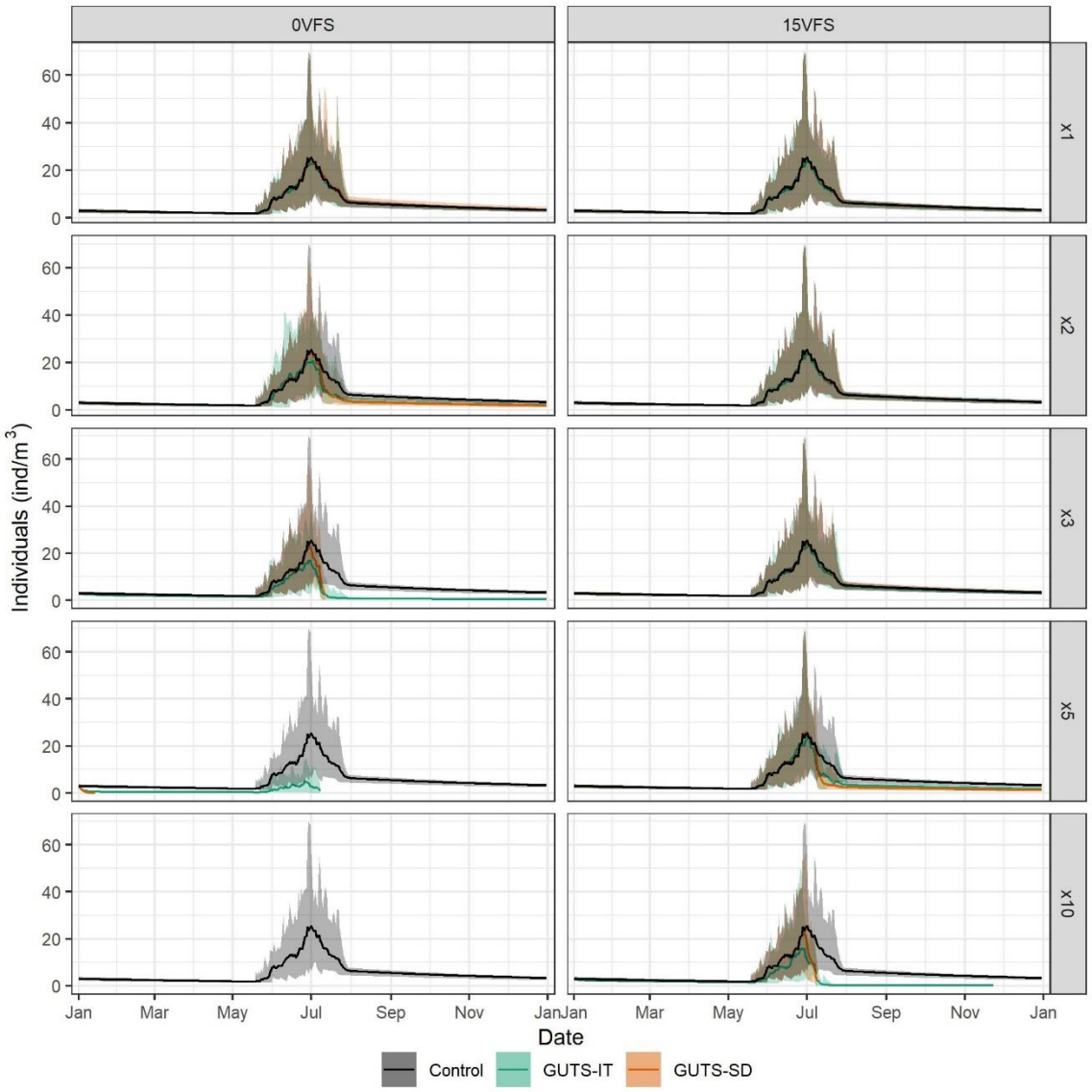


Figure S23. Dynamics of Topeka shiner population abundance (individuals/m^3) during the exposure year with 0VFS (left column) and 15VFS (right column) oxbow exposure profiles applied. Multiplication factors between 1 and 5 were applied to the 0VFS profile and between 1 and 10 to the 15VFS profile. Biomasses of exposed populations are shown in comparison to non-exposed populations (control). Lethal effects to the Topeka shiners were either simulated using GUTS-IT or GUTS-SD and combined with sublethal effects. Solid lines show the mean and shaded areas the range of outputs from 20 simulation repetitions.

6.3. Population-level exposure-effects relationships

As described in the main manuscript, from the end-of-year population-level effects, a dose-response relationship was derived using the BMDS tool (U.S. Environmental Protection Agency, 2018). Effects derived from model outputs can be used to identify candidate point of departures (POD). The POD is defined as the highest dose (multiplication factor) at which no adverse effects are observed (NOAEL). The most conservative NOAEL(s) were identified from the simulated effects of benzovindiflupyr on Topeka Shiner population biomass and abundance. In addition, a benchmark dose (BMD) analysis was conducted on the selected critical endpoints. BMD should allow for a more accurate selection of a POD than the NOAEL approach, which is limited by dose levels (multiplication factors) applied in the study. The use of the BMD methodology was preferred for the estimation of a POD for many reasons, including consideration of the shape of the entire dose-response curve and estimation of the experimental variability associated with the calculated dose-response relationship. Use of BMD methods involved fitting mathematical models to the observed dose-response data and provides a BMD and its 95% lower confidence limit (BMDL) associated with a pre-determined benchmark response (BMR). The BMDL was then used in lieu of the NOAEL or LOAEL as the POD. A benchmark response (BMR) of 1 standard deviation was applied to the continuous models given the effects data was continuous data with measures of variability with a negative trend. The effects data were not amenable to dichotomous models.

After fitting models to the data sets, the following procedure for model selection was applied. First, models were rejected if the p-value for global goodness of fit was <0.1 (Test 4).

There are four tests of interest for continuous data concerning differences in responses and or variances in responses.

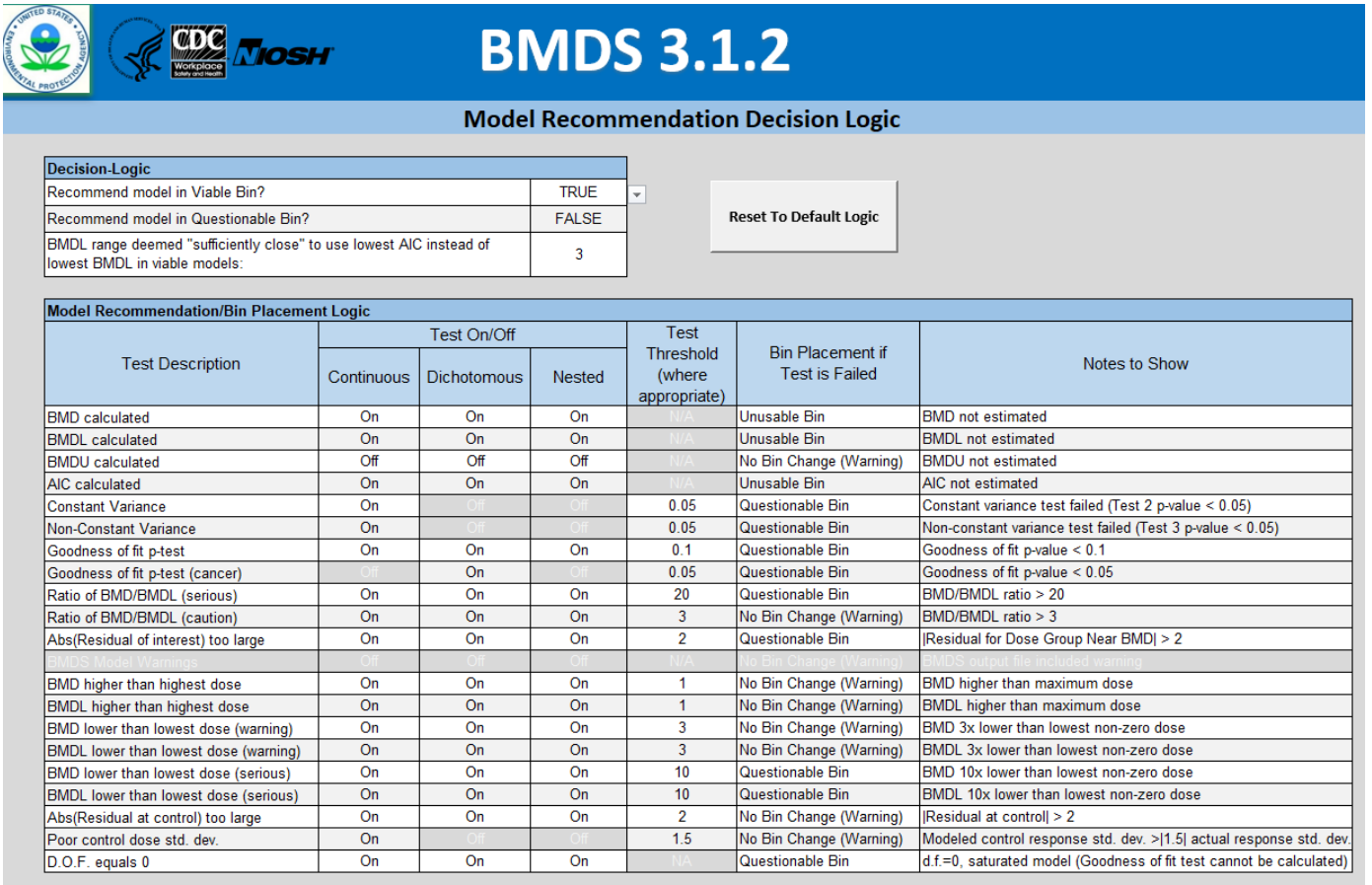
- Test 1 – Do responses and/or variances differ among dose levels? (Is the model statistically significantly different than the data?)
    - It is only appropriate to use models that show a difference between dose levels, $p > 0.05$.
- Test 2 – Are variances homogenous?
    - This test provides if a constant variance model is appropriate or a non-homogenous variance model is needed.
    - Constant variance test failed ($p < 0.05$)
- Test 3 - Are variances adequately modeled?
    - Nonconstant variance test failed ($p < 0.05$)
- Test 4 – Does the model fit the data? “Global”
    - This test is the global goodness-of-fit test and informs if modifications are needed for the data needed (e.g., log-scale doses, drop highest dose) or the data are not amenable to modeling; $p > 0.1$.

Models were rejected if they did not appear to adequately fit the low-dose region of the dose-response relationship, based on an examination of graphical displays (visual inspection) of the data and scaled residuals (difference between estimated curve and actual data points). If the BMDL estimates from the remaining models were “sufficiently close” (with a criterion of within twofold for “sufficiently close”; defined as 3-fold variance), then the model with the lowest Akaike’s Information Criteria (AIC) was selected. Akaike’s Information Criteria—a measure of information loss from a dose-response model that can be used to compare a set of models. The model with the lowest AIC among a specified set of models is considered the “best.” If two or more models shared the lowest AIC, an average of the BMDLs would be used, averaging was not used in this assessment because for the occasions in which models shared the lowest AIC, a selection was made based on visual fit and lowest scaled residues. If the BMDL estimates

from the remaining models are not sufficiently close, some model dependence was assumed. Additionally, for continuous models, constant variance models were used for model parsimony; however, nonconstant variance was run and evaluated and model parsimony was judged to be the reasonable method for this analysis.

For BMR selection, statistical and biological factors were considered. For continuous data, the preferred approach for defining the BMR is to use a pre-established value. This value should represent a minimal biologically significant response (e.g., there is substantial precedence for using a 10% change in weight for organ and body weights and a 5% change in weight for fetal weight). In the absence of a well-established cut-point, a BMR of 1 (control) standard deviation from the control mean may be used. For this data set on Topeka Shiner all runs were continuous models with a BMR of 1 SD.

The decision tree for acceptability is presented in Figure S24. The US EPA BMDS is primarily used to determine a POD or BMDL; however, in this case model fit was an additional objective.



BMDS 3.1.2

Model Recommendation Decision Logic

Decision-Logic	
Recommend model in Viable Bin?	TRUE
Recommend model in Questionable Bin?	FALSE
BMDL range deemed "sufficiently close" to use lowest AIC instead of lowest BMDL in viable models:	3

Reset To Default Logic

Model Recommendation/Bin Placement Logic

Test Description	Test On/Off			Test Threshold (where appropriate)	Bin Placement if Test is Failed	Notes to Show
	Continuous	Dichotomous	Nested			
BMD calculated	On	On	On	N/A	Unusable Bin	BMD not estimated
BMDL calculated	On	On	On	N/A	Unusable Bin	BMDL not estimated
BMDU calculated	Off	Off	Off	N/A	No Bin Change (Warning)	BMDU not estimated
AIC calculated	On	On	On	N/A	Unusable Bin	AIC not estimated
Constant Variance	On	Off	Off	0.05	Questionable Bin	Constant variance test failed (Test 2 p-value < 0.05)
Non-Constant Variance	On	Off	Off	0.05	Questionable Bin	Non-constant variance test failed (Test 3 p-value < 0.05)
Goodness of fit p-test	On	On	On	0.1	Questionable Bin	Goodness of fit p-value < 0.1
Goodness of fit p-test (cancer)	Off	On	Off	0.05	Questionable Bin	Goodness of fit p-value < 0.05
Ratio of BMD/BMDL (serious)	On	On	On	20	Questionable Bin	BMD/BMDL ratio > 20
Ratio of BMD/BMDL (caution)	On	On	On	3	No Bin Change (Warning)	BMD/BMDL ratio > 3
Abs(Residual of interest) too large	On	On	On	2	Questionable Bin	|Residual for Dose Group Near BMD| > 2
BMDS Model Warnings	Off	Off	Off	N/A	No Bin Change (Warning)	BMDS output file included warning
BMD higher than highest dose	On	On	On	1	No Bin Change (Warning)	BMD higher than maximum dose
BMDL higher than highest dose	On	On	On	1	No Bin Change (Warning)	BMDL higher than maximum dose
BMD lower than lowest dose (warning)	On	On	On	3	No Bin Change (Warning)	BMD 3x lower than lowest non-zero dose
BMDL lower than lowest dose (warning)	On	On	On	3	No Bin Change (Warning)	BMDL 3x lower than lowest non-zero dose
BMD lower than lowest dose (serious)	On	On	On	10	Questionable Bin	BMD 10x lower than lowest non-zero dose
BMDL lower than lowest dose (serious)	On	On	On	10	Questionable Bin	BMDL 10x lower than lowest non-zero dose
Abs(Residual at control) too large	On	On	On	2	No Bin Change (Warning)	|Residual at control| > 2
Poor control dose std. dev.	On	Off	Off	1.5	No Bin Change (Warning)	Modeled control response std. dev. >|1.5| actual response std. dev.
D.O.F. equals 0	On	On	On	NA	Questionable Bin	d.f.=0, saturated model (Goodness of fit test cannot be calculated)

Figure S24. BMDS Model Decision Logic.

In the Tables S46-S54, the results from the BMD runs determining the POD and the best fitting functions the simulated effects from the 0VFS and 15VFS exposure profiles with multiplication factors (doses) applied. Three functions tested in BMDS provided acceptable fits for all data sets: frequentist exponential degree 3, frequentist exponential degree 5, and the frequentist Hill function. We chose the frequentist

exponential degree 3 as the most parsimonious best fit across all data sets because it requires the fit of 3 parameters in contrast of 4 parameters that are fit to data for exponential degree 5 and the Hill functions. The following equation corresponds to the frequentist exponential degree 3 function:

$$\mathrm{M}(dose) = \mathrm{a}\, e^{-(b\, dose)^d}$$

In the equation, a is the control level (background response), b is the slope (> 0) of the function and d is the power (> 1). The parameters providing the best fit of the frequentist exponential degree 3 function to the Topeka shiner population endpoints are listed in Table S45. The resulting dose response curves along with the effects data are presented in the main manuscript (Figure 5).

Table S45. Parameters of the frequentist exponential degree 3 function fit to the end-of-year Topeka shiner population biomass (g C/m2) and abundance (#/m3) using BMDS.

Exposure profile	Lethal effects simulation	Population-level endpoint	a	b	d
0VFS	GUTS-IT	Biomass	0.218 g C/m^2	0.484	2.778
0VFS	GUTS-SD	Biomass	0.214 g C/m^2	0.503	5.362
15VFS	GUTS-IT	Biomass	0.215 g C/m^2	0.208	3.986
15VFS	GUTS-SD	Biomass	0.215 g C/m^2	0.216	6.143
0VFS	GUTS-IT	Abundance	3.376 #/m^3	0.424	3.421
0VFS	GUTS-SD	Abundance	3.363 #/m^3	0.488	18.0*
15VFS	GUTS-IT	Abundance	3.266 #/m^3	0.180	4.344
15VFS	GUTS-SD	Abundance	3.311 #/m^3	0.200	12.938

* Parameter estimate fell within the tolerance boundaries set by BMDS, and was bounded to the listed value.

Table S46. Summary of Dose Response Model Curve Fitting for Mortality With or Without Vegetative Filter Strip in Biomass and Individuals of Topeka Shiner to Benzovindiflupyr

Effect	POD type	POD	Comment
0VFS			
Biomass (GUTS-IT)	NOAEL	1.5	
Biomass (GUTS-IT)	BMDL	0.8	Table S47, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
Biomass (GUTS-SD)	NOAEL	1.5	
Biomass (GUTS-SD)	BMDL	1.2	Table S48, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
Abundance (GUTS-IT)	NOAEL	1.5	
Abundance (GUTS-IT)	BMDL	1.4	Table S49, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
Abundance (GUTS-SD)	NOAEL	1.5	
Abundance (GUTS-SD)	BMDL	1.8	Table S50, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
15VFS			
Biomass (GUTS-IT)	NOAEL	5	
Biomass (GUTS-IT)	BMDL	2.5	Table S51, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
Biomass (GUTS-SD)	NOAEL	5	
Biomass (GUTS-SD)	BMDL	2.9	Table S52, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
Abundance (GUTS-IT)	NOAEL	5	
Abundance (GUTS-IT)	BMDL	3.0	Table S53, Hill model, continuous BMR = 1SD Lowest AIC and scaled residuals form M3 and M5
Abundance (GUTS-SD)	NOAEL	5	
Abundance (GUTS-SD)	BMDL	3.5	Table S54, Hill M3, or M5 models, continuous BMR = 1SD; all three have similar AIC and scaled residuals

Table S47. Summary of BMD modeling results for population biomass with 0VFS exposure profile and lethal effects modeled using GUTS-IT; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	-453.945	-3.221	-3.2217	0.335357189	0.286173736	poor goodness of fit
Exponential (M3)	**0.05691**	**-618.736**	**1.7166**	**-0.6291**	**0.851297379**	**0.768089629**	**Acceptable visual fit; goodness of fit does not pass Test 4 and questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	-453.945	-3.221	-3.2216	0.335358	0.286173	poor goodness of fit
Exponential (M5)	**0.02330**	**-616.743**	**1.7045**	**-0.6218**	**0.852532**	**0.768986**	**Acceptable visual fit; goodness of fit does not fit Test 4 and questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.00507**	**-613.695**	**0.5301**	**-0.0452**	**0.968811**	**0.883881**	**Lowest AIC, acceptable visual fit, and lowest scaled residuals suggest best fit of the model to the data; goodness of fit does not pass, questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	-458.322	4.6000	0.67368	0.720586777	0.683336202	poor goodness of fit
Polynomial 4°	<0.0001	-458.322	4.6000	0.67368	0.720586777	0.696198063	poor goodness of fit
Polynomial 3°	<0.0001	-458.322	4.6000	0.67370	0.720586777	0.639275125	poor goodness of fit
Polynomial 2°	<0.0001	-458.322	4.6000	0.67370	0.720586777	0.639275125	poor goodness of fit
Power	<0.0001	-458.322	4.6000	0.67373	0.720588603	0.639233077	poor goodness of fit
Linear	<0.0001	-458.322	4.6001	0.6739	0.720596313	0.639269199	poor goodness of fit

Table S48. Summary of BMD modeling results for population biomass with 0VFS exposure profile and lethal effects modeled using GUTS-SD; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	-397.9077	-3.25863	-3.25863	0.42825	0.358149	poor goodness of fit
Exponential (M3)	**0.574859**	**-625.0453**	**0.13790**	**0.2760084**	**1.25443**	**1.16466**	**Acceptable visual fit; goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	-397.9078	-3.26105	-3.261054	0.427978	0.358149	poor goodness of fit
Exponential (M5)	**0.567768**	**-623.9014**	**0.126363**	**0.29077**	**1.255472**	**1.166731**	**Lowest AIC, acceptable visual fit, goodness of fit passes Test 4; and questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.63422**	**-624.1228**	**0.04720**	**0.617077**	**1.303989**	**1.233465**	**Acceptable visual fit, goodness of fit passes Test 4, lowest scaled residuals suggest best fit of the model to the data; questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	-410.9504	4.138085	-0.395236	0.835116	0.770449	poor goodness of fit
Polynomial 4°	<0.0001	-410.9504	4.1380	-0.395217	0.835118	0.801694	poor goodness of fit
Polynomial 3°	<0.0001	-410.9504	4.138088	-0.395224	0.835118	0.736884	poor goodness of fit
Polynomial 2°	<0.0001	-410.9504	4.13809	-0.395217	0.835118	0.736884	poor goodness of fit
Power	<0.0001	-410.9504	4.138072	-0.395247	0.835116	0.736874	poor goodness of fit
Linear	<0.0001	-410.9504	4.138095	-0.395213	0.835118	0.736884	poor goodness of fit

Table S49. Summary of BMD modeling results for population abundance with 0VFS exposure profile and lethal effects modeled using GUTS-IT; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	248.9333	-3.62772	-3.627727	0.478914	0.402121	poor goodness of fit
Exponential (M3)	**0.240254**	**77.87730**	**0.693109**	**-0.851834**	**1.205586**	**1.102487**	**Acceptable visual fit; goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	248.9333	-3.62740	-3.62740	0.47893	0.402123	poor goodness of fit
Exponential (M5)	**0.140555**	**79.59754**	**0.648423**	**-0.811710**	**1.214105**	**1.10733**	**Acceptable visual fit, goodness of fit passes Test 4; and questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.98688**	**75.699630**	**-0.09621**	**-0.029876**	**1.35289**	**1.25245**	**Lowest AIC, acceptable visual fit, goodness of fit passes Test 4, lowest scaled residuals suggest best fit of the model to the data; questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	207.31761	3.804916	-1.898923	0.720487	0.648881	poor goodness of fit
Polynomial 4°	<0.0001	207.31761	3.804916	-1.89892	0.720487	0.639098	poor goodness of fit
Polynomial 3°	<0.0001	207.31761	3.804916	-1.898923	0.720487	0.639098	poor goodness of fit
Polynomial 2°	<0.0001	207.31761	3.804915	-1.898924	0.720487	0.639098	poor goodness of fit
Power	<0.0001	207.31761	3.804915	-1.898924	0.720487	0.639099	poor goodness of fit
Linear	<0.0001	207.31761	3.804916	-1.898924	0.720487	0.639098	poor goodness of fit

Table S50. Summary of BMD modeling results for population abundance with 0VFS exposure profile and lethal effects modeled using GUTS-SD; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	302.06591	3.579668	-3.587381	0.610990077	0.5014093	poor goodness of fit
Exponential (M3)	**0.002299**	**106.07185**	**-0.00439**	**-0.594947**	**1.816773787**	**1.667916**	**Acceptable visual fit; goodness of fit does not pass Test 4, questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	304.06591	3.579708	-3.587306	0.610993952	0.501409	poor goodness of fit
Exponential (M5)	**0.030749**	**100.35333**	**-0.00478**	**-0.61543**	**1.811540648**	**1.6653882**	**Acceptable visual fit; goodness of fit does not pass Test 4, questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.031381**	**100.30843**	**-0.01594**	**-0.637186**	**1.780560923**	**1.605288**	**Lowest AIC, acceptable visual fit, lowest scaled residuals suggest best fit of the model to the data; goodness of fit does not pass Test 4, questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	264.80773	2.963429	-2.564960	0.872970223	0.7683438	poor goodness of fit
Polynomial 4°	<0.0001	264.80773	2.963502	-2.564924	0.872963965	0.7687913	poor goodness of fit
Polynomial 3°	<0.0001	264.80773	2.963425	-2.564965	0.872969925	0.768790	poor goodness of fit
Polynomial 2°	<0.0001	264.80773	2.963343	-2.56515	0.872952044	0.7687910	poor goodness of fit
Power	<0.0001	266.33345	2.868083	-2.189256	0.720487	0.639099	poor goodness of fit
Linear	<0.0001	264.8077	2.96334	-2.565158	0.720487	0.639098	poor goodness of fit

Table S51. Summary of BMD modeling results for population biomass with 15VFS exposure profile and lethal effects modeled using GUTS-IT; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	-431.0757	0.251291	-3.840520	0.937561989	0.7922481	poor goodness of fit
Exponential (M3)	**0.333646**	**-586.4681**	**-0.46624**	**0.1358373**	**2.696905136**	**2.4427617**	**Acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	-431.0757	0.251286	-3.840528	0.937561989	0.7922481	poor goodness of fit
Exponential (M5)	**0.218460**	**-584.8282**	**-0.47392**	**0.1438897**	**2.698779106**	**2.4441125**	**Acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.338821**	**-585.7059**	**-0.28082**	**0.2331529**	**2.731139602**	**2.5180511**	**Lowest AIC, acceptable visual fit, goodness of fit pass Test 4, lowest scaled residuals suggest best fit of the model to the data; questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	-478.1910	0.144655	-2.397064	1.340990067	1.2040017	poor goodness of fit
Polynomial 4°	<0.0001	-478.1910	0.144659	-2.397059	1.340990067	1.2238327	poor goodness of fit
Polynomial 3°	<0.0001	-478.1910	0.144632	-2.397097	1.340990067	1.1933049	poor goodness of fit
Polynomial 2°	<0.0001	-478.1910	0.144632	-2.397097	1.340990067	1.1932377	poor goodness of fit
Power	<0.0001	-476.5818	0.159509	-2.048351	1.464539754	1.2033694	poor goodness of fit
Linear	<0.0001	-478.191	0.144609	-2.39711	1.341	1.932	poor goodness of fit

Table S52. Summary of BMD modeling results for population biomass with 15VFS exposure profile and lethal effects modeled using GUTS-SD; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	-389.614	0.350781	-3.662287	1.060314178	0.8817098	poor goodness of fit
Exponential (M3)	**0.940944**	**-601.8417**	**-0.07499**	**0.1118456**	**3.145427704**	**2.8877966**	**Acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	-389.6147	0.350774	-3.662289	1.060314178	0.8817098	poor goodness of fit
Exponential (M5)	**0.831238**	**-599.8687**	**-0.05527**	**0.1063260**	**3.141608238**	**2.8878649**	**Acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.870939**	**-599.9620**	**-0.02517**	**0.142502**	**3.115369404**	**2.9404184**	**Lowest AIC, acceptable visual fit, goodness of fit pass Test 4, lowest scaled residuals suggest best fit of the model to the data; questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	-423.6496	3.300190	-2.239541	1.613912582	1.4334608	poor goodness of fit
Polynomial 4°	<0.0001	-423.6496	3.300190	-2.239541	1.613912582	1.5428785	poor goodness of fit
Polynomial 3°	<0.0001	-423.6496	3.300190	-2.239541	1.613912582	1.4284758	poor goodness of fit
Polynomial 2°	<0.0001	-423.6496	3.30019	-2.239541	1.613912582	1.4284866	poor goodness of fit
Power	<0.0001	-421.7397	3.23924	-2.077253	1.688534005	1.4307314	poor goodness of fit
Linear	<0.0001	-423.6496	3.300190	-2.239541	1.613913	1.428576	poor goodness of fit

Table S53. Summary of BMD modeling results for population abundance with 15VFS exposure profile and lethal effects modeled using GUTS-IT; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	223.1431	-0.54124	-3.552564	1.150081	0.969448	poor goodness of fit
Exponential (M3)	**0.346658**	**106.95311**	**-0.10927**	**0.5838405**	**3.402167**	**2.928332**	**Acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	223.14316	-0.54123	-3.552563	1.150081	0.969448	poor goodness of fit
Exponential (M5)	**0.50661**	**107.00602**	**-0.10956**	**0.5901032**	**3.393898**	**2.944899**	**Acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.51852**	**106.95958**	**-0.08495**	**0.612664**	**3.362946**	**2.951969**	**Lowest AIC, acceptable visual fit, goodness of fit pass Test 4, lowest scaled residuals suggest best fit of the model to the data; questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	145.60379	2.573114	-1.608433	1.905112	1.501767	poor goodness of fit
Polynomial 4°	<0.0001	145.60379	2.573117	-1.60843	1.90511	1.501881	poor goodness of fit
Polynomial 3°	<0.0001	145.60379	2.573118	-1.608435	1.90511	1.501881	poor goodness of fit
Polynomial 2°	<0.0001	145.60379	2.573117	-1.608435	1.90511	1.501881	poor goodness of fit
Power	<0.0001	140.81093	2.337187	-1.248821	2.118786	1.707107	poor goodness of fit
Linear	<0.0001	155.44163	-1.15390	-3.36263	1.304448	1.161597	poor goodness of fit

Table S54. Summary of BMD modeling results for population abundance with 15VFS exposure profile and lethal effects modeled using GUTS-SD; BMR = 1 std. dev. change from control mean.

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Exponential (M2)	<0.0001	260.76371	-0.05529	-3.712640	1.210569	1.007754	poor goodness of fit
Exponential (M3)	**0.934840**	**100.3507 7**	**2.02E^{-06}**	**0.0318202**	**4.233781**	**3.457082**	**Lowest AIC, acceptable visual fit. goodness of fit pass Test 4; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Exponential (M4)	<0.0001	260.76371	-0.05529	-3.712644	1.210567	1.00776	poor goodness of fit
Exponential (M5)	**0.97755**	**101.9702 6**	**9.21E^{-07}**	**0.031707**	**4.229989**	**3.455481**	**Acceptable visual fit. goodness of fit pass Test 4, lowest scaled residuals suggest best fit of the model to the data; questionable model with constant variance test failed (Test 2 p-value < 0.05)**
Hill	**0.977515**	**101.9703 4**	**-6.11E^{-05}**	**0.0289310**	**4.116465**	**3.402789**	**Acceptable visual fit, goodness of fit pass Test 4; questionable model with test 2 constant variance test failed (Test 2 p-value < 0.05)**
Polynomial 5°	<0.0001	209.5364	2.512542	-2.474180	1.82469	1.477665	poor goodness of fit
Polynomial 4°	<0.0001	209.5364	2.512542 471	-2.4741625 38	1.824697	1.429899	poor goodness of fit
Polynomial 3°	<0.0001	209.5364	2.512550 552	-2.4741905 07	1.824684	1.429888	poor goodness of fit
Polynomial 2°	<0.0001	209.5364	2.512550 409	-2.4741900 34	1.824684	1.429864	poor goodness of fit
Power	<0.0001	205.03533 02	2.269095 804	-1.9289517 97	2.133026	1.672327	poor goodness of fit

Model[a]	Goodness of fit		Scaled Residual		BMD_{1SD} (dose)	$BMDL_{1SD}$ (dose)	Basis for model selection
	p-value (p > 0.1)	AIC	Dose Group near BMD	Control Dose Group			
Linear	<0.0001	209.5315279	2.713467654	-3.221071872	4.13797	3.402885	poor goodness of fit

6.4. Population recovery

Population recovery time was defined as the number of simulated years until exposed populations reached control-level biomass and abundance. In the main manuscript, recovery trajectories are presented for population biomasses after reductions due to exposures to benzovindiflupyr (Figure 6). Figure S25 shows corresponding recovery for Topeka shiner abundance. Recovery in abundance was delayed compared to the recovery of biomass: numbers of individuals remained at their reduced level (year 6) for the year following the exposure (year 7). Abundance increased in the following year until control levels were reached. As observed for population biomass, higher reductions in abundance due to the exposure resulted in longer recovery times. Populations did not recover if they were reduced to very low numbers at the end of the exposure year (Figure S25, 0VFS x5).

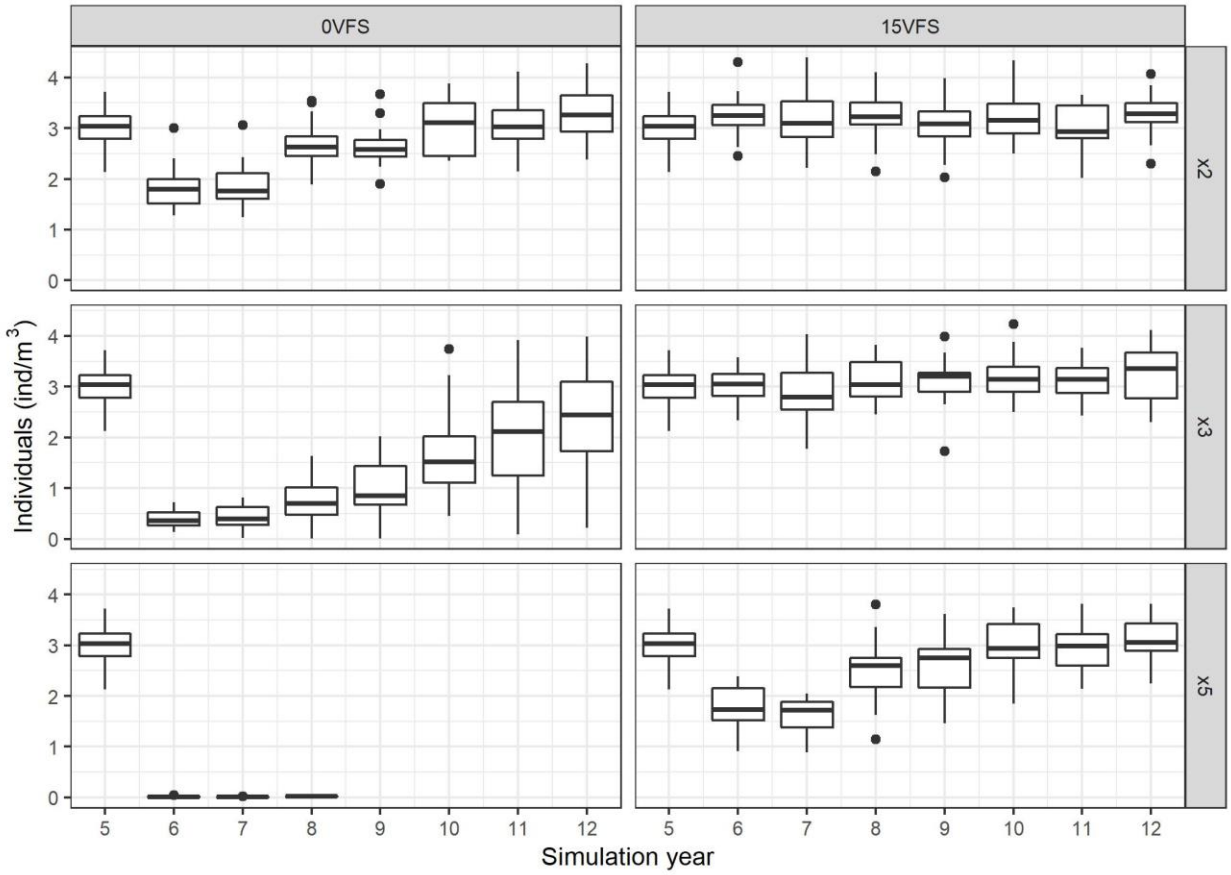


Figure S25. Recovery of Topeka shiner population abundance (individuals/m) after exposure to the single-year 0VFS (left column) and 15VFS (right column) oxbow exposure profile. Simulation year 6 corresponds to the exposure year. Lethal effects were simulated with GUTS-IT and combined with sublethal effects. Multiplication factors 2, 3 and 5 are shown as examples. Medians as a percentage of control from the 20 simulation repetitions are shown; boxes delineate the interquartile range, showing the 25th and 75th percentiles. Whiskers extend up to 1.5 times the interquartile range, and outliers are beyond the whiskers.

6.5. Separating lethal and sublethal effects

In the simulation results presented in the main manuscript, exposures to benzovindiflupyr were simulated to affect Topeka shiner growth (through consumption inhibition; sublethal effects) and survival rate (lethal effects).

To better understand the role of lethal and sublethal effects on Topeka shiner population properties, we simulated the two effects pathways separately. For these exploratory simulations, a single exposure profile was used. We chose the 0VFS x2 profile because it caused considerable effects on end-of-year population biomass (<50% of control biomass) but not complete population collapse (>10% of control biomass) in the simulations with combined effects. Intermediate effect levels were assumed to be most likely compounded of sublethal and lethal effects. Simulation sets were conducted applying only lethal effects, using either GUTS-IT or GUTS-SD. Sublethal effects were also simulated separately using the 0VFS x2 exposure, including no direct lethal effects.

Sublethal effects alone did not have a large impact on population biomass for the tested exposure profile: on average, biomass dropped to 91% of control level. The average individual number was slightly increased compared to controls, suggesting that the limited sublethal effects did not result in increased mortality. Reductions in abundance at the end of the exposure year were similar (median ~50%) between simulations with combined affects and simulations applying lethal effects only. Population biomasses at the end of the exposure year declined more when both lethal and sublethal effects were simulated (Figure S26).

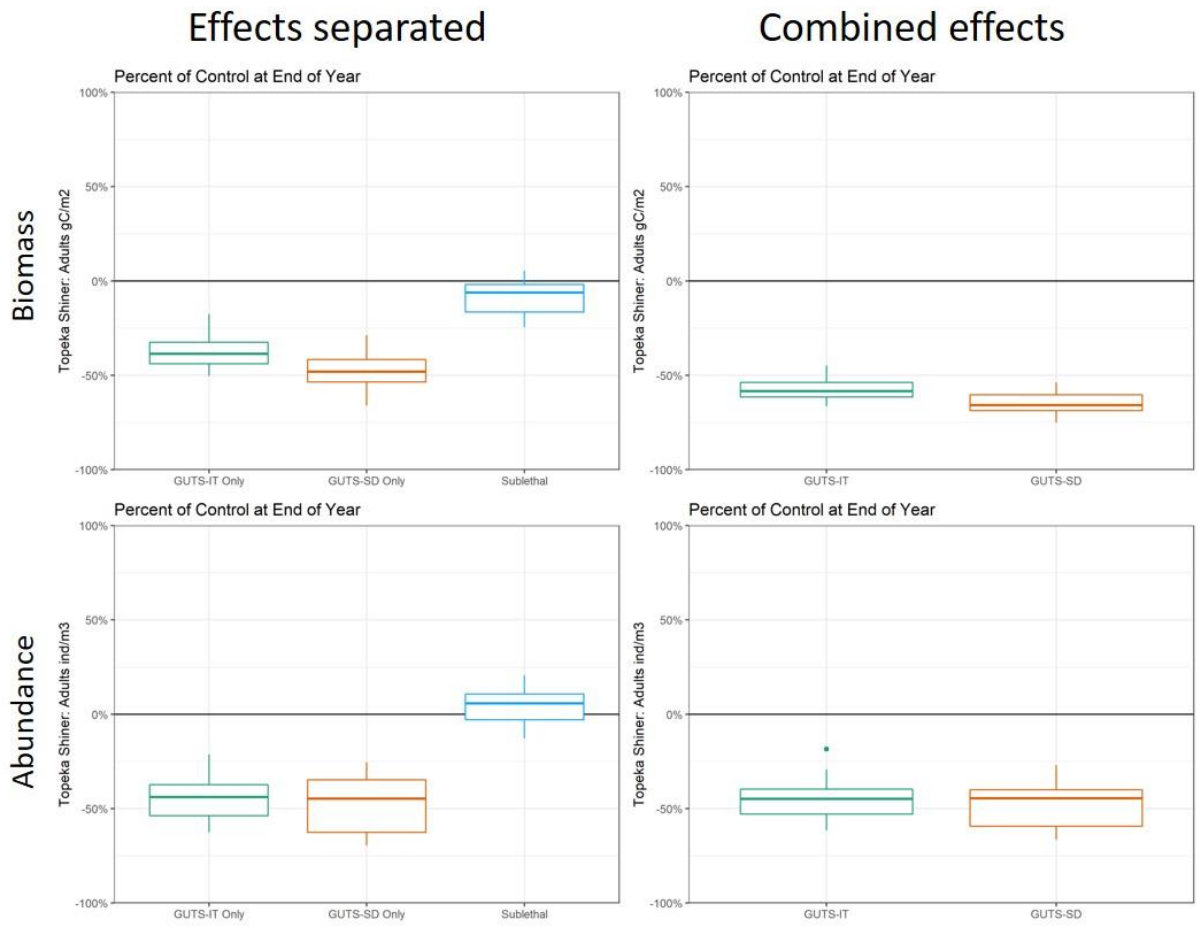


Figure S26. End-of-year Topeka shiner biomass (g C/m^2; top) and abundance (individuals/m^3; buttom) for the 0VFS x2 exposure profile. Effects are shown as percent of control. Simulations with only lethal, only sublethal and combined effects are shown. Lethal effects were either simulated using GUTS-IT or GUTS-SD.

From the simulations with the separate effects, an expectation of combined additive effects can be derived: the proportion of the control biomass observed if effects were simulated in combination should equal the proportion of control from lethal effects only times the proportion of control from sublethal effects only. However, the observed effects on population biomass in the simulations with combined effects exceeded this expectation (Table S55). The difference between the expected additive effects and the effects observed in the simulations with combined effects resulted from immature (subadult) and adult fish experiencing slowed growth prior to spawning: subadults that did not reach adult minimum size did not spawn and smaller adults produced fewer eggs than larger adults. This effect on growth resulted in a lower number of eggs produced by the population. A large fraction of the adults subsequently died due to lethal effects following the peak exposure which occurred during the spawning season, removing modeled density-dependent background mortality of the early life stages. Accordingly, the combined effects observed reflect an interaction between timing of peak exposure and density dependence in offspring survival.

Table S55. Population-level effects on Topeka shiner biomass at the end of the exposure year with 0VFS x2 exposure profile applied. The average percentage of population biomass relative to control simulations without exposure are listed. Expected effect levels (from simulations with separate lethal and sublethal effects) are compared to observed levels of combined effects (lethal and sublethal).

Effects combination	Expected % of control biomass from separate effects runs	Observed % of control biomass from combined effect runs	Difference
GUTS-IT + sublethal	57%	42%	15%
GUTS-SD + sublethal	47%	36%	11%

Topeka shiner abundance was not negatively affected by sublethal effects only, and the effect on abundance from lethal effects only did not clearly differ from combined effect simulations at the end of the exposure year. However, the population recovery from the effects was delayed in the combined effect simulations compared to simulations with only lethal effects. Recovery of population abundance was delayed for almost another year when combined effects were simulated (see also section 6.4). In contrast, abundance considerably increased in the first year after exposure if only lethal effects were simulated (Figure S27).

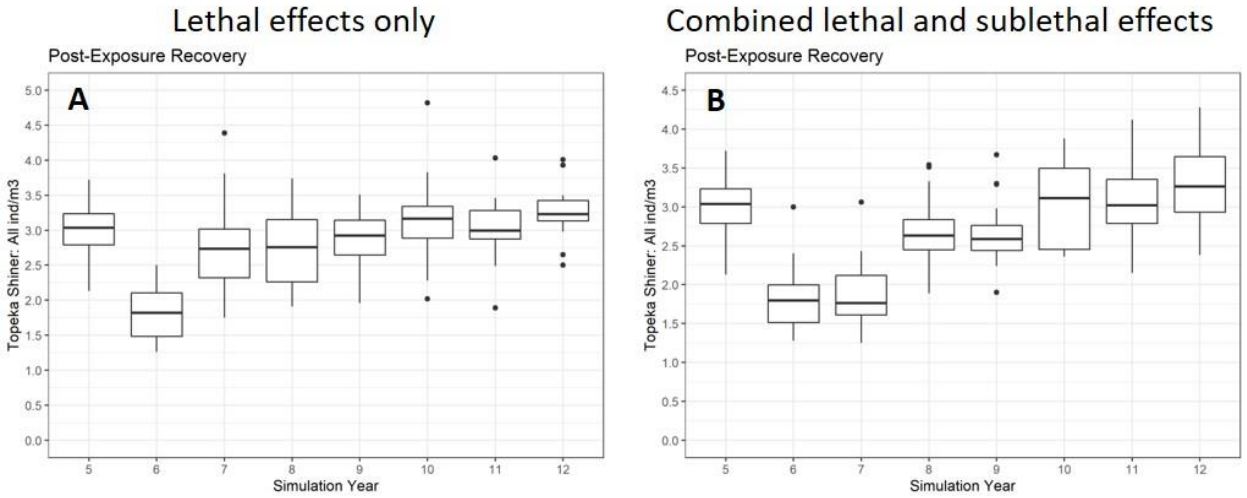


Figure S27. Recovery of abundance (individuals/m^3) in the simulated Topeka shiner population after exposure to 0VFS x2 in simulation year 6. Lethal effects were simulated with GUTS-IT. Simulation year 5 corresponds to the baseline condition prior to the exposure year. No exposure to benzovindiflupyr was simulated in years 7-12. A: Only lethal effects simulated, applying GUTS-IT; B: Only lethal effects simulated, applying GUTS-SD; C: Lethal effects (GUTS-IT) combined with sublethal effects; D: Lethal effects (GUTS-SD) combined with sublethal effects.

7. REFERENCES

Accolla, C., Nerini, D., Maury, O., Poggiale, J.-C., 2015. Analysis of functional response in presence of schooling phenomena: An IBM approach. Progress in Oceanography 134, 232–243.

Ashauer R, Thorbek P, Warinton JS, Wheeler JR, Maund S. 2013. A method to predict and understand fish survival under dynamic chemical stress using standard ecotoxicity data. Environmental Toxicology and Chemistry 32:954-965.

Bakevich BD, Pierce CL, Quist MC. 2013. habitat, fish species, and fish assemblage associations of the Topeka shiner in west-central Iowa. North American Journal of Fisheries Management 33: 1258-1268. DOI: 10.1080/02755947.2013.839969

Bartell, S.M., Brain, R.A., Hendley, P., Nair, S.K., 2013. Modeling the potential effects of atrazine on aquatic communities in midwestern streams. Environmental Toxicology and Chemistry 32, 2402–2411.

Bartell, S.M., Schmolke, A., Green, N., Roy, C., Galic, N., Perkins, D., Brain, R. 2019. A Hybrid Individual-Based and Food Web–Ecosystem Modeling Approach for Assessing Ecological Risks to the Topeka Shiner (*Notropis topeka*): A Case Study with Atrazine. Environmental Toxicology and Chemistry 38: 2243–58.

Benke, A. C., Huryn, A. D. 2017. Secondary Production and Quantitative Food Webs. In: Methods in Stream Ecology (Third Edition), Editor(s): Gary A. Lamberti, F. Richard Hauer. Academic Press, p. 235-254.

Berman, T. 1978. *Peridinium cinctum* fa. *westii* (Lemm.) Lef.: general biochemical features. In: Lake Kinneret (Ed. C. Serruya), pp. 269–270. Dr Junk Publishers, The Hague.

Bigg, M. A., 1981. Harbour seal - *Phoca vitulina* and *P. largha*. In: Handbook of marine mammals. Edited by S. H. Ridgway and R. J. Harrison, Academic Press, London. Vol. Vol. 2 pp. 1-27.

Blower, S. M. and Dowlatabadi, H. 1994. Sensitivity and uncertainty analysis of complex models of disease transmission: an HIV model as an example. International Statistical Review, 62, 229–243

Brey, T. 2001. Population dynamics in benthic invertebrates. A virtual handbook. Alfred Wegener Institute for Polar and Marine Research, Germany. http://www.awi-bremerhaven.de/Benthic/Ecosystem/FoodWeb/Handbook/main.html

Brey, T., Rumohr, H., and Ankar, S. 1988. Energy content of macrobethic invertebrates:general conversion factors from weight to energy. J. Exp. Mar. Biol. Ecol., 117:271-278.

Brody, S. 1945. Bioenergetics and Growth, Reinhold, New York.

Bryan, S.D., C.A. Soupir, W.G. Duffy, and C.E. Freiburger. 1996. Caloric densities of three predatory fishes and their prey in Lake Oahe, South Dakota. Journal of Freshwater Ecology 11: 153-161.

Campbell, Scott W, Cody S Szuwalski, Vernon M Tabor, and Frank DeNoyelles. 2016. Challenges to Reintroduction of a Captive Population of Topeka Shiner (*Notropis topeka*) into Former Habitats in Kansas. Transactions of the Kansas Academy of Science 119 (1): 83–92.

Cauffopé, G., and S.J.J. Heymans. 2005. Energy contents and conversion factors for sea lion's prey. In Guenette, S., and V. Christensen (editors). 2005. Food web models and data for studying fisheries and environmental impacts on Eastern Pacific ecosystems. Fisheries Centre Research Reports 13: 225-237.

Churchill, E. P. and W. H. Over. 1938. Fishes of South Dakota. South Dakota Department of Fish and Game, Pierre. 87 pp.

Cross, F. B. and J. T. Collins. 1995. Fishes in Kansas. University of Kansas Natural History Museum, University Press of Kansas, Lawrence. 315 pp.

Cummins, K.C. and J.C. Wuycheck. 1971. Caloric equivalents for investigations in ecological energetics. Verhandlungen der Internationalen Vereinigung für Theoretische und Angewandte Limnologie 18: 1-158.

Dahle, S.P. 2001. Studies of Topeka Shiner (*Notropis topeka*) Life History and Distribution in Minnesota. Master Thesis. University of Minnesota.

Deslauriers, David, Steven R. Chipps, James E. Breck, James A. Rice and Charles P. Madenjian. 2017. Fish Bioenergetics 4.0: An R-Based Modeling Application, Fisheries, 42:11, 586-596.

Duffy, W.G. 1998. Population dynamics, production, and prey consumption of fathead minnows (*Pimephales promelas*) in prairie wetlands: a bioenergetics approach. Canadian Journal of Fisheries and Aquatic Sciences 54: 15-27.

Durbin, E.G., and A.G. Durbin. 1981. Assimilation efficiency and nitrogen excretion of a filter-feeding planktivore, the Atlantic menhaden *Brevoortia tyrannus* (Pisces: Clupeidae). Fishery Bulletin 79: 601-616.

Evans-White, M. A., Stelzer, R. S. and Lamberti, G. A. 2005. Taxonomic and regional patterns in benthic macroinvertebrate elemental composition in streams. Freshwater Biology, 50: 1786-1799.

Fernández-Reiriz, M. J., U. Labarta, and M.J. Ferreiro. 1993. Effect of commercial enrichment diets on the dietary value of rotifer *Brachionus plicatilis*. Aquaculture 112: 195-206.

Gould and Nichols (1998) Gould, W. R. and Nichols, J. D. 1998. Estimation of temporal variability of survival in animal populations. Ecology 79: 2531-2538.

Graeb, B.D.S., Mangan, M.T., Jolley, J.C., Wahl, D.H., Dettmers, J.M., 2006. Ontogenetic Changes in Prey Preference and Foraging Ability of Yellow Perch: Insights Based on Relative Energetic Return of Prey. Transactions of the American Fisheries Society 135, 1493–1498.

Grimm, V., Berger, U., Bastiansen, F., Eliassen, S., Ginot, V., Giske, J., Goss-Custard, J., Grand, T., Heinz, S. K., Huse, G., Huth, A. and et al. 2006. A standard protocol for describing individual-based and agent-based models. Ecological Modelling, 198, 115–126.

Hanson, P. C., T. B. Johnson, D. E. Schindler, and J. F. Kitchell. 1997. Fish bioenergetics 3.0 software for Windows. University of Wisconsin Center for Limnology, Sea Grant Institute, Technical Report WISCU-T-97-001, Madison, Wisconsin.

Hartman, K. J. 2017. Bioenergetics of Brown Bullhead in a changing climate. Transactions of the American Fisheries Society 146:634–644.

Hatch, J. T. and S. Besaw. 2001. Food use in Minnesota populations of the Topeka shiner (*Notropis topeka*). Journal of Freshwater Ecology. 16(2): 229-233.

Hunt, G. L. J., Burgeson, B., and Sanger, G. A., 1981. Feeding ecology of seabirds of the eastern Bering Sea. In: The Eastern Bering Sea Shelf: Oceanography and Resources. Edited by D. W. C. Hood, J.A., NOAA, Univ. of Washington Press, Seattle, Washington. Vol. 2 pp. 629-647.

Hunt, G. L. J., Kato, H., and McKinnel, S. M., 2000. Predation by marine birds and mammals in the subarctic Pacific Ocean. North Pacific Marine Science Organisation, Sidney, BC, Canada, PICES Scientific Report, 14. 165 pp.

Jager T, Zimmer EI. 2012. Simplified dynamic energy budget model for analysing ecotoxicity data. Ecological Modelling 225: 74-81.

Jangaard, P. M. 1974. The capelin (*Mallotus villosus*): Biology, distribution, exploitation. utilization and composition. Fish. Res. Board Can. Bull., 186.

Jeeja, P.K., I. Joseph, and P. Raj. 2011. Nutritional composition of rotifer (*Brachionus plicatilis* Muller) cultured using selected natural diets. Indian Journal of Fisheries 58(2): 59-65.

Kerns, H. A. 1983. Aspects of the life history of the Topeka shiner, *Notropis topeka* (Gilbert), in Kansas. Unpublished thesis. Museum of Natural History, University of Kansas, Lawrence. 32 pp.

Kerns, H.A., and J.L. Bonneau. 2002. Aspects of the life history and feeding habits of the Topeka shiner (*Notropis topeka*) in Kansas. Transactions of the Kansas Academy of Science 105 (3–4): 125–42.

Kitchell, J. F., D. J. Stewart, and D. Weininger. 1977. Applications of a bioenergetics model to Yellow Perch (*Perca flavescens*) and Walleye (*Stizostedion vitreum vitreum*). Journal of the Fisheries Research Board of Canada 34:1922–1935.

Klekowski, R.Z., and E.A. Shushkina. 1966. Ernährung, Atmung, Wachstum und Energie-Umformung in *Macrocyclops abbidus* (Jur.). Verh. Int. Ver. Limnol. 16: 399-418.

Koehle JJ. 2006. The effects of high temperature, low dissolved oxygen, and Asian tapeworm infection on growth and survival of the Topeka shiner, *Notropis topeka*. MS Thesis, University of Minnesota.

Laurence, G.C. 1976. Caloric content of some North Atlantic calanoid copepods. Fishery Bulletin 78: 218-220.

Laybourn, J.E.M., and J.M. Stewart. 1975. Studies on consumption and growth in the ciliate *Colpidium campylum* Stokes. J. Anim. Ecol. 44: 165-174.

Ling S.W. 1966. Feeds and feeding of warm-water fishes in ponds in Asia and the Far East. In: FAO World Symposium on Warm-Water Pond Fish Culture, Rome.

Linzmaier, S.M., Twardochleb, L.A., Olden, J.D., Mehner, T., Arlinghaus, R., 2018. Size-dependent foraging niches of European Perch *Perca fluviatilis* (Linnaeus, 1758) and North American Yellow Perch *Perca flavescens* (Mitchill, 1814). Environ Biol Fish 101, 23–37.

Luecke, C., and D. Brandt. 1993. Estimating the energy density of daphnid prey for use with rainbow trout bioenergetics models. Transactions of the American Fisheries Society 122: 386–389.

Mackinson, S. 1996. System definition and primary production. In: Mass-balance models of North-eastern Pacific ecosystems. Edited by D. Pauly and V. Christensen, Fisheries Center, University of British Columbia, Vancouver, BC. Vol. 4: pp. 63-64.

Morris, W.F., and D.F. Doak. 2002. Quantitative Conservation Biology: Theory and Practice of Population Viability Analysis. Sinauer Associates Inc., Sunderalnd, MA, USA.

Peters, R.H., and J.A. Downing. 1984. Empirical analysis of zooplankton filtering and feeding rates. Limnology and Oceanography 29: 763-784.

Pflieger, W. L. 1975. The fishes of Missouri. Missouri Department of Conservation. 343 pp.

Pflieger, W. L. 1997. The fishes of Missouri. Missouri Department of Conservation. 382 pp.

Platt, T., and B. Irwin. 1973. Caloric content of phytoplankton. Limnol. Oceanogr. 18: 306-310.

R Project for Statistical Computing. www.r-project.org.

Reynolds, C.S. 1984. The Ecology of Freshwater Phytoplankton. Cambridge University Press, Cambridge.

Rogerson, A. 1979. Energy content of *Amoeba proteus* and *Tetrahymena pyriformis* (Protozoa). Canadian Journal of Zoology 57: 2463-2465.

Ross, S.T. 2013. Ecology of North American freshwater fishes. University of California Press, Berkley and Los Angeles, California.

Rudstam, L.G. 1989. A bioenergetic model for *Mysis* growth and consumption applied to a Baltic population of *Mysis mixta*. Journal of Plankton Research 11: 971-983.

Schmolke, A., Bartell, S.M., Roy, C., Green, N., Galic, N., Brain, R., 2019. Species-specific population dynamics and their link to an aquatic food web: A hybrid modeling approach. Ecological Modelling 405, 1–14.

Schneider, D.W. 1992. A bioenergetics model of zebra mussel, *Dreissena polymorpha*, growth in the Great Lakes. Canadian Journal of Fisheries and Aquatic Sciences 49: 1406-1416.

Schneider, J.C., P.W. Laarman, and H. Gowing. 2000. Chapter 17: Length-weight relationships. Manual of Fisheries Survey Methods II, Michigan Department of Natural Resources (http://www.dnr.state.mi.us/publications/pdfs/IFR/manual/SMII%20Chapter17.pdf)

Schrank, S. J., Guy, C. S., Whiles, M. R., Brock, B. L. 2001. Influence of Instream and Landscape-Level Factors on the Distribution of Topeka Shiners *Notropis topeka* in Kansas Streams. Copeia 2001(2):413-421.

Sladecek, V., Sladeckova, A. 1963. Relationship between wet weight and dry weight of the periphyton. Limnology and Oceanography 8: 309-311.

Slobodkin, L.B., and S. Richman. 1961. Calories/gm in species of animals. Nature 191: 299.

Smith, R. L., Paul, A. J., and Paul, J. M. 1986. Effect of food intake and temperature on growth and conversion efficiency of juvenile wall eye pollock (*Theragra chalcogramma* Pallas): a laboratory study. J. Cons. CIEM, 42:241-253.

Snow, N.B. 1972. The effect of season and animal size on the caloric content of *Daphnia pulicaria* Forbes. Limnology and Oceanography 17: 909-913.

Spencer, D.F., F.J. Ryan, and G.G. Ksander. 1997. Construction costs for some aquatic plants. Aquatic Botany 56: 203-214.

Stark, William J, Jason S Luginbill, and Mark E Eberle. 2002. Natural History of a Relict Population of Topeka Shiner (*Notropis Topeka*) in Northwestern Kansas. Transactions of the Kansas Academy of Science 105 (3): 143–52.

Tabor, R.A., Warner, E.J., Fresh, K.L., Footen, B.A., Chan, J.R., 2007. Ontogenetic Diet Shifts of Prickly Sculpin in the Lake Washington Basin, Washington. Transactions of the American Fisheries Society 136, 1801–1813.

Theilacker, G.H., and M.F. McMaster. 1971. Mass culture of the rotifer *Brachionus plicatilis* and its evaluation as a food for larval anchovies. International Journal on Life in Oceans and Coastal Waters 10(2): 183-188.

Thornton, K. W., Lessem, A. S. 1978. A Temperature Algorithm for Modifying Biological Rates, Transactions of the American Fisheries Society 107: 284-287.

Van Winkle, W., Jager, H. I., Railsback, S. F., Holcomb, B. D., Studley, T. K., Baldrige, J. E. 1998. Individual-based model of sympatric populations of brown and rainbow trout for instream flow assessment: model description and calibration. Ecological Modelling 110: 175-207.

Vijverberg, J., and T.H. Frank. 1976. The chemical composition and energy contents of copepods and cladocerans in relation to their size. Freshwater Biology 6: 333-345.

Waters, T. F. 1977. Secondary Production in Inland Waters. Advances in Ecological Research 10: 91-164.

Werner, E.E., Gilliam, J.F., 1984. The Ontogenetic Niche and Species Interactions in Size-Structured Populations. Annual Review of Ecology and Systematics 15, 393–425.

Wiebe, W. J., Johannes, R. E., Webb, K. L. 1975. Nitrogen Fixation in a Coral Reef Community. Science 188: 257-259.

Wilensky U. 1999. NetLogo. http://ccl.northwestern.edu/netlogo/. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL, USA.

Witte, Christopher C. 2008. "Effects of Temperature, Photoperiod, and Substrate on the Maturation and Reproductive Behavior of the Topeka Shiner (*Notropis topeka*)." University of Missouri-Columbia. Master Thesis.

Wynne D., N.J. Patni, S. Aaronson, and T. Berman. 1982. The relationship between nutrient status and chemical composition of *Peridinium cinctum* during the bloom in Lake Kinneret. Journal of Plankton Research 4: 125-136.

York DO. 2010. SYN545192 – Early life-stage toxicity test with fathead minnow (Pimephales promelas). Final report to Syngenta Crop Protection, LLC. Springborn Smithers Laboratories, Wareham, Massachusetts. 53 p.