



A simulation-based evaluation of management actions to reduce the risk of contaminants of emerging concern (CECs) to walleye in the Great Lakes Basin



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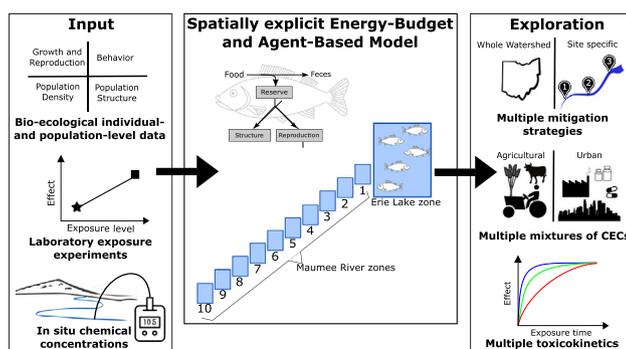
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HIGHLIGHTS

- We modeled the effectiveness of two mitigation strategies (large vs small scale).
- We explored the impact of hypothetical toxicokinetics and CEC mixture types.
- Small-scale mitigation is more effective when it focuses on spawning sites.
- Toxicokinetics are more important to evaluate small-scale mitigation effectiveness.
- Population characteristics are more important to evaluate large-scale mitigation.

GRAPHICAL ABSTRACT



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ABSTRACT

Contaminants of emerging concern (CECs) are ubiquitous, present in complex chemical mixtures, and represent a threat to the Great Lake ecosystem. Mitigation strategies are needed to protect populations of key species, but knowledge about ecological and biological effects of CECs at the population level are limited. In this study, we combined laboratory data on CEC effects at the individual-level with in-situ CEC concentration data in a walleye (*Sander vitreus*) population model to simulate the effectiveness of different CEC mitigation strategies in the Maumee River and Lake Erie. We compared the effectiveness of moderate mitigation (50% reduction in exposure level) of an entire watershed versus intensive mitigation (reduction of exposure to a level that does not affect walleye) of single river sites for three CEC mixture scenarios (agricultural, urban, and combined). We also explored the impact of hypothetical chemical toxicokinetics (the time course of chemicals in walleye) on the relative effectiveness of the mitigation strategies. Our results suggest that when CECs impact fecundity, single-site mitigation is more effective when it focuses on spawning sites and nearby downstream sites that are substantially impaired. Our simulations also suggest that chemical toxicokinetics are important when evaluating single-site mitigation strategies, but that population characteristics, such as stage-specific mortality rate, are more important when evaluating watershed mitigation strategies. Results can be used to guide fisheries management, such as choosing habitat restoration sites, and identify key knowledge gaps that direct future research and monitoring.

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1. Introduction

The Great Lakes represent one fifth of the world's surface freshwater, provide water for communities and industries, support numerous and valuable ecosystems and their services, are regional hotspots of biodiversity, and generate billions of dollars annually via jobs and recreation (Allan et al., 2013). However, chemical pollution threatens Great Lakes ecosystems, the services that they provide, and the wildlife that they support (Allan et al., 2013; Danz et al., 2007). Human activities have introduced complex mixtures of organic compounds to the environment, but regulations since the 1960s have been effective at reducing the occurrence of many of these compounds (Elliott et al., 2017). However, some classes of chemicals, termed Contaminants of Emerging Concern (hereafter CECs), remain a concern for public and ecosystem health (Barber et al., 2013; Kolpin et al., 2002). CECs are ubiquitous in aquatic environments (Barber et al., 2013; Kolpin et al., 2002), including in the Great Lakes Basin (Baldwin et al., 2016; Choy et al., 2017; Elliott et al., 2017), and may cause adverse biological effects (Baldwin et al., 2016; Brain et al., 2005; Cipoletti et al., 2019; Relyea, 2009; Thomas et al., 2017). Many CECs are unregulated because they are new to the market and/or their occurrence in the environment has increased. They include pharmaceuticals, personal care products, some pesticides, flame retardants, and solvents that are often present in complex chemical mixtures (Elliott et al., 2018).

Estimating population-level effects of CEC mixtures and evaluating management strategies requires information about the CECs that are present in the environment and their individual-level effects. The US Geological Survey identified the most common CECs in the Great Lakes Basin and their environmental concentrations (Elliott et al., 2017), and identified a dichotomy of CECs in agricultural- and urban-influenced stream environments (Elliott et al., 2018). Atrazine, bisphenol A (BPA), bromacil, diethyl-meta-toluamide, estrone (E1), metolachlor, nonylphenol (NP), and tributoxethyl phosphate were consistently detected in water samples from rivers surrounded by agricultural landscapes, whereas BPA, diethyl-meta-toluamide, desvenlafaxine, E1, fexofenadine, galaxolide, metformin, methyl-1H-benzotriazole, NP, sulfamethoxazole, and tributoxethyl phosphate were the most commonly detected CECs in urban landscapes. Laboratory exposure of fathead minnows (*Pimephales promelas*), a widely used toxicity test species for which standard protocols have been developed (Ankley and Villeneuve, 2006), to these mixtures revealed a significant impact on reproductive endpoints, reducing egg production by up to 81% when fish were exposed to the urban mixture (Schoenfuss et al., 2020) and by up to 33% when exposed to the agricultural mixture (Cipoletti, 2018).

Environmental management strategies generally aim to protect populations or groups of populations, rather than individuals. Nevertheless, they often rely on experimental results measuring effects of toxicants at the individual level, while population-level effects are not necessarily proportional to these individual-level responses (Forbes et al., 2008; Vaugeois et al., 2020). Complex interactions of individuals with each other and their environment can intensify or mitigate the population-level effects of a stressor. Moreover, experimentally detecting impacts at the population level is challenging because of the spatiotemporal scales that are needed to detect changes in population dynamics. Nevertheless, it is essential to rely on population-level outcomes to set an effective management strategy. Population models can be used to extrapolate population-level effects of CECs and other stressors from individual-level effects while taking into account population-level processes. These models are valuable tools for protecting and managing fish populations because they can improve our understanding of the population-level impacts of CECs, compare different mitigation strategies, and identify important factors in population recovery.

Population models often use in-situ data on system characteristics, and exposure is integrated in a spatially explicit model in which exposure is variable over space and time. In these cases, organisms face varying exposure conditions, as in the wild, but unlike long-term exposure experiments in the laboratory. Thus, Toxicokinetic-Toxicodynamic (TK-TD)

models are recommended for simulating individual-level effects of exposure to toxicants (Ashauer and Escher, 2010). Toxicokinetics is the study of the time course of toxicant concentration in an organism at the site of toxic action, which encompasses absorption, distribution, biotransformation, and elimination; and toxicodynamics link toxicant concentration in an organism at the site of toxic action to effects on the individual organism (Ashauer et al., 2011). We developed an Individual-Based Model (IBM) because this modeling technique can easily integrate individual-level effects of stressors and TKTD models (Accolla et al., 2020). Our IBM incorporates Dynamic Energy Budget (DEB) theory (Kooijman, 2010) and published data to explore individual- and population-level impacts of exposure to different mixtures of CECs. Our model represents a walleye (*Sander vitreus*) population in the Maumee River and Lake Erie. Walleye is an economically important fish species that supports commercial and recreational fisheries in the Great Lakes region that are worth millions of dollars annually (Pandit et al., 2013; Roseman et al., 2012). The Maumee River is one of the major U.S. watersheds in the Great Lakes Basin (Forsyth et al., 2016), and is substantially impacted by both agricultural and urban activities (Baldwin et al., 2016; Choy et al., 2017; Elliott et al., 2017). We incorporated in-situ data from previous studies (Choy et al., 2017; Elliott et al., 2017) to estimate exposure to CECs along the river, and used laboratory data on the effects of CECs on individual fish (Cipoletti, 2018; Schoenfuss et al., 2020) to determine the effects associated with long-term exposure at different levels. Our goal was to compare how different management strategies (a moderate mitigation of the entire watershed versus an intensive mitigation of single river sites) could impact walleye population density. Although TK-TD models are recommended for spatially explicit models of toxicant exposure (Ashauer and Escher, 2010), we accounted for different toxicokinetics assumptions (fast, moderate, and slow), and assessed their impact on the effectiveness of mitigation strategies in order to better understand how much precision of chemical toxicokinetics is required. Moreover, because the data required to parametrize TK-TD models are often lacking, especially when dealing with mixtures of toxicants, we used a simplified approach to consider the influence of temporally variable exposure. This approach, which consisted of simulating different exposure durations prior to reproduction, accurately approximated a one-compartment toxicokinetic model with the same uptake and elimination rates. We assessed the effectiveness of the two mitigation strategies under the three toxicokinetics assumptions, and for three CEC mixture types (agricultural, urban and combined). We assumed the position of a manager who was observing a walleye population under stress. Population characteristics (based on published data) were the same before the start of the mitigation for every mixture type, toxicokinetic assumption, and mitigation strategy. Our simulations then estimate the effectiveness of different management actions under different toxicological contexts to protect walleye populations. Results can be used to guide fisheries management decision making, such as choosing habitat restoration sites, and identify key knowledge gaps that direct future research and monitoring.

2. Materials and methods

2.1. Study system and species

Our study focuses on the Maumee River, which is the largest U.S. watershed in the Great Lakes Basin (Forsyth et al., 2016). Seventy seven and a half percent of this watershed is covered by agricultural lands, 11.5% is covered by urban lands (Forsyth et al., 2016), and CECs are often detected at levels that can cause biological impacts to fish (Baldwin et al., 2016; Choy et al., 2017; Elliott et al., 2017). Cipoletti et al. (2019, 2020) found that contaminants were detected in every water and fish tissue sample from this watershed, and that they tended to have the greatest impact on reproductive endpoints. Watershed characteristics, in-situ CEC concentration measurements, and the stresses observed on resident fish make the Maumee River a particularly relevant case study for modeling.

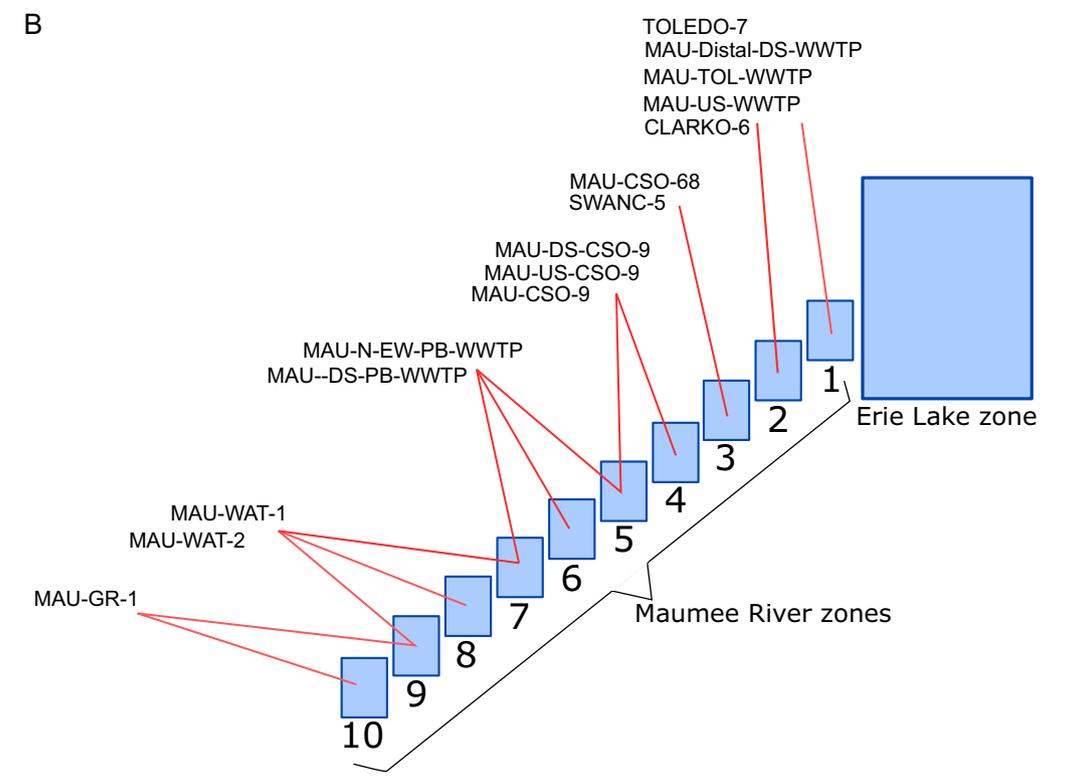
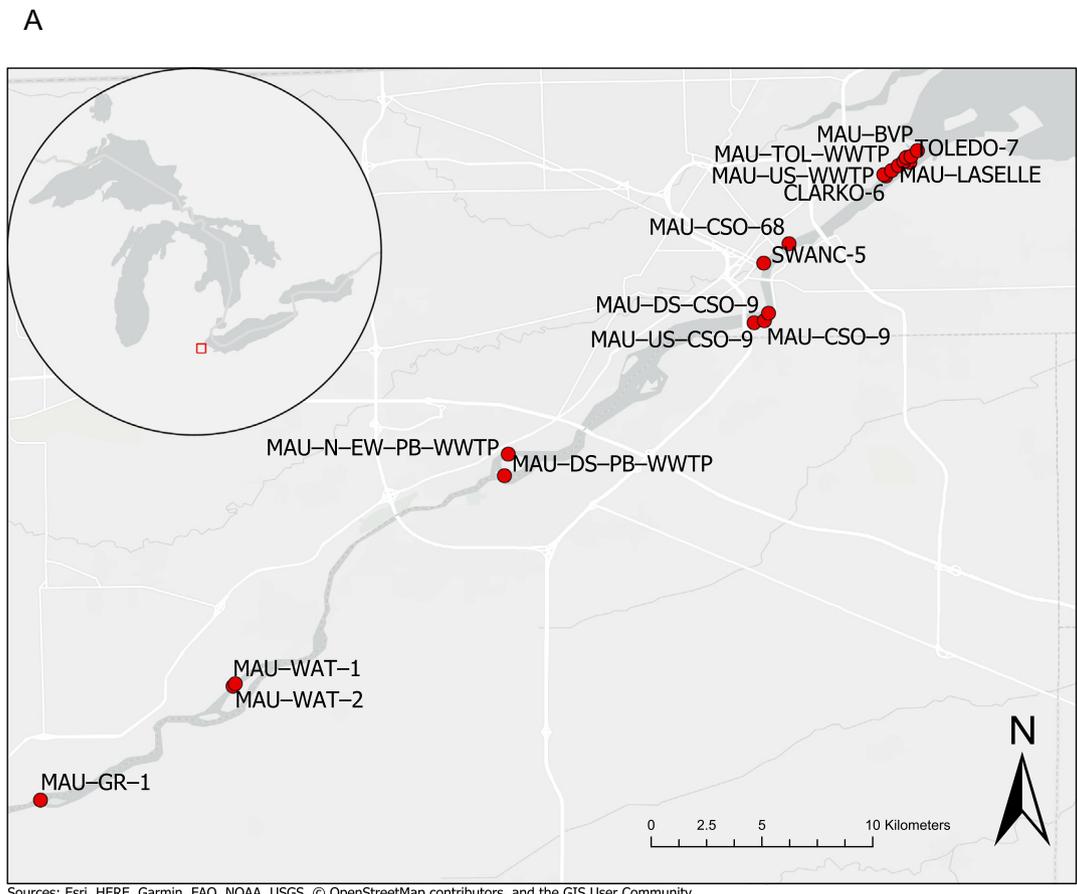


Fig. 1. USGS sampling sites along the Maumee River and correspondence between USGS sites and modeled zones. Chemical concentrations and the correspondence between USGS sites and modeled zones can be found in Supplemental Information, Sections 2.13.2 and 2.13.3. On the map in the upper panel, dark gray is water, light gray is land, white lines are roads, and dotted gray lines are state boundaries.

We focused on walleye because of its socio-economic importance. Walleye are a popular game fish, and commercial and recreational fisheries are worth millions of dollars annually in the Great Lakes region (Pandit et al., 2013; Roseman et al., 2012). Moreover, there is a great deal of published information (spawning site locations, spawning site fidelity, population density, population structure, migration timing) with which to parametrize our population model.

2.2. Model

The life cycle of individual walleye is described through their metabolism using DEB theory (Kooijman, 2010). The DEB model was calibrated using published data on important processes such as growth and reproduction. The parameters of the standard DEB model were estimated using the co-variation method (Lika et al., 2011), which uses the simplex method to simultaneously minimize the weighted sum of squared deviations between model predictions and observations for a considerable number of data sets (Supplemental Information, Section 3.1). We simulated population dynamics via an IBM. Individual-level effects of CECs are modeled as impacts to an energetic pathway of the DEB model (Supplemental Information, Section 2.13.1) based on laboratory toxicity data (Cipoletti, 2018; Schoenfuss et al., 2020). The IBM includes population processes, such as migration and reproduction, and realistically describes the walleye population in the Maumee River and Lake Erie. The DEB-IBM was calibrated to reproduce published observations and estimates of the reproductive season, the distribution of reproducing individuals in the river, spawning site fidelity, population density, and population structure (Supplemental Information, Sections 3.2 and 6.2). We used in-situ measurements of CEC concentrations (Elliott et al., 2017) to determine the exposure regime in the river during the year (Fig. 1) (Supplemental Information, Sections 2.13.2 and 2.13.3).

2.2.1. Purpose

Our model estimates the population-level effects caused by the exposure of walleye to two mixtures of CECs (agricultural and urban). It uses in-situ CEC concentration data (Elliott et al., 2017) and the results

of laboratory toxicity tests (Cipoletti, 2018; Schoenfuss et al., 2020) to assess the potential effects of two CEC mitigation strategies (watershed-wide and moderate vs. site-specific and intensive) on a Lake Erie walleye population that spawns in the Maumee River. We also simulated different exposure durations prior to reproduction to account for different toxicokinetics (see below).

2.2.2. Basic principles

The model is based on DEB theory for describing the energetics of individuals. The DEB model describes how individuals feed, allocate energy for growth and reproduction, and die of aging and/or starvation. The parameters of the DEB model are species-specific, and were estimated from published, individual-level data (Supplemental Information, Section 3.1). We chose to implement the scaled version of the DEB model (Kooijman et al., 2008), because it is a simplification of the standard DEB model.

The degree of food limitation in our model depends on both fish density and the logistic growth parameter for food. We introduced predation as a third, external source of mortality because DEB theory only represents mortality due to aging and starvation. The individual dies in a given time step if a randomly selected number (continuous uniform distribution $U(0,1)$) is less than the stage-specific probability of dying from predation. In this study, we considered a stage-specific, density-independent, predation mortality rate and an indirect competition for food from which density-dependence emerged.

2.2.3. Entities, state variables, and scales

There are two types of entities in the model: individual fish and spatial unit. We used the scaled version of the DEB model with metabolic acceleration to represent the energy budget of individuals. Individuals are characterized by six state variables (Supplemental Information, Table 1): structure (L , in cm); scaled reserve (U_E , $d \cdot cm^{-2}$); scaled maturity (U_H , $d \cdot cm^{-2}$); scaled reproduction (U_R , $d \cdot cm^{-2}$); damage-inducing compounds (\hat{q}), expressed as aging acceleration; and damage (\hat{h}), expressed as hazard rate. For more details and an introduction to DEB theory, see Jusup et al. (2017); Kooijman (2010); Nisbet et al.

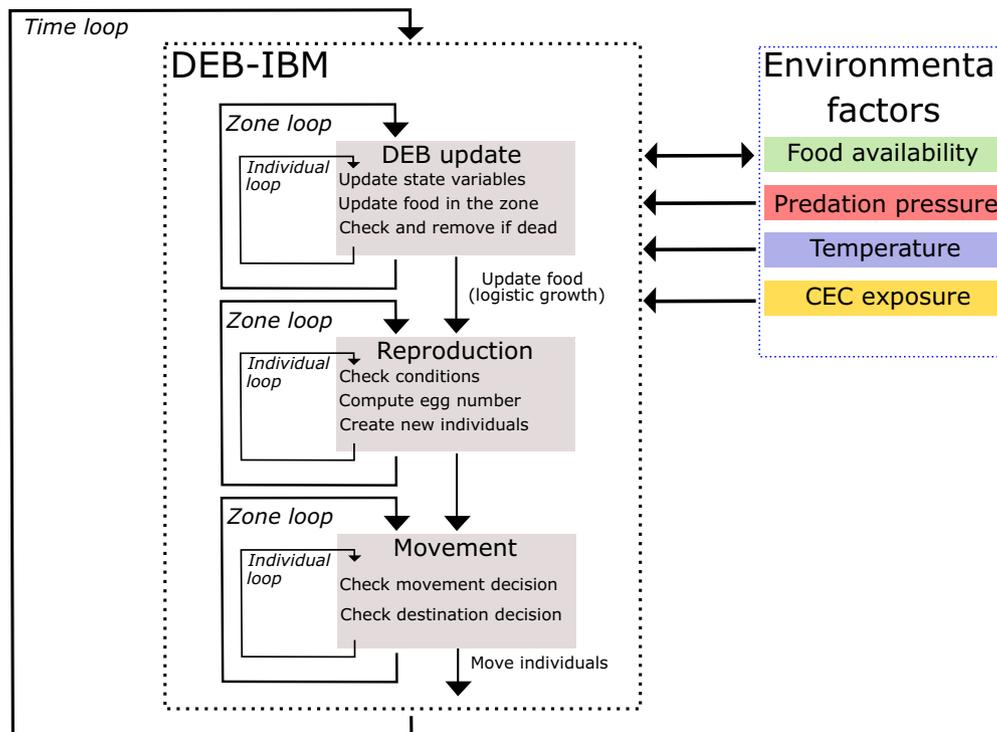


Fig. 2. Schematic description of the walleye population model processes and scheduling. Individuals are first listed by zone, then they update their DEB state variables. Food is updated before the next step. Individuals are listed by zone and proceed to reproduction. Finally, Individuals are listed by zone and movement occurs as a stochastic process.

(2000); Sousa et al. (2010). All model parameters and equations are reported in Tables 2 and 3 in Supplemental Information, respectively. The aging of individuals follows Martin et al. (2012). Briefly, aging in DEB theory is based on the evidence that damage-inducing compounds (i.e., free radicals) cause irreversible damage to DNA, and that the probability of dying by aging is proportional to the amount of damage. Aging is therefore described in terms of two state variables: damage-inducing compounds (\dot{q}), and damage (h). We followed the same methodology as Martin et al. (2012), based on Kooijman et al. (1989), to set variability among individuals. We introduced a normally distributed, scatter multiplier ($\mu = 1$ and $\sigma = 0.05$) to account for inter-individual variability in six of the standard DEB parameters (half-saturation coefficient, energy investment ratio, the scaled maturity thresholds for hatching, birth, metamorphosis, and puberty).

The model has 10 spatial units that each represent a 1-ha zone of the Maumee River, plus one zone representing 10-ha of Western Lake Erie. The five most upstream river zones are potential spawning areas according to Dufour (2012), Hayden et al. (2018), and Schmidt (2016). Each zone is characterized by five state variables: the density of the first food item ($X_1, \text{J} \cdot \text{m}^{-2}$), the density of the second food item ($X_2, \text{J} \cdot \text{m}^{-2}$), temperature (T , in $^{\circ}\text{C}$), surface area (in m^2), and the stress factor (s). The stress factor, which reflects the impact of a stressor on a physiological mode of action, is calculated based on in situ and laboratory data. In situ data allowed us to estimate time series of exposure level per zone, and laboratory data allowed us to link exposure level to individual-level effects on reproduction (supplemental information, Section 2.13). It is then used to calculate the effect of the stressor on reproduction by impacting the reproduction efficiency parameter (κ_R) as follows: $\kappa_R = \kappa_{R0} * (1 - s)$. We introduced two food items because walleye diets change with ontogeny (Galarowicz and Wahl, 2005; Uphoff et al., 2019). Both food item densities change once during each daily time step according to a logistic growth equation and fish consumption. The logistic growth function has two parameters: daily intrinsic growth rate (aE in d^{-1} for both food items) and carrying capacity ($kE1$ in $\text{J} \cdot \text{m}^{-2}$ for food item 1, $kE2$ in $\text{J} \cdot \text{m}^{-2}$ for food item 2) (Supplemental Information, Section 2.10). All river zones have the same water temperature (range from 0.1 to 29.5 $^{\circ}\text{C}$ during the year). The Lake Erie zone has a specific seasonal temperature profile (range from 0.5 to 23.9 $^{\circ}\text{C}$ during the year). The daily changes in river temperature were gathered from online temperature data that were recorded in 2016 in the Maumee River (<https://waterdata.usgs.gov/nwis>). The daily changes in lake temperature were gathered from online temperature data of average temperature near Cleveland (1981–2010) (https://www.weather.gov/cle/avg_lake_erie_water_temps). We estimated the stress factor (s) from the results of individual-level in-situ and laboratory experiments (Supplemental Information, Section 2.13).

Model integration followed the classical Runge-Kutta method using the Apache Commons Math library (release 3) with a daily time step.

2.2.4. Process overview and scheduling

The model executes the following actions at each time step (Fig. 2):

1) Individuals are listed by zone, and then the model updates their DEB state variables (Supplemental Information, Section 2.8.1). This update can result in three forms of mortality: starvation (i.e., an inability to pay maintenance costs), aging, or predation (modeled as a stage-dependent survival rate to predation). Starvation is deterministic (i.e., depends on a state variable), and death by aging and predation are stochastic (i.e., depend on random selection). Both starvation death and aging death are based on individual energetics and interactions with the environment. The starvation module allows a starving fish to reallocate energy that is used for reproduction or maturity to somatic maintenance. Starvation does not cause fish to shrink, and a fish dies if it fails to pay its maturity and somatic maintenance. Predation was implemented in the IBM as a stage-dependent cause of death. Dead individuals are removed before the next action. The densities of both food items are updated after each individual eats, and then allowed to increase according to the logistic growth function after all individuals have eaten.

2) Individuals are listed by zone, and then reproduction occurs (Supplemental Information, Section 2.8.2). Individuals select their reproduction area before the beginning of each reproduction season. Individuals that reproduced the previous year select the same reproduction area with a 70% fidelity rate (Hayden et al., 2018). If an individual selects a reproduction area for the first time, or does not select the same area as the previous year, then this area is randomly selected. The probability of selecting a given river zone is zone-specific, and was set in accordance with observed egg density in the Maumee River (Schmidt, 2016) (Supplemental Information, Section 2.12.2). Thus, Sites 6 and 7 were the most frequently selected spawning sites (there is less reproduction in upstream sites and no reproduction in Sites 1 to 5). Only adults that have allocated the minimum amount of energy to reproduction ($U_R, \text{d} \cdot \text{cm}^{-2}$) can reproduce. In addition, females can only reproduce if they are in their selected spawning site and share a spawning zone with at least one male that is also ready to reproduce.

3) Individuals are listed by zone, and then movement occurs. Movement is a stochastic process (Supplemental Information, Section 2.8.3) that depends on an individual's life stage (e.g., upstream migration of adults, eggs do not move, larvae drift downstream), its current location (e.g., no movement by adults if they are in their selected spawning site), and the time of year (e.g., to match reproductive season).

2.3. Linking CEC exposure and individual-level effects in a spatially explicit model

The individual-level responses of walleye to CEC mixtures are unknown, so we modeled them after the results of experiments involving fathead minnow (*Pimephales promelas*). Egg production declined by up to 81% when fathead minnows were exposed to the urban mixture (Schoenfuss et al., 2020) and by up to 33% when exposed to the agricultural mixture (Cipoletti, 2018). However, the gonadosomatic index (GSI) was not significantly impacted in either case. These results suggest that exposure to CECs probably reduced egg production by impacting oocytes during final maturation and ovulation. Based on this laboratory work, our model assumed the same response intensity to CEC exposure in walleye (81 and 33% reduction of egg production), by impacting the egg maturation process (i.e., increasing the cost of converting reproductive energy into eggs).

Although it is recommended to use Toxicokinetic-Toxicodynamic (TK-TD) models to simulate individual-level effects of exposure to toxicants over time, especially when exposure is variable (Ashauer and Escher, 2010), the appropriate data were lacking for our study. Fish in the fathead minnow laboratory toxicity study were exposed to a constant concentration of CECs for their entire lifespan, and so internal and external CEC concentrations had likely reached equilibrium. In contrast, wild fish are exposed to different mixture levels of CECs depending on both time and location. Without appropriate data to simulate how internal concentrations of CECs adjust to different exposure conditions, we used a simple approach to consider the influence of temporally variable exposure (e.g., that could occur from differences in TK of chemicals in the CEC mixture) by simulating three exposure durations prior to reproduction. For each exposure duration, we assumed that the individual-level effect at time t was equal to the average individual-level effect associated with the exposure levels encountered during the exposure duration. Averaging over the last 5 days corresponded to fast toxicokinetics, i.e. a relatively rapid attainment of equilibrium between internal and external CEC concentrations. Correspondingly, the 15- and 30-day exposures represented moderate and slow toxicokinetics, respectively. Our methodology reflects the idea of individual memory of exposure to toxicants. For a fast toxicokinetics, only the exposure history of the last few days needs to be considered, while it is longer for slower toxicokinetics. This approach is also in accordance with the mode of action of the CEC mixtures (impacting egg production but not accumulated energy for reproduction) and timing of egg maturation and ovulation of our species of interest. Walleye GSI rises during autumn with the onset of exogenous

vitellogenesis and a corresponding increase in mean oocyte diameter (Malison and Held, 1996). They do not begin final maturation until just before spawning (Malison and Held, 1996).

Our method accurately approximates a one-compartment toxicokinetic model with the same uptake and elimination rates (Supplemental Information, Section 6.3), but is probably specific to our case because CECs affected egg production, not the growth or survival of eggs or other life stages. Consequently, only the recent exposure needed to be taken into account. Also, the CEC mode of action in our study did not impact the size distribution of reproducing adults (egg production is linked to adult size) or their annual exposure history (no impact on movement behavior).

2.4. Simulations

Food density is set to carrying capacity in all zones at the beginning of each simulation, and is identical for all simulations. We selected a high carrying capacity because food-limited populations tend to show a reduced effect of stressors (Vaugeois et al., 2020). All simulations began by introducing 30 new individuals per zone (eggs that will reach the larval stage) on day 93 of the simulation. We then repeated this introduction of new individuals for the subsequent three years to initialize our model with cohorts of different life stages. Each CEC mixture scenario (urban, agricultural, and combined – see below) has specific effects on individuals that depend on exposure concentration. Exposure concentrations varied in time and space consistent with field monitoring data (Supplemental Information, Section 2.13). Simulations included an initial, 35-year period during which populations were allowed to stabilize. Baseline observations of the simulated populations were made during the subsequent 5 years, and management strategies were implemented beginning in year 40 and lasting until year 50.

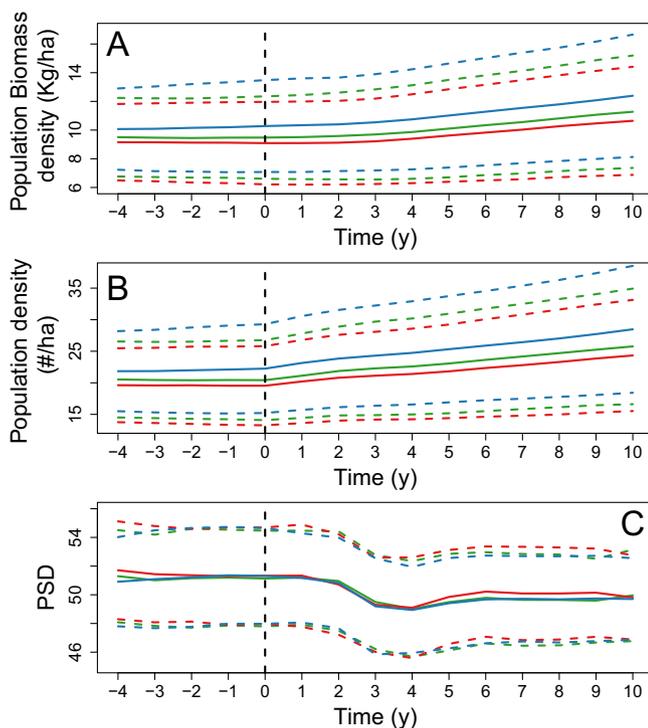


Fig. 3. Modeled yearly averaged walleye population biomass density (A), density (B) and Proportional Stock Distribution (PSD, C) before and after a 50% reduction of agricultural CEC mixture for the three toxicokinetic scenarios (fast in blue, moderate in red, slow in green) in the Maumee River and Lake Erie. Continuous lines are the average of 400 replicates, dotted lines are the standard deviation. The vertical dotted line marks the change in CEC exposure. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

We collected observations (average of 400 replicates) on fish density for different age groups, biomass density and Proportional Stock Density (hereafter PSD; the ratio of the number of individuals ≥ 38 cm to the number of individuals ≥ 25 cm (Anderson, 1980)). We simulated three CEC mixture scenarios: (1) Urban mixture; (2) Agricultural mixture; (3) Combined mixture. For the first two scenarios, all zones are exclusively under urban or agricultural exposure. The third scenario assumed that river zones 1–6 and the lake zone were exposed to urban CECs, and that river zones 7–10 were exposed to the agricultural mixture (river zones from 7 to 10) following (Cipoletti et al., 2020) (Supplemental Information, Section 2.13.2 and 2.13.3). For each of the three CEC mixture scenarios, we assessed the effectiveness of hypothetical management actions by measuring how average population density over the last 10 years of the simulation was impacted by a (i) 50% reduction in the effects of the CEC mixture on individuals for all sites, which would correspond to a moderate mitigation of the entire watershed; or (ii) 100% reduction in the effects of the CEC mixture on individuals for one river site at a time, which would correspond to an intensive mitigation of specific sites within the watershed. For each mitigation strategy, we assessed the impact of accounting for different toxicokinetics (fast, moderate, and slow).

We adjusted some stage-specific survival rate parameters by 5–8% under the urban and combined mixtures so that population densities were consistent with the literature (see Section 3.2 and Table 13 of the Supplemental Information).

3. Results

3.1. Responses to moderate, whole-watershed CEC mitigation

Walleye biomass density, population density, and PSD were similar for all the toxicokinetics assumptions for the agricultural (Fig. 3), urban (Fig. 4) and combined mixture (Fig. 5) scenarios. When

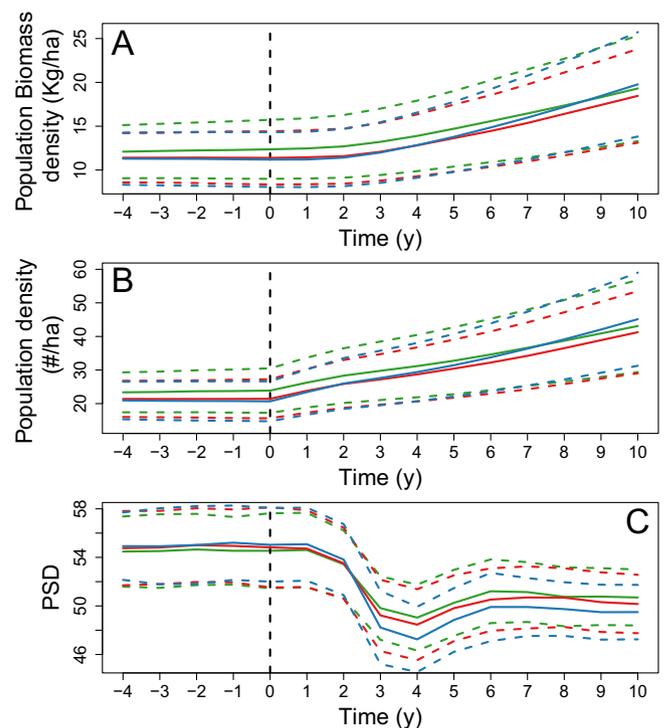


Fig. 4. Modeled yearly averaged walleye population biomass density (A), density (B) and Proportional Stock Distribution (PSD, C) before and after a 50% reduction of urban CEC mixture for the three toxicokinetic scenarios (fast in blue, moderate in red, slow in green) in the Maumee River and Lake Erie. Continuous lines are the average of 400 replicates, dotted lines are the standard deviation. The vertical dotted line marks the change in CEC exposure. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

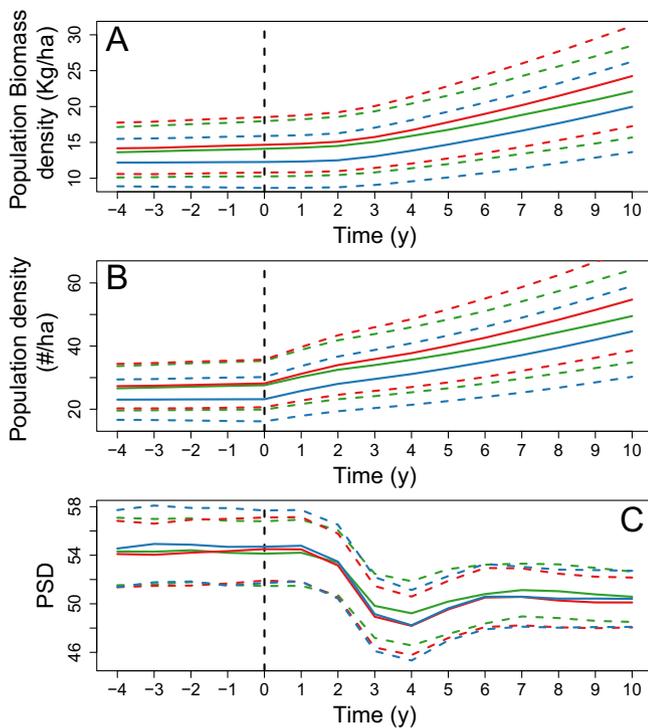


Fig. 5. Modeled yearly averaged walleye population biomass density (A), density (B) and Proportional Stock Distribution (PSD, C) before and after a 50% reduction of combined CEC mixture for the three toxicokinetic scenarios (fast in blue, moderate in red, slow in green) in the Maumee River and Lake Erie. Continuous lines are the average of 400 replicates, dotted lines are the standard deviation. The vertical dotted line marks the change in CEC exposure. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

comparing among the different mixture scenarios, biomass density, population density and PSD were similar before the start of mitigation (as intended) but different afterward.

After an approximately two-year lag, biomass density increased linearly by about 25, 55, and 66% following 10 years of whole-watershed mitigation of agricultural (Fig. 3A), urban (Fig. 4A), and combined (Fig. 5A) CEC exposure, respectively. Whereas the trajectories associated with the three toxicokinetics assumptions (fast, moderate, or slow) were parallel for the agricultural mixture, they crossed for the urban mixture, and were non-parallel but non-intersecting for the combined mixture. Population density increased linearly immediately after the start of mitigation by about 33, 114, and 96% for the agricultural (Fig. 3B), urban (Fig. 4B), and combined (Fig. 5B) CEC exposure scenarios, respectively. Likewise, depending on the assumed toxicokinetics, population density trajectories remained parallel for the agricultural mixture, crossed for the urban mixture, and were non-parallel but non-intersecting for the combined mixture. PSD trajectories before and after the start of mitigation were similar, decreasing from 55 to 49% for the agricultural (Fig. 3C), urban (Fig. 4C), and combined (Fig. 5C) CEC exposure scenarios.

3.2. Effectiveness of mitigation strategies and impact of toxicokinetics

The effectiveness of a single-site mitigation strategy for walleye in the Maumee River and Lake Erie depended on site choice, the CEC mixture, and CEC toxicokinetics. The effectiveness of whole watershed mitigation varied with toxicokinetics, but only for some CEC mixture scenarios.

The single-site mitigation of agricultural CECs had less of an effect on population density than whole-watershed mitigation regardless of toxicokinetics (Fig. 6). Single-site mitigation was relatively ineffective

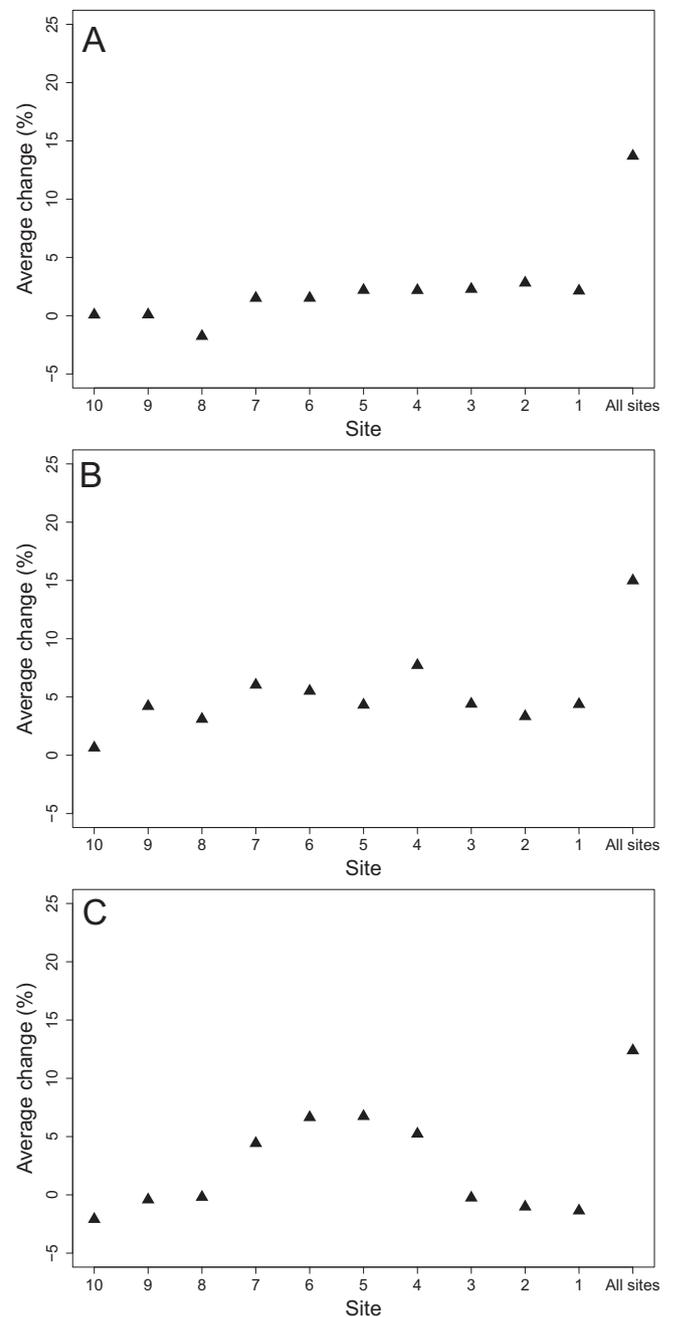


Fig. 6. Comparison of modeled mitigation strategy effectiveness for the agricultural mixture in the Maumee River and Lake Erie. 10-year average walleye population density change (y-axis) for different mitigation strategies (x-axis) and for the toxicokinetic scenarios: slow toxicokinetic scenario (A), moderate toxicokinetic scenario (B), fast toxicokinetic scenario (C). Site numbers increase from 1 (downstream) to 10 (upstream) (see Fig. 1). whole watershed mitigation is marked as "All sites". Reproduction was highest on Sites 6 and 7, and moderate on Sites 8 to 10.

when toxicokinetics were slow (Fig. 6A), benefitted most sites when toxicokinetics were moderate (Fig. 6B), and only benefitted Sites 4–7 when toxicokinetics were fast (Fig. 6C). The effectiveness of whole watershed mitigation was not impacted by toxicokinetics for this exposure type.

Single site mitigation was generally more effective at improving population density for the urban mixture (Fig. 7) than it was for the agricultural mixture. Responses varied from effectively no change in population density (Sites 8–10) to increases of ~5% (Sites 1–6) and ~20% (Site 7) when toxicokinetics were slow (Fig. 7A). These relative

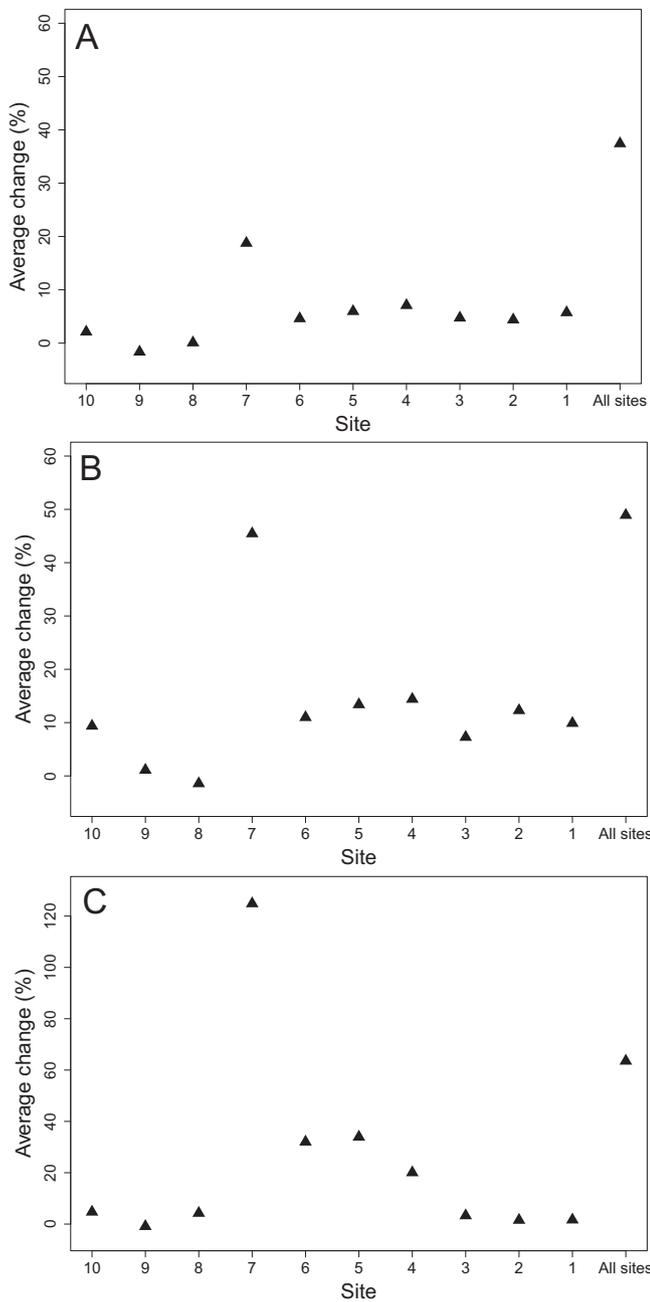


Fig. 7. Comparison of modeled mitigation strategy effectiveness for the urban mixture scenario. 10-year average walleye population density change (y-axis) for different mitigation strategies (x-axis) and for the three toxicokinetic scenarios: slow toxicokinetic scenario (A), moderate toxicokinetic scenario (B), fast toxicokinetic scenario (c). Single river site mitigation is numbered from 1 (downstream) to 10 (upstream), whole watershed mitigation is marked as “All sites”. Reproduction occurs on Site 6 to 10, and more frequently on Sites 6 and 7.

differences were generally preserved when toxicokinetics were moderate, albeit at higher percentages (Fig. 7B). The Site 7 response was so high that it was almost equal to the response of population density to whole-watershed mitigation. The response at this site exceeded the whole-watershed response when toxicokinetics were fast (Fig. 7C). Responses also increased for Sites 4–6, but were close to zero for Sites 1–3 and 8–10. Unlike with the agricultural exposure, whole watershed mitigation was impacted by toxicokinetics assumptions. It was about 38, 50 and 62% for the slow, moderate and fast toxicokinetics, respectively.

The response of population density to the single-site mitigation in the combined CEC scenario was intermediate to the responses to agricultural and urban mixture scenarios (Fig. 8). Single-site mitigation

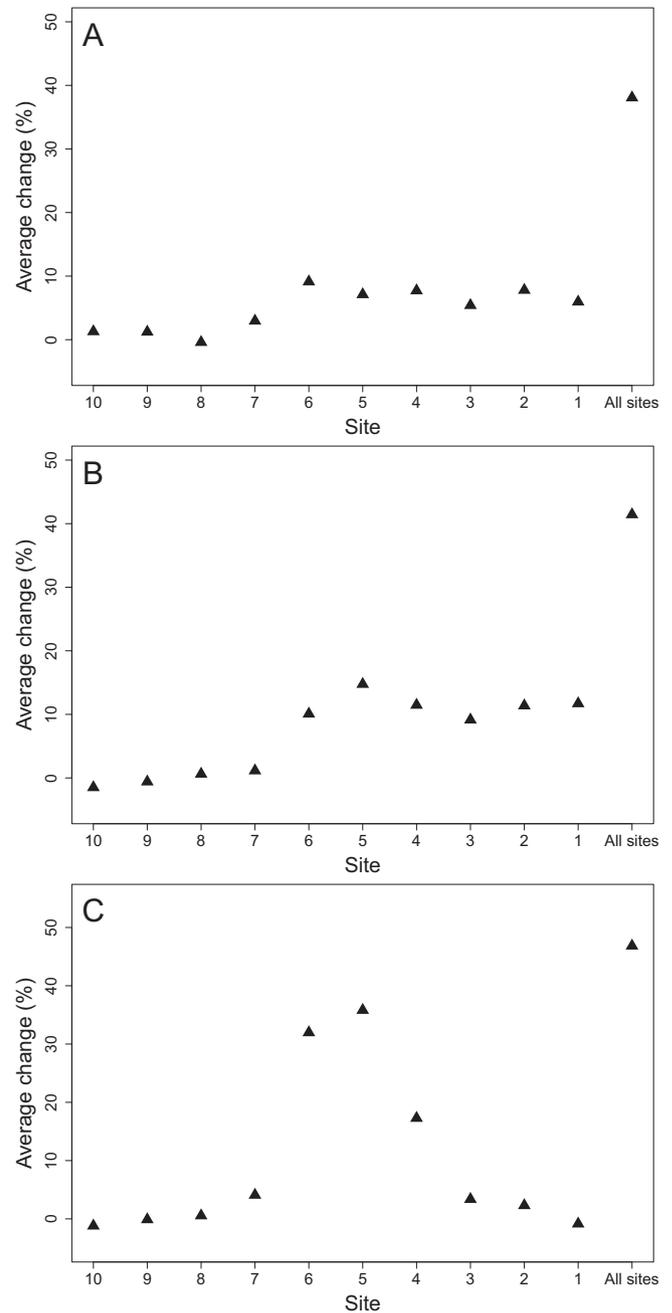


Fig. 8. Comparison of modeled mitigation strategy effectiveness for the combined mixture. 10-year average walleye population density change (y-axis) for different mitigation strategies (x-axis) and for the three toxicokinetic scenarios: slow toxicokinetic scenario (A), moderate toxicokinetic scenario (B), fast toxicokinetic scenario (c). Single river site mitigation is numbered from 1 (downstream) to 10 (upstream), whole watershed mitigation is marked as “All sites”. Reproduction occurs on Site 6 to 10, and more frequently on Sites 6 and 7.

was relatively effective for Sites 1–6 (urban influenced sites) but not Sites 7–10 (agricultural influenced sites) when toxicokinetics were slow (Fig. 8A) or moderate (Fig. 8B), and only benefitted Sites 4–7 when toxicokinetics were fast (Fig. 8C). The response to single-site mitigation at these three sites was almost as high as the response to mitigation across the whole watershed. The estimation of the whole watershed mitigation was less impacted by toxicokinetics than with the urban mixture, but more than with the agricultural mixture. The effectiveness was ~38% when toxicokinetics was slow, and ~42 and 46% for moderate and fast toxicokinetics, respectively.

4. Discussion

Our study used published individual- and population-level data to build a realistic model that simulates walleye population dynamics in the Maumee River and Lake Erie. We modeled the effects of CECs on individual walleye by using chemical effect data from the fathead minnow. According to acute 50% lethal concentrations (LC50s), perciformes tend to be more sensitive to toxicants than fathead minnow (Teather and Parrott, 2006). Nevertheless, there is no evidence that LC50s and chronic effects on reproduction are correlated. Some studies have reported different ratios among different chemicals for the same species (Bisson and Hontela, 2002; Nakashima and Suzuki, 1965) and different ratios for the same chemical between two species (Lacroix and Hontela, 2004). This is because different endpoints have different biological backgrounds; a percent reduction in reproduction or survival does not have the same ecological consequences (Jager, 2011, 2015). Given limited data on the relative sensitivity to reproductive effects of CECs on walleye and fathead minnow, our focus herein is on the qualitative differences between mitigation strategies, rather than on their quantitative differences. Our objective is to guide fisheries management decision-making, such as choosing habitat restoration sites, and to identify key knowledge gaps that direct future research and monitoring. Our focus is thus on the development of a realistic walleye population model that can simulate any level of chemical impacts on walleye reproduction.

Our model generated realistic population-level responses to mitigation. For example, whereas population density increased quickly in response to a rapid increase in reproductive investment, biomass density did not increase for ~2 years because new individuals took time to grow. This dynamic was reflected in changes to population size structure. PSD decreased after two years, indicating that the population was composed of many small individuals. Finally, the strongest population density increase (~115%) is within the range of variation that is observed for Walleye populations in Lake Erie (Dippold et al., 2020; Nate et al., 2011).

Walleye populations across the three mixture scenarios were similar prior to, but not after, watershed mitigation. The increases in biomass density and population density were largest for the urban CECs and smallest for the agricultural CECs. These differences were partly due to the varied effect of exposure levels by zone on individual reproduction. Individual-level effects on reproduction were lower for the agricultural mixture (18 to 33% reduction) than for the urban mixture (33 to 49%). Consequently, reducing the effect-level by 50% represented a smaller reduction (9 to 16.5%) for the agricultural mixture than for the urban mixture (16.5 to 24.5%). The number and locations of high-, moderate-, and low-impacted zones were also important because walleye must pass through downstream sites to reach upstream spawning areas. Whereas urban CECs were present at higher concentrations at several downstream sites, the agricultural CECs were more evenly distributed throughout the river.

Assumptions about CEC toxicokinetics had little effect on the effectiveness of whole-watershed mitigation for the agricultural mixture, but were more important for the urban and the combined mixture scenarios. The differences observed were due to differences in some population parameters, which were required to have similar realistic initial populations (same population size and PSD between all CEC scenarios, all in accordance with the literature). All parameters for the different toxicokinetics assumptions were the same for the agricultural mixture, in which the effectiveness of watershed mitigation was not influenced by toxicokinetics assumptions. For the urban and combined mixtures, in which different toxicokinetics assumptions led to small differences (non-parallel trajectories after the start of watershed mitigation), two parameters varied by 5 to 8% depending on toxicokinetics assumptions (see Section 3.2 and Table 13 of the Supplemental Information). These variations are smaller than the range of variation observed when estimating stage-dependent survival rates (for instance survival rate of

age 5 and older walleye is between 0.64 and 0.77, and between 0.6 and 0.7 for age 2 fish in Hayden et al. (2018)). This result suggests that it is more important to accurately capture population characteristics (e.g., stage-specific predation rates) and individual-level effects of the CEC mixture than chemical toxicokinetics when assessing the effectiveness of a whole-watershed mitigation strategy. Although chemical toxicokinetics are important to consider when evaluating stressor effects for spatially explicit population models, our results suggest that this may not be necessary when evaluating the effectiveness of a whole watershed mitigation strategy. Toxicokinetic models simulate how quickly internal CEC concentrations equilibrate with environmental CEC concentrations. However, when the decline of external concentration is homogenous and synchronous in space and time, all individuals will have a similar decline of their internal concentration, even if the exposure level is non-homogeneously distributed and temporally variable. Of course, this only holds if individual movement behavior remains unaffected by chemical exposure. Further study is needed to determine the extent to which this result applies when considering other modes of action of chemicals and other fish species.

Chemical toxicokinetics appear to be an important factor when predicting the effectiveness of site-specific mitigation, regardless of mixture type. The walleye in our model migrated to the river annually to spawn. The rate at which their internal chemical concentration adjusted to lower CEC concentrations in a mitigated area had a considerable population-level impact. Our results showed that knowledge of these rates is important for accurately assessing the effectiveness of a site-specific mitigation plan. Mitigation is predicted to have a strong impact when the internal adjustment is fast, and almost no impact when the adjustment is slow. The importance of accounting for chemical toxicokinetics applies to any organism evolving in an environment with non-homogenous or time-varying toxicant levels (Ashauer et al., 2006, 2007). Our study contributes to this literature and underlines the importance of performing tests that enable accounting for toxicokinetics of chemicals in assessing risks to populations in the field. Ideally, this information should be available for all chemicals when dealing with mixtures, because patterns of toxic effects in time differ among chemicals, and time patterns differ among endpoints of interest (Baas et al., 2010). This is particularly challenging when the number of chemicals in a mixture is large and varies in time or space, and a topic for which more research is needed. Information about the time that is required for fish to recover from individual-level effects could be important when choosing a management strategy.

Our results indicate that site-specific mitigation is most likely to be effective for CECs that primarily impact reproduction when it involves the highly impaired downstream areas through which adult walleye migrate, and the upstream sites in which they ultimately spawn. Sites 6 and 7 were the most frequently selected spawning sites (there is less reproduction in upstream sites and no reproduction in Sites 1 to 5). Consequently, mitigation of Sites 1 to 7 reduced CEC impacts for a larger number of fish, whereas mitigation of sites further upstream affected fewer fish and consequently had less of an impact on the population. Mitigating downstream sites that were closer to spawning sites had a greater impact on population recovery. The extent to which the mitigated site was impaired was also an important factor that increased population recovery. For instance, although Sites 6 and 7 are both spawning areas that had the same exposure level to urban CECs, Site 7 mitigation was more effective because it was closer to other spawning sites. Conversely, Sites 6 and 7 were associated with different exposure levels for the combined mixture. Site 6 was exposed to the urban mixture, and Site 7 was under a low agricultural exposure. In this scenario, it was most effective to mitigate Site 6 and Site 5 immediately downstream. This result indicates that mitigating sites that are downstream of, and more impaired than, spawning sites may be more effective than mitigating weakly impaired spawning sites.

Our watershed mitigation strategy was representative of general actions to reduce the release of CECs into the environment, like new

legislation to restrict the use of CECs, or investment in infrastructure (e.g., wastewater treatment) to reduce CEC levels at source of input. These actions are often more costly or difficult to implement but, as our study shows, can be more effective than localized mitigation. However, localized mitigation is likely to be more cost-effective. For instance, it is relatively easy to establish vegetative buffer strips that are effective at reducing agricultural runoff (Arora et al., 1996; Caron et al., 2010). Our study suggests that a localized mitigation strategy can be effective when applied at appropriate sites, especially when stress levels are high and involve CECs with rapid toxicokinetics. In practice, the effectiveness of single site mitigation could be higher than estimated in our study. Some site-specific mitigation strategies, like river restoration, can also increase fish abundance by increasing survival rates, habitat quality, and habitat carrying capacity (Roni, 2019), which we did not take into account. Moreover, we did not include effects of site mitigation on downstream sites. Nevertheless, our study highlights that the intensity of CEC effects, their toxicokinetics, and information about stage-dependent survival rates influence the effectiveness of mitigation strategies, and are therefore important factors to consider. Economical and societal impacts should also be assessed when weighing mitigation options, but this is beyond the scope of our study.

Some results of our study are qualitatively generalizable to other species and river systems. For instance, the increased effectiveness of site-specific mitigation when applied on reproduction sites is likely generalizable to other species for chemicals impacting reproduction efficiency. We also found that the required level of precision of different types of data that are needed to accurately estimate the effectiveness of a mitigation strategy varied depending on the mitigation strategy itself. Precise knowledge of chemical toxicokinetics was not important for whole watershed mitigation, but did influence site-specific mitigation strategies. In contrast, having precise, stage-dependent survival rates was more important to assess the effectiveness of whole watershed mitigation. This result is probably generalizable to other species and toxicants as it relates to the context-specific importance of toxicokinetics versus population characteristics. However, further study is needed to confirm this. The quantitative results of our study are likely specific to the mode of action of the CEC mixtures and the species of interest. For instance, even closely related species with similar ecology and experiencing similar individual-level effects can exhibit different population-level effects (Accolla et al., 2019). Moreover, different individual-level modes of action have different population-level effects (Accolla et al., 2019; Galic et al., 2018; Vaugeois et al., 2020). Consequently, further work is needed to better understand how these quantitative results could apply to closely related species with similar ecology, or for the same species for different stressor modes of action.

In this study, we place ourselves in the perspective of managing a population under an unknown stress intensity-level due to CEC exposure impacting egg maturation (same starting population for every mixture scenario and toxicokinetics assumption). We built a modeling approach to represent hypothetical TK-TD assumptions when data are limited, and showed the possible impact of different management strategies on an ecosystem of concern. Such modeling approaches are crucial to improving risk assessment and inform management decisions (Forbes et al., 2019). They can highlight the importance of particular exposure scenarios (e.g., urban vs agricultural), and identify the information that is likely to improve model predictions. Our work would be even more valuable if coupled with frequent monitoring of the ecosystem of interest, which would allow us to improve and adapt the TK-TD approach to new situations and/or system knowledge.

CRediT authorship contribution statement

MV, PAV, SHM and VEF conceptualized the study. MV performed the modeling work. MV, PAV, SHM and VEF analyzed simulation data. MV led the writing of the first draft, all authors substantially contributed to revisions.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2020.144326>.

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Supplemental Information:

TRACE document

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

Vaugeois M., Venturelli P. A., Hummel S. L., and Forbes V. E., 2021: A simulation-based evaluation of management actions to reduce the risk of contaminants of emerging concern (CECs) to walleye in the Great Lakes Basin.

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

The rationale of this document is as follows:

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

and uses the updated standard terminology and document structure in:

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

and:

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

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1. Problem formulation

This TRACE element provides supporting information on the decision-making context in which the model will be used; the types of model clients or stakeholders addressed; a precise specification of the question(s) that should be answered with the model, including a specification of necessary model outputs; and a statement of the domain of applicability of the model, including the extent of acceptable extrapolations. This document rationale is based on Augusiak et al. (2014), Grimm et al. (2014), and Schmolke et al. (2010).

Summary:

The model we present in this document aims to estimate population-level effects caused by exposure to different mixtures of Contaminants of Emerging Concern (CECs). Based on in-situ CEC concentration data (Elliott et al., 2017) and laboratory individual-level effect data (Cipoletti, 2018; Schoenfuss et al., 2020), we assess the potential effects of different management strategies on a walleye population in Lake Erie and the Maumee River. We also accounted for different toxicokinetics assumptions (fast, moderate, and slow), and assessed their impact on the effectiveness of mitigation strategies.

The life cycle of Walleye (*Sander vitreus*) is described through their metabolism using the Dynamic Energy Budget (DEB) theory (Kooijman, 2010) that was calibrated using published data (section [3.1](#)). We represent the population through an Individual-Based Model (IBM). Individual-level effects of CECs are represented by impacting an energetic pathway of the DEB model (section [2.13.1](#)) based on laboratory data (Cipoletti, 2018; Schoenfuss et al., 2020). Laboratory individual-level effects data were assessed on fathead minnow (*Pimephales promelas*). The IBM includes population processes, such as migration and reproduction, and realistically describes the walleye population in the Maumee River and Lake Erie. The DEB-IBM was calibrated to reproduce literature data on reproductive season, location of reproducing individuals in the river, spawning site fidelity, age-specific population densities, and population structure (sections [3.2](#) and [6.2](#)). We used *in-situ* data of CEC water concentrations (Elliott et al., 2017) to determine the exposure regime in the river during the year (sections [2.13.2](#) and [2.13.3](#)).

2. Overview, Design concepts, Details

This TRACE element provides supporting information on the model. It provides a detailed written model description. The Overview, Design concepts, Details (ODD) protocol (Grimm et al., 2010, 2006) is recommended as a standard format for individual/agent-based models and other simulation models. For

complex sub-models, it should include concise explanations of the underlying rationale. Model users should learn what the model is, how it works, and what guided its design.

Summary:

Here we present the complete model description following the ODD designed for describing individual-based models.

The model description follows the ODD protocol (Grimm et al., 2010, 2006). The model uses a DEB-IBM approach (Martin et al., 2012) and is developed in Java using the "SimAquaLife" framework (Dumoulin, 2007), which is an individual-based, process-oriented framework for simulating aquatic life. The code is available in supplemental information of the main manuscript.

2.1. Purpose

Our model estimates population-level effects caused by exposure to two mixtures of CECs (agricultural and urban). It uses in-situ CEC concentration data (Elliott et al., 2017) and the results of laboratory toxicity tests (Cipoletti, 2018; Schoenfuss et al., 2020) to assess the potential effects of two CEC mitigation strategies (watershed-wide and moderate vs. site-specific and intensive) on a Lake Erie walleye population that spawns in the Maumee River. We also simulated different exposure durations prior to reproduction to account for different toxicokinetics.

2.2. Basic principles

The model is based on DEB theory for describing the energetics of individuals. The DEB model describes how individuals feed, allocate energy for growth and reproduction, and die of aging and/or starvation. Parameters of the DEB model are species specific and were estimated based on an extended set of published individual-level data.

The degree of food limitation in our model depends on both fish density and the logistic growth parameter for food. We introduced predation as a third, external source of mortality because DEB theory only represents mortality due to aging and starvation. At each time step, if a randomly selected number (continuous uniform distribution $U(0,1)$) is less than the stage-specific probability of dying from predation, then the individual dies. In this study, we considered a stage-specific, density-independent, predation mortality rate and an indirect competition for food from which density-dependence emerged.

2.3. Entities, state variables, and scales

There are two types of entities in the model: individual fish and spatial unit. We used the scaled version of the DEB model with metabolic acceleration to represent the energy budget of individuals. Individuals are characterized by six state variables (Table 1): structure (L , in cm); scaled reserve (U_E , d.cm⁻²); scaled maturity (U_H , d.cm⁻²); scaled reproduction (U_R , d.cm⁻²); damage-inducing compounds (\dot{q}), expressed as aging acceleration; and damage (\dot{h}), expressed as hazard rate. For more details and an introduction to DEB theory, see Jusup et al. (2017), Nisbet et al. (2000), Sousa et al. (2010), and van der Meer (2006). All model parameters and equations are reported in Tables 2 and 3, respectively.

The aging of individuals follows Martin et al. (2012). Briefly, aging in DEB theory is based on the idea that damage-inducing compounds (*i.e.*, free radicals) cause irreversible damage to DNA, and that the probability of dying by aging is proportional to the amount of damage. Aging is therefore described in terms of the state variables damage-inducing compounds (\dot{q}), and damage (\dot{h}).

We introduced a normally distributed, scatter multiplier ($\mu = 1$ and $\sigma = 0.05$) to account for inter-individual variability in six of the standard DEB parameters (half-saturation coefficient, energy investment ratio, the scaled maturity thresholds for hatching, birth, metamorphosis, and puberty).

Table 1: State variables of the scaled DEB model.

Name	Notation	Dimension
Volumetric structural length	L	Cm
Scaled reserve	U_E	d.cm ⁻²
Scaled maturity	U_H	d.cm ⁻²
Scaled reproduction	U_R	d.cm ⁻²
Aging acceleration	\dot{q}	d ⁻¹
Hazard rate	\dot{h}	d ⁻¹
Food item 1 density	X_1	J.m ⁻²
Food item 2 density	X_2	J.m ⁻²

The model has 10 spatial units that each represent a 1-ha zone of the Maumee River, plus one zone representing 10-ha of Western Lake Erie. The five most upstream river zones are potential spawning zones based on Dufour (2012), Hayden et al. (2018) and Schmidt (2016). Each zone is characterized by five state variables: the first food item density (X_1 , J.m⁻²), the second food item density (X_2 , J.m⁻²), temperature (T , in

C), surface area (in m^2), and the stress factor (s) the calculation of which is based on *in-situ* data and laboratory data (see section 2.13). Both food item densities change once during each daily time step according to a logistic growth equation and fish consumption. The logistic growth function has two parameters: daily intrinsic growth rate (aE in d^{-1} for both food items) and the carrying capacity ($kE1$ in $J.m^2$ for food item1, $kE2$ in $J.m^2$ for food item 2) (see section 2.10). Temperature is homogenous in a zone and is the same for all the river zones (range from 0.1 to 29.5 °C during the year). The zone representing Lake Erie has a different temperature profile (range from 0.5 to 23.9 °C during the year). The daily changes in river temperature were gathered from online temperature data that were recorded in 2016 in the Maumee River (<https://waterdata.usgs.gov/nwis>). The daily changes in lake temperature were gathered from online temperature data of average temperature near Cleveland (1981-2010) (https://www.weather.gov/cle/avg_lake_erie_water_temps).

Model integration followed the classical Runge-Kutta method using the Apache Commons Math library (release 3) with a daily time step.

Table 2: Parameters of the scaled abj DEB model for walleye. wd stands for without dimensions.

Name	Notation	Dimension
Standard parameters		
Fraction of mobilized energy to soma	κ	wd
Fraction of mobilized energy fixed in eggs	κ_R	wd
Somatic maintenance rate coefficient	κ_M	d^{-1}
Maturity maintenance rate coefficient	κ_j	d^{-1}
Scaled maturity at hatching	U_H^h	$d.cm^{-2}$
Scaled maturity at birth	U_H^b	$d.cm^{-2}$
Scaled maturity at metamorphosis for female	U_H^j	$d.cm^{-2}$
Scaled maturity at puberty for female	U_H^p	$d.cm^{-2}$
Scaled maturity at metamorphosis for male	U_H^{jm}	$d.cm^{-2}$
Scaled maturity at puberty for male	U_H^{pm}	$d.cm^{-2}$
Energy conductance	\dot{v}	$cm. d^{-1}$
Energy investment ratio	g	wd
Aging parameters		
Weibull aging acceleration	\ddot{h}_a	d^{-2}

Gompertz stress coefficient	S_G	wd
Auxiliary parameters		
Digestion efficiency of food to reserve	κ_x	wd
Chemical potential of reserve	μ_x	mol ⁻¹
Surface area-specific maximum ingestion rate	$\{j_{xAm}\}$	L ⁻² .t ⁻¹
Surface-area-specific searching rate	$\{F_m\}$	l.cm ⁻² .d ⁻¹
Arrhenius temperature	T_A	K
Reference temperature	T_{ref}	K

2.4. Process overview and scheduling

Individuals are listed by zone, and then the model executes the following actions at each time step for each zone:

- Individuals update their DEB state variables (see section [2.8.1](#)): Organisms feed and grow in structure and maturity. For individuals, this update can result in three forms of mortality: starvation (*i.e.*, an inability to pay maintenance costs), aging, or predation (stage-dependent survival rate to predation). Starvation is deterministic (*i.e.*, depends on a state variable), and death by aging and predation are stochastic (*i.e.*, depend on random selection). Both starvation death and death by aging are based on individual energetics and interactions with the environment. Predation is a stage-dependent, external cause of death. Dead individuals are removed before the next action. After each individual update, the density of both food items is updated (what one individual has eaten is removed). When all individuals of one zone have been updated, both food items are updated according to their logistic growth function.
- Reproduction (see section [2.8.2](#)): Only adults with a minimum amount of energy allocated to reproduction (U_R , d.cm⁻²) are able to reproduce. Females can only reproduce if they share a spawning zone with a male that is also ready to reproduce and if they are in their selected spawning site.
- Movement (see section [2.8.3](#)): Movement is the last action and is dependent on the life stage of the organism (*e.g.* upstream migration of adults), its current location (*e.g.* no movement for adults if they are in their selected spawning site), and the time of the year (*e.g.* to match the reproductive season).

2.5. Design concepts

2.5.1. Basic principles

The model is based on Dynamic Energy Budget theory for describing the energetics of individuals. The DEB model describes how individuals feed, allocate energy for growth and reproduction, and die of aging, predation, and/or starvation. Food in our model is limited by both fish density and the logistic growth parameter of food defined in spatial units. DEB theory allows for the representation of two kinds of mortality: aging and starvation. We also introduced mortality due to predation.

2.5.2. Emergence

The following variables emerge from the behavior of individuals, their metabolism, the indirect interactions of individuals through competition for food, and predation: fish population density, the average spawning interval, total biomass, and Proportional Stock Density (PSD, ratio of the number of individuals ≥ 38 cm over the number of individuals ≥ 25 cm).

2.5.3. Adaptation

The model does not contain adaptive behavior. DEB parameters differ among individuals, but they stay constant over the simulation of each individual. The model is also free of evolutionary adaptation; parameter values for new individuals in the model are set identically as in the initialization process.

2.5.4. Objectives

The objective of the study is to simulate a realistic walleye population in the Maumee River and western Lake Erie under realistic CEC exposure in order to assess the impacts of different management strategies.

2.5.5. Learning

There is no learning process in the model.

2.5.6. Prediction

There is no prediction in the model.

2.5.7. Sensing

The only sensing process in the model is the detection by females of the presence of males in the river zone. If reproductive males (*i.e.*, reproduction buffer is greater than the threshold for reproduction, see section [2.12.1](#)) are present in the river zone, then females can reproduce.

2.5.8. Interactions

Individuals interact directly via reproduction, and indirectly via competition for food.

2.5.9. Stochasticity

Some DEB parameters vary among individuals. We followed the same methodology as Martin et al. (2012), based on Kooijman et al. (1989), to set variability among individuals. Briefly, the surface area specific maximum ingestion rate $\{j_{xAm}\}$ is multiplied by a scatter multiplier to introduce differences between individuals. It impacts six DEB parameters: the half-saturation coefficient K which is multiplied by the scatter multiplier; the energy investment ratio g , which is divided by the scatter multiplier, the scaled maturity threshold for hatching U_H^h , birth U_H^b , metamorphosis U_H^j and puberty U_H^p , which are divided by the scatter multiplier because we use the scaled DEB model (which is the standard DEB model scaled by $\{\dot{P}_{Am}\}$, see Kooijman et al. (2008) for more details on scaling the standard DEB model).

Other sources of stochasticity include the order in which organisms are updated, the probabilities of dying by aging or predation (section [2.8.1](#)), the selection of the reproduction site for the coming reproduction season, and the decision to move (section [2.8.3](#)).

2.5.10. Collectives

There is no aggregation behavior in the model.

2.5.11. Observations

We collected observations on fish density for different age groups, eggs per reproductive event per female, total biomass, and PSD.

We assessed the efficiency of different management actions. We compared how average population size for the last 10 years of the simulation was impacted when we:

- decreased the effects of the CEC mixtures on individuals for all sites by 50%, which would correspond to a moderate remediation of the entire watershed;
- decreased the effects of the CEC mixtures on individuals by 100% for one river site at a time, which would correspond a complete remediation of one localized site.

2.6. Initialization

Food density is set to carrying capacity in all zones at the beginning of each simulation. All simulations began by introducing 30 new individuals per zone (eggs that will reach larval stage) at day 93 of the simulation. Each mixture (urban or agricultural) has specific effects on individuals that depend on the exposure intensity. Exposure to a contaminant mixture varies in time and space as described in section 2.13. Fish are exposed to this exposure regime for the first 35 years of simulation. We start observing the population at year 35 for a 20 year period. We start the different management scenarios at year 40.

We introduced variability among individuals as described in section 2.5.9. The initial set of DEB parameters (*i.e.*, the one on which we apply a scatter multiplier) is the one from the parameterization of the individual DEB model (see section 3.1). The initial values of the DEB state variables are $L = 0.001$, $U_R = 0$, $U_H = 0$. The initial amount of scaled reserve U_E is calculated for each individual using the bisection method from Martin et al. (2012). Briefly, this method determines the initial amount of scaled reserve via adaptive trial and error so that the reserve density (E/V) of the offspring at birth is similar to the reserve density of the mother when she produces the offspring.

2.7. Input data

The model uses a single year of daily water temperature data for all river zones and years, and another one for the lake zone. River data were recorded in 2016 in the Maumee River, and can be downloaded from the USGS website (<https://waterdata.usgs.gov/nwis>). Lake data are average temperatures measured near Cleveland (1981-2010) (https://www.weather.gov/cle/avg_lake_erie_water_temps).

We also imputed stress factor (s) series for each zone based on laboratory and *in-situ* data (see section 2.13).

Table 3: Equations of the scaled abj DEB model for ectotherms.

Differential equations

$$\frac{dU_E}{dt} = S_A - S_C$$

$$\frac{dL}{dt} = \frac{1}{3} \left(\frac{\dot{v} S_C}{g L^2_A} - \dot{\kappa}_M L \right)$$

$$\frac{dU_H}{dt} = (1 - \kappa) S_C - S_J \text{ if } U_H < U_H^p, \quad \text{else } \frac{dU_H}{dt} = 0$$

$$\frac{dU_R}{dt} = 0 \text{ if } U_H < U_H^p, \quad \text{else } \frac{dU_R}{dt} = (1 - \kappa) S_C - S_J$$

$$\frac{d\ddot{q}}{dt} = \left(\ddot{q} \left(\frac{L}{L_m} \right)^3 S_G + h_a \right) e \left(\frac{\dot{v}}{L} - \frac{3}{L} dL \right) - \frac{3}{L} dL \ddot{q} \text{ with } L_m = \frac{\dot{v}}{g \dot{\kappa}_M}$$

$$\frac{dh}{dt} = \ddot{q} - \frac{3}{L} dL \dot{h}$$

Flux equations

$$S_A = c(T) f(X) L^2 \text{ if } U_H \geq U_H^h, \text{ else } S_A = 0$$

$$S_C = c(T) L^2 \frac{g e}{g + e} \left(1 + \frac{L \dot{\kappa}_M}{\dot{v}} \right)$$

$$S_J = c(T) \dot{\kappa}_J U_H$$

Scaled food and temperature functions

$$f(X) = \frac{X}{X + K}, \text{ with } K = \frac{\{J_{XAm}\} \mu_X}{\{\dot{F}_m\}}$$

$$c(T) = \exp \left(\frac{T_A}{T_{ref}} - \frac{T_A}{T} \right)$$

2.8. Sub-models

The model includes 3 sub-models: the DEB sub-model, which includes DEB state variables (updated daily), death due to starvation, death due to aging, death due to predation, and food dynamics; the reproduction sub-model, which describes when individuals reproduce and how they update their corresponding state variables; and the movement sub-model, which describes how organisms move depending on their maturity level and ability to reproduce. Each sub-model is looped over all zones before moving to the next sub-model.

2.8.1. DEB sub-model

For each zone:

- For each individual in the zone:
 - Calculate the average stress-level exposure over the lifetime of each fish.
 - Calculate the change in reserve due to feeding and mobilized energy.
 - If maturity is less than the maturity threshold for puberty, then calculate the change in maturity. Otherwise, calculate the change in reproduction buffer.
 - Calculate the change in length.
 - If the change in length is less than 0, then recalculate structure, reserves, maturity, and reproduction buffer based on starvation rules (see section [2.9](#)).
 - Calculate the change in aging acceleration and hazard based on aging (*i.e.*, the probability of dying due to aging, see section [2.11](#)).
 - Calculate the change in food density based on feeding (see section [2.10](#)).
 - Update the DEB state variables.
 - If a randomly selected number (continuous uniform distribution $U(0,1)$) is less than the probability of dying from aging, then die. The probability of dying from aging at a moment t is $1 - H$, where H is the integral from 0 to t of \dot{h} .
 - If a randomly selected number (continuous uniform distribution $U(0,1)$) is less than the probability of dying from predation, then die. The probability of dying from predation is stage-dependent and is calculated from the parameter: annual, stage-dependent probability of survival from predation (values reported in section [3.2](#)). Death by predation at the egg and larval stages are not computed daily to improve simulation time. When a female reproduces, only the eggs that will survive up to the end of the larval stage are introduced into the model. All stages are defined by the amount of energy invested in maturity U_H . We defined the egg stage from fertilization to hatching ($U_H < U_H^h$), larval stage from hatching to metamorphosis

$(U_H^h < U_H < U_H^j)$, juvenile stage from metamorphosis to start of investment into reproduction
 $(U_H^j < U_H < U_H^p)$, and adult stage afterward ($U_H > U_H^p$).

Update food densities for all zones after they have all been updated (see section [2.10](#)).

2.8.2. **Reproduction sub-model**

For each zone:

- If the environmental temperature is $>4^{\circ}\text{C}$ and $< 11^{\circ}\text{C}$ and the zone is a spawning zone:
 - List all individuals that are ready to reproduce (*i.e.*, reproduction buffer is greater than the threshold for reproduction, see section [2.12.1](#)).
 - Allow reproduction by females that are ready to reproduce and sharing a spawning zone with at least one male that is also ready to reproduce and if the current zone is the same as the individual's selected reproduction zone. The choice of the reproduction zone is set up in the movement sub-model (section [2.8.3](#)). Because the time step is daily, both males and females can only reproduce once per day:
 - * calculate the initial amount of energy in eggs.
 - * calculate the number of spawned eggs that were fertilized, and update female reproduction buffer accordingly (see section [2.12.1](#)).
 - * randomly select a male among those in that zone that are ready to reproduce.
 - * calculate the amount of energy needed for the reproduction event for the male (whole energy content of the buffer for reproduction) and update the male reproduction buffer.
 - * create new female individuals by setting the number of new females to half the number of fertilized eggs spawned (ceiling function, sex ratio 1:1) multiplied by the annual egg and larval survival rate to predation (we only introduce eggs and larvae that would survive predation). The initial amount of energy is calculated based on

reserve density of the mother using the bisection method. The parameter values for each new individual are set as in the initialization (section [2.6](#)).

* create male individuals by setting the number of new males to half the number of fertilized eggs spawned (flooring function, sex ratio 1:1) multiplied by the annual egg and larval survival rate to predation. Rules for parameter values and initial amount of energy are the same as for females.

2.8.3. Movement sub-model

For each zone:

- Once a year, before the reproductive season, fish select their future spawning zone. This process is described in section [2.12.2](#).
- Movement of fish depends on their life stage, their current zone location, and the time of the year:
 - If the fish DEB stage is embryonic (egg and non-feeding larvae): set the current zone as the movement destination whatever the location and time of the year.
 - If the fish DEB stage is juvenile: if the current location is a river zone and a randomly selected number (continuous uniform distribution $U(0,1)$) is less than the probability to move (set to 0.5), then set the next downstream zone as the movement destination; otherwise set the current zone as the movement destination.
 - If the fish DEB stage is adult:
 - If the fish is ready to reproduce (*i.e.*, reproduction buffer is greater than the threshold for reproduction, see section [2.12.1](#)):
 - if the time of the year is between April and end of May (between day 60 and 121 for males, and between days 76 to 121 for females) (reproduction period - Mion et al. (1998); Roseman et al. (1999)):
 - if the current location is not the selected reproduction site and if a randomly selected number (continuous uniform distribution $U(0,1)$) is less than the probability to move (set to 0.5),

then set the next zone upstream as the movement destination;
otherwise set the current zone as the movement destination.

- if the time of the year is not between April and end of May, then set the next downstream zone as the movement destination.
- If the fish is not ready to reproduce, then set the next zone downstream (if the current zone is the lake zone, then current zone) as the movement destination.

Update the position of all fish once all zones have been updated.

2.9. Starvation

Individuals interact indirectly through competition for a limited food resource. Some individuals die of starvation as a result of this competition. Although many starvation strategies can be implemented with DEB theory (Kooijman, 2010; Martin et al., 2012), we implemented the following strategy because it is the most realistic for fish. DEB theory specifies that organisms use energy to grow and reproduce based on available energy in the reserve compartment. This reserve compartment is fuelled by the assimilation process. The assimilation flux is weakened when food is scarce, and the energy content of the reserve compartment may be insufficient for growth, maintenance, and reproduction/maturation. Individuals enter starvation when they cannot pay their maintenance cost (*i.e.*, when $\frac{[E]}{[E_m]} < \frac{L}{L_m}$). Growth is no longer possible at this point ($\frac{dL}{dt} = 0$), and somatic maintenance is prioritized. If the organism has not reached puberty, then its level of maturity may decrease, otherwise available energy for reproduction may decrease. The individual dies when the reserve is empty and, for non-adults, maturity decreases to 0. The individual also dies if the mobilized energy is less than the energy that is needed for maintenance.

2.10. Food density update

There are two food items in the model. Walleye diet ontogenetic shift to piscivory occurs during their first year and is size dependent (Galarowicz and Wahl, 2005; Uphoff et al., 2019). We fixed the diet shift size to 6.2 cm based on Uphoff et al. (2019). Fish feed on the first item when they are below this size, and the second food item when they are larger. The first food item represents zooplankton, other invertebrates and small fishes; the second item represents larger fishes only.

Resource density for both food items ($\text{J}\cdot\text{m}^{-2}$), is modeled as a generic logistic function.

$$\frac{dX_1}{dt} = c(T) a_e X_1 \left(1 - \frac{X}{K_{E1}}\right), \text{ and}$$

$$\frac{dX_2}{dt} = c(T) a_e X_2 \left(1 - \frac{X}{K_{E2}}\right),$$

where a_e ($\text{J}\cdot\text{J}^{-1}\cdot\text{d}^{-1}$) is the intrinsic growth rate, K_{E1} and K_{E2} ($\text{J}\cdot\text{m}^{-2}$) are carrying capacities of food item 1 and 2, respectively. The amount of food that an individual eats is determined by its energetic parameters. The resource density is updated after each individual eats in a time step. We prevented the total depletion of food by introducing a lower resource density below which individuals cannot feed. We fixed this value to 0.1 times the individual half saturation coefficient (K). The resource density is updated according to the logistic function after all individuals have eaten in a time step.

2.11. Aging

The aging process is described in DEB theory as the consequence of irreparable damage caused by free radicals or related reactive oxygen species (ROS). These damage-inducing compounds accumulate at a rate that is proportional to the mobilization rate, and the probability of dying is proportional to the amount of damage that is induced. The two state variables that describe aging mortality are thus the acceleration at which damage-inducing compounds accumulate, \dot{q} (t^{-2}), and the hazard or death rate \dot{h} (t^{-1}), proportional to the damage density. The differential equations for these two variables can be found in Table 3. The integral of \dot{h} over time gives the conditional probability of dying at time $t + \Delta t$ given that an organism has survived up to t . The survival probability is calculated from the hazard rate as follows (Kooijman, 2010):

$$\frac{dPr(a>t)}{dt} = -Pr(a > t) \dot{h}(t),$$

where a is the age of death of the organism. Therefore, the survival function at time t is:

$$R(t) = \exp^{-\int_0^t h(\varepsilon)d\varepsilon}.$$

The mortality probability at t is calculated as $m(t) = 1 - R(t)$.

2.12. Reproduction

2.12.1. Ability to reproduce and computation of the number of eggs produced:

We introduced a calibrated parameter ($R_{Threshold} = 13.8648$) so that individuals were deemed ready to reproduce when $\frac{U_R}{L^3} \geq R_{Threshold}$.

The number of fertilized eggs is calculated from the number of spawned eggs as

$$NB_{EF} = asr_E FR \frac{U_R}{\kappa_R},$$

where asr_E is the egg annual survival rate (*i.e.* the proportion of eggs that will survive to the larval stage), and FR is the proportion of fertilized eggs, a constant value extracted from the literature (Bozek et al., 2011):

$$FR = 0.76.$$

2.12.2. Selection of the reproduction site:

Zones are numbered from 1 to 10 from downstream to upstream. Fish that reproduced during the last reproductive season will choose to go back to the same location with a 70% probability as reported in Hayden et al. (2018). Selection is achieved via a randomly selected number (continuous uniform distribution $U(0,1)$). If this number is less than the probability of choosing the same reproduction site (0.7), then they will choose the same site. If a fish has not reproduced during the previous reproductive season, or if the randomly selected number is above 0.7, then they randomly select a reproduction site as follows: a random integer is selected (poisson distribution ($P(1)$)), to which six is added so that the mean of the distribution will be 7 and the minimal selected value will be 6. If the randomly selected number is above 10 (maximum number of river sites), it is set to 6. This way, there is no reproduction occurring in sites 1 to 5 and most of the reproduction events occur in sites 6 and 7, in accordance with observed egg densities in the Maumee River (Schmidt 2016).

2.13. Effects of stressors

We modeled only sublethal effects of CECs on reproduction, and the stressor intensity (s) was determined as defined in the following subsections. Effects on reproduction are simulated as a reduction in one parameter value: $\kappa_R = \kappa_R (1 - s)$. We did not consider any intergenerational effect, and no damage is passed to the following generation.

2.13.1. Laboratory mixtures and measured effects:

Two CEC mixtures were created based on the results of a two-way cluster analysis of 559 water samples conducted by US Geological Survey (USGS) to identify the most frequently detected CECs in the Great Lakes Basin and their environmental concentrations (Elliott et al., 2017). This analysis revealed a dichotomy of CECs in agricultural- and urban-influenced streams. Atrazine, bisphenol A (BPA), bromacil, diethyl-metoluamide, estrone (E1), metolachlor, nonylphenol (NP), and tributoxyethyl phosphate were consistently detected in water samples from rivers surrounded by agricultural landscapes, and BPA, diethyl-metoluamide, desvenlafaxine, E1, fexofenadine, galaxolide, metformin, methyl-1H-benzotriazole, NP, sulfamethoxazole, and tributoxyethyl phosphate in urban landscapes. Composition of the two laboratory mixtures are reported in Tables 4 and 5.

Table 4: Composition of the laboratory made agricultural mixtures in ng/L.

	Metolachlor	4-nonylphenol	Atrazine	BP A	Bromacil	Estrone	DEET	Tris(2-butoxyethyl) phosphate
Agr. Low	17	18.8	40	6	12	2.4	20	210
Agr. Medium	170	188	400	60	120	24	200	2100
Agr. High	1700	1880	4000	600	1200	240	2000	21000

Table 5: Composition of the laboratory made urban mixtures in ng/L.

	4-nonylphenol	5-methyl-1H-benzotriazole	BPA	Estro ne	HHC B	DEET	Tris(2-butoxyethyl) phosphate
Urban Ultra Low	43.55	136.61	131.88	0	2.28	87.17	156.61
Urban Super Low	133.07	142.72	30.05	0	19.55	67.19	940.68
Urban Low	322.14	2820.7	163.69	0	69.06	201.93	837.66
Urban	1201.64	3173.57	1817.	0	1396.	1263.3	11284.23

Medium			13		12		
Urban High	3151.28	19297.01	7554. 64	10	1852. 05	4413.2 3	19125.5
Urban Super High	9242.66	49053.59	17960 .6	26.1	3612. 75	10127. 35	40693.84

Exposure experiments were conducted at Saint-Cloud State University (SCSU) on fathead minnows (*Pimephales promelas*), and effects on reproduction were assessed for the two mixtures at different levels. Results are from Cipoletti (2018) and Schoenfuss et al. (2020) reported in Tables [6](#) and [7](#).

Table 6: Measured effects on reproduction (eggs production) compared to EtOH for two generations of fathead minnow exposed to different agricultural mixtures.

	Low/EtOH	Med/EtOH	High/EtOH
Generation 1	+6.6%	+20%	-28.9%
Generation 2	+4.22%	-18.1%	-32.6%

Table 7: Measured effects on reproduction (eggs production) compared to Blank for two generations of fathead minnow exposed to different urban mixtures.

	UL/Blank	SL/Blank	L/Blank	Med/Blank	H/Blank	SH/Blank
Generation 1	-54.3%	-48.9%	-33.3%	-42.2%	-80.3%	-58.4%
Generation 2	-69.8%	-88.1%	-82.8%	-71.7%	-88.1%	-84.3%

2.13.2. Measured mixture concentrations in the different zones:

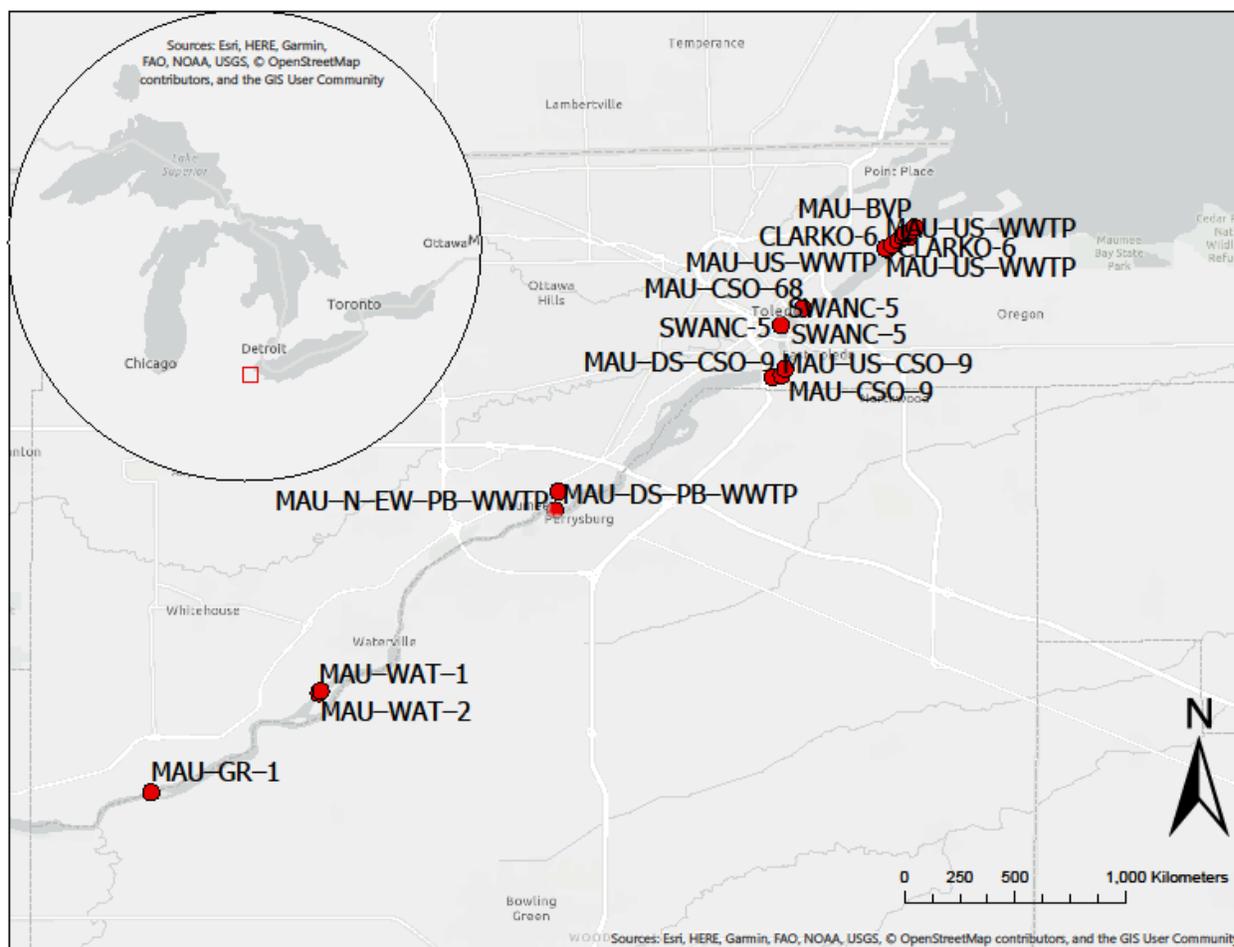


Figure 1: USGS sampling sites along the Maumee River.

USGS data were collected between 2010 and 2012 at 19 stations along the Maumee River (Figure 1). Stations were sampled in mid-April (earliest 04/17) to early May (latest 05/04), and in September (earliest 9/18) to October (latest 10/06). Results are shown in Figures 2, 3, 4, 5, and 6. For the agricultural mixture, we present the Tris(2-butoxyethyl) Phosphate (Figures 2) and all the other chemical (Figure 3) measurements separately for y-axis convenience.

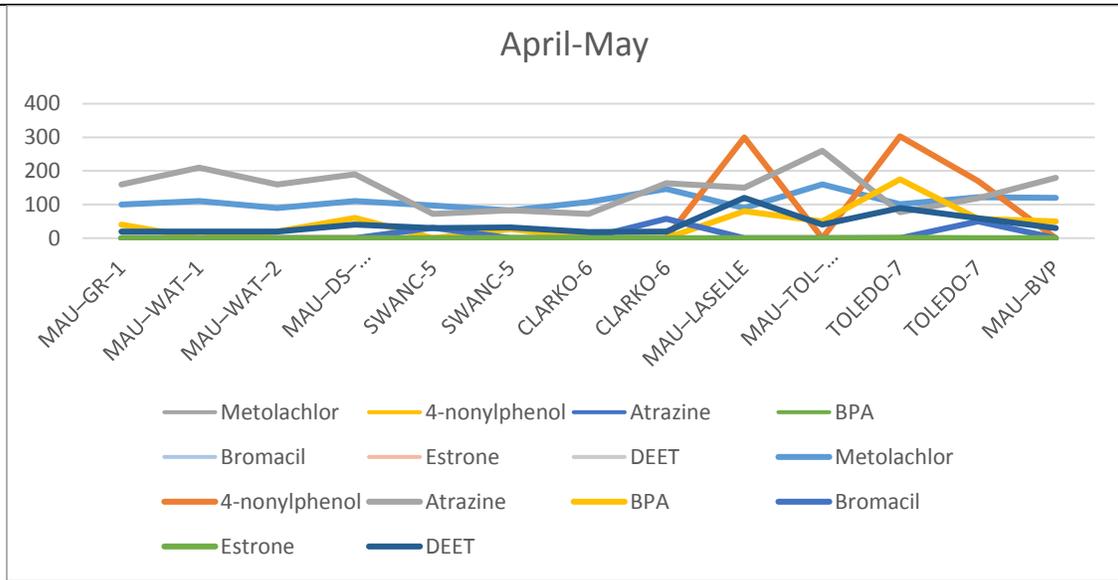


Figure 2: USGS agricultural mixture measurements (concentrations in ng/L; y-axis) for April-May at different stations (x-axis).

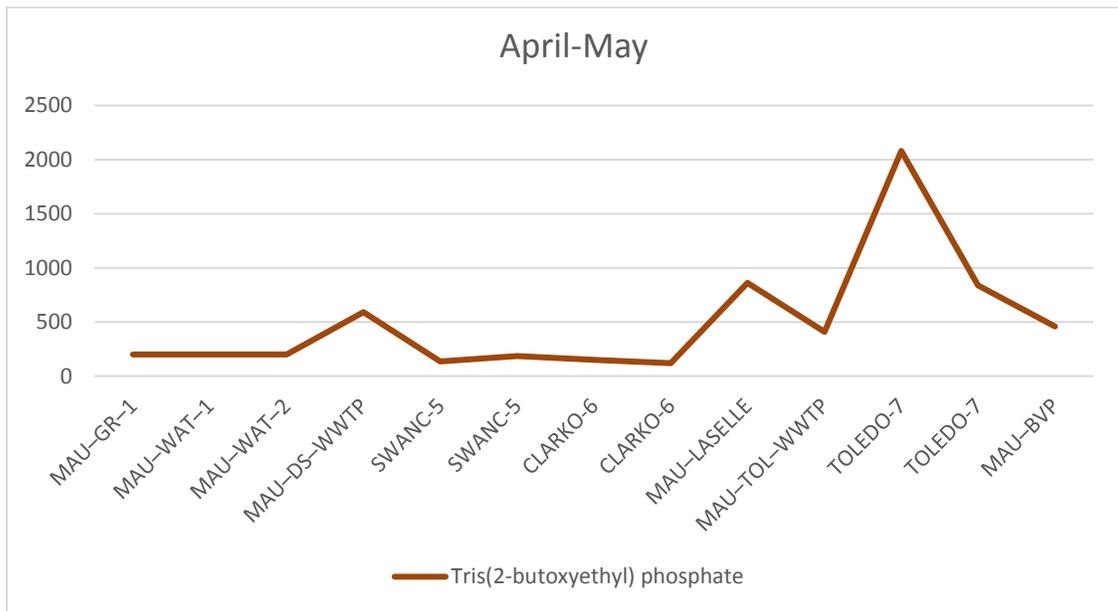


Figure 3: USGS agricultural mixture (Tris(2-butoxyethyl) Phosphate) measurements (concentrations in ng/L; y-axis) for April-May at different stations (x-axis).

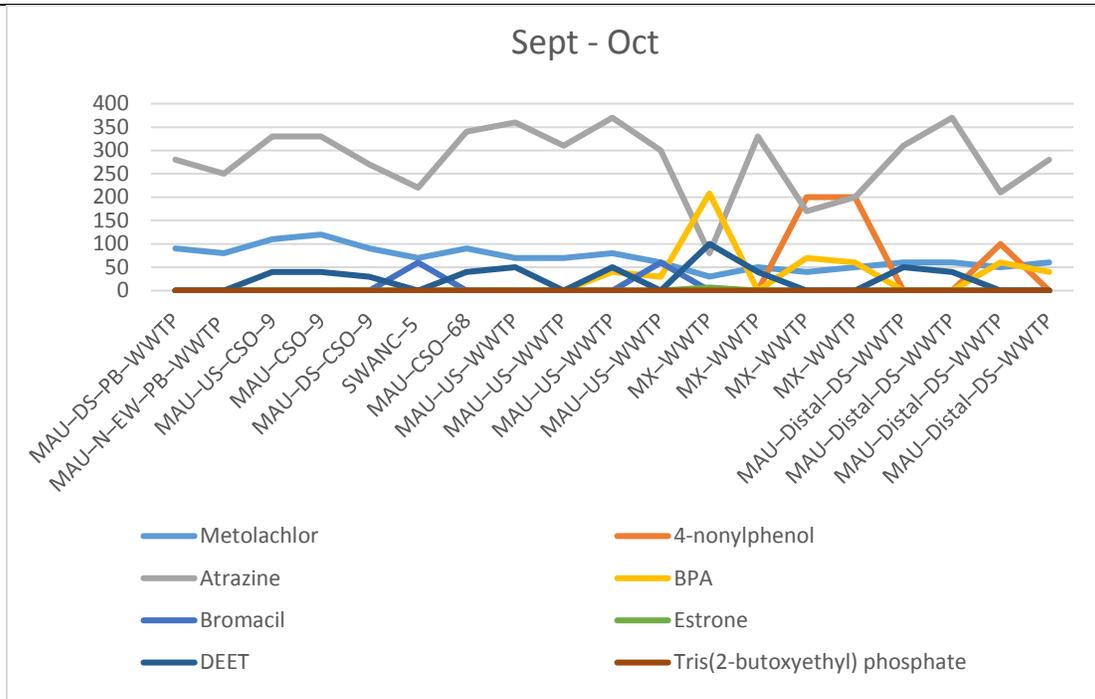


Figure 4: USGS agricultural mixture measurements (concentrations in ng/L; y-axis) for September-October at different stations (x-axis).

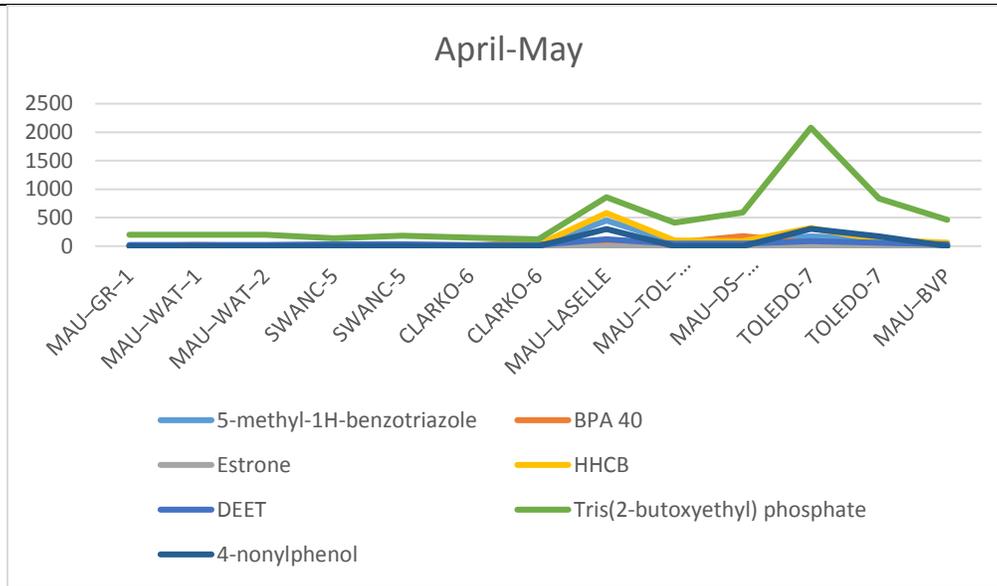


Figure 5: USGS urban mixture measurements (concentrations in ng/L; y-axis) for April-May at different stations (x-axis).

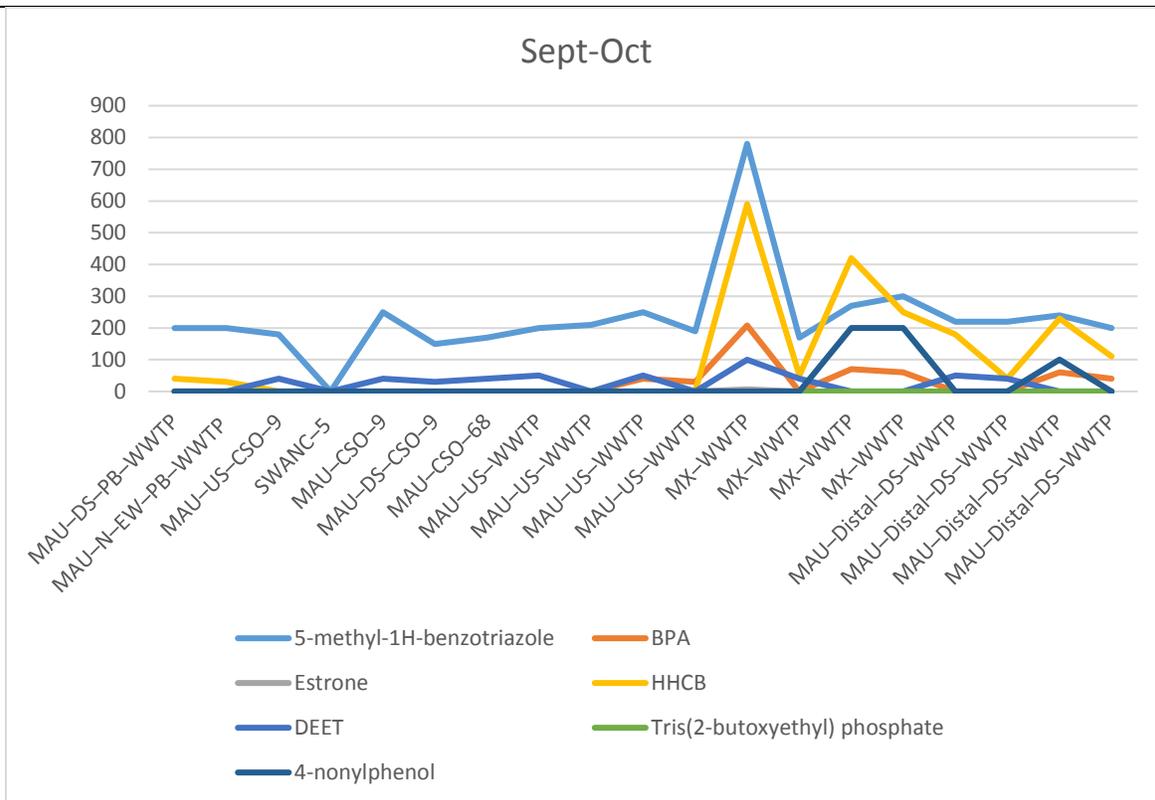


Figure 6: USGS urban mixture measurements (concentrations in ng/L; y-axis) for September-October at different stations (x-axis).

2.13.3. Modeled effects per zone:

The exposure level for each zone was determined based on the USGS measurements compared to the SCSU mixture composition.

We modeled 10 river zones that correspond to the Maumee River, and one zone that corresponds to Lake Erie. Zones are approximately 5km apart and represent 1-ha each (10-ha for Lake Erie).

We assigned stations to modeled zones based on their proximity (Table 8), and then estimated exposure in a zone for April-May and September-October by comparing the measured concentrations of chemicals

from the stations assigned to the zone to the concentration of chemicals in the laboratory mixtures. For each chemical contained in a mixture, every time a concentration at a station was above its concentration in a laboratory mixture, we estimated the level of exposure of this chemical to be the level of the mixture above. After repeating the same procedure for each chemical of a mixture, we took the highest exposure level as the exposure level of the station at this period of the year. For instance, MX-WWTP has a BPA concentration that is higher than the Agricultural Mixture Medium in September-October, so we considered the level of exposure to be Agricultural Mixture High for this chemical. With the same procedure, we found the exposure level for DEET, Estrone, Atrazine and Metolachlor at this same station and at the same period to be Agricultural Mixture Medium. Overall, we considered the exposure level of the MX-WWTP station in September-October to be Agricultural Mixture High because of the BPA concentration.

Phosphorus and Nitrogen concentrations are higher from December to June in the Maumee River (Stow et al., 2015). Consequently, we considered that our estimated April-May exposure level was applicable to the period from early December to late June, and our September-October exposure level was applicable to the period from early July to late November. For the zone representing a part of Erie Lake (numbered 0), we assumed that the exposure level was one level lower than the last river zone because fewer chemicals of concern are found in lakes compared to rivers (Elliott et al., 2018). We obtained the exposure Tables [9](#) and [10](#) for the urban and agricultural CEC mixture simulations, respectively. We created a third mixture scenario in which zones 10 to 7 are under agricultural influence, and zones 6 to 0 are under urban influence.

Table 8: USGS station assignment to the different modeled zones.

Modeled Zone	Assigned stations
10 – River	MAU-GR-1
9 – River	MAU-GR-1, MAU-WAT-1, MAU-WAT-2
8 – River	MAU-WAT-1, MAU-WAT-2
7 – River	MAU-WAT-1, MAU-WAT-2, MAU-DS-WWTP, MAU-N-EW-PB-WWTP

6 - River	MAU-DS-WWTP, MAU-N-EW-PB-WWTP
5 - River	MAU-DS-WWTP, MAU-N-EW-PB-WWTP, MAU-US-CSO-9, MAU-CSO-9, MAU-DS-CSO-9
4 - River	MAU-US-CSO-9, MAU-CSO-9, MAU-DS-CSO-9
3 - River	SWANC-5, MAU-CSO-68
2 - River	CLARKO-6, MAU-US-WWTP, MAU-LASELLE
1 - River	MAU-TOL-WWTP, MX-WWTP, TOLEDO-7, MAU-DS-WWTP, MAU-Distal-DS-WWTP, MAU-BVP
0 - Lake	MAU-TOL-WWTP, MX-WWTP, TOLEDO-7, MAU-DS-WWTP, MAU-Distal-DS-WWTP, MAU-BVP

Table 9: Determined effects per zone for urban mixture exposure.

Zone	Dec.,1 – June,30	July,1 – Nov.30
10	Urban Low	Urban Low
9	Urban Low	Urban Low
8	Urban Super Low	Urban Low
7	Urban Super Low	Urban Low
6	Urban Super Low	Urban Low
5	Urban Super Low	Urban Low
4	Urban Super Low	Urban Low
3	Urban Low	Urban Low
2	Urban Medium	Urban Low
1	Urban Medium	Urban Medium
0	Urban Low	Urban Low

Table 10: Determined effects per zone for agricultural mixture exposure.

Zone	Dec.,1 – June,30	July,1 – Nov.30
10	Agr. Medium	Agr. Medium
9	Agr. Medium	Agr. Medium

8	Agr. Medium	Agr. Medium
7	Agr. Medium	Agr. Medium
6	Agr. Medium	Agr. Medium
5	Agr. Medium	Agr. Medium
4	Agr. Medium	Agr. Medium
3	Agr. Medium	Agr. Medium
2	Agr. Medium	Agr. Medium
1	Agr. High	Agr. High
0	Agr. Medium	Agr. Medium

2.13.4. Linking CEC exposure and individual-level effects

The individual-level responses of walleye to CEC mixtures are unknown, so we modeled them after the results of experiments involving fathead minnow (*Pimephales promelas*) Egg production declined by up to 81% when fathead minnows were exposed to the urban mixture (Schoenfuss et al., 2020) and by up to 33% when exposed to the agricultural mixture (Cipoletti, 2018). However, in both cases the gonadosomatic index (GSI) was not significantly impacted. These results suggest that exposure to CECs reduced egg production by impacting oocytes during final maturation and ovulation. Based on this laboratory work, our model assumed the same response intensity to CEC exposure in walleye (81 and 33% reduction of egg production), by impacting the egg maturation process (*i.e.*, increasing the cost of converting reproductive energy into eggs).

Although it is recommended to use Toxicokinetic-toxicodynamic (TK-TD) models to simulate individual-level effects of exposure to toxicants over time, especially when exposures are variable (Ashauer and Escher, 2010), the appropriate data were lacking for our study. Fish in the fathead minnow laboratory toxicity study were exposed to a constant concentration of CECs for their entire lifespan, so internal and external CEC concentrations had likely reached equilibrium, while wild fishes are exposed to space- and time-varying levels of CECs. Moreover, we scaled exposure level to effect level because the stoichiometry of lab-tested mixtures was not always constant between levels of exposure. Without appropriate data to simulate how internal concentrations of CECs adjust to different exposure conditions, we used a simple approach to consider the influence of temporally variable exposure (e.g., as a result of differences in TK of chemicals in the CEC mixture) by simulating three exposure durations prior to reproduction. For each exposure duration,

we considered that the individual-level effect at time t was equal to the average individual-level effect associated with the exposure levels encountered during the exposure duration. Averaging over the last 5 days corresponded to fast toxicokinetics, *i.e.*, a relatively rapid attainment of equilibrium between internal and external CEC concentrations. Correspondingly, the 15- and 30-day exposures represented moderate and slow toxicokinetics, respectively. This approach is also in accordance with the mode of action of the CEC mixtures (impacting egg production but not accumulated energy for reproduction) and timing of egg maturation and ovulation of walleye. Walleye GSI rises during autumn with the onset of exogenous vitellogenesis and a corresponding increase in mean oocyte diameter (Malison and Held, 1996). They do not begin final maturation until just before spawning (Malison and Held, 1996).

Our method accurately approximates a one-compartment toxicokinetic model with same uptake and elimination rates (section 6.3), but is probably specific to our case because CECs affected egg production, not the growth or survival of eggs or other life stages. Consequently, only the recent exposure needed to be taken into account. Also, the CEC mode of action in our study did not impact the size distribution of reproducing adults (egg production is linked to adult size) or their annual exposure history (no impact on movement behavior).

2.14. Shape and temperature corrections

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

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

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

$$sc = \frac{L_j}{L_b} \text{ if } U_H > U_H^j$$

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

The second modification is the multiplication of the assimilation rate by the correction for temperature, $c(T)$. Every energy flow is influenced by this modification because temperature affects all metabolic rates (see Table [3](#)).

3. Data evaluation

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

Summary:

Here we provide information on the type of data that were used to parameterize the individual properties. This pertains mostly to the parameterization of the DEB model. The parameters related to population properties are fairly uncertain, and model results are sensitive to them. They were calibrated to represent demographic patterns found in the literature.

3.1. DEB parameterization

This section presents a model representing the full life cycle of walleye (*Sander vitreus*). This model describes the growth, reproduction and maintenance at the individual scale based on the Dynamic Energy Budget (DEB) theory (Kooijman, 2010). It is a DEB model with type M acceleration, which means that metabolism accelerates during a part of the life cycle. This model is a one-parameter extension of the standard DEB model.

This section is organized as follows: First, we briefly describe the standard DEB model and the type M acceleration. Then, we briefly introduce our parameter estimation method. Finally, we present the data that were used in this parameter estimation, and compare model outputs to empirical data.

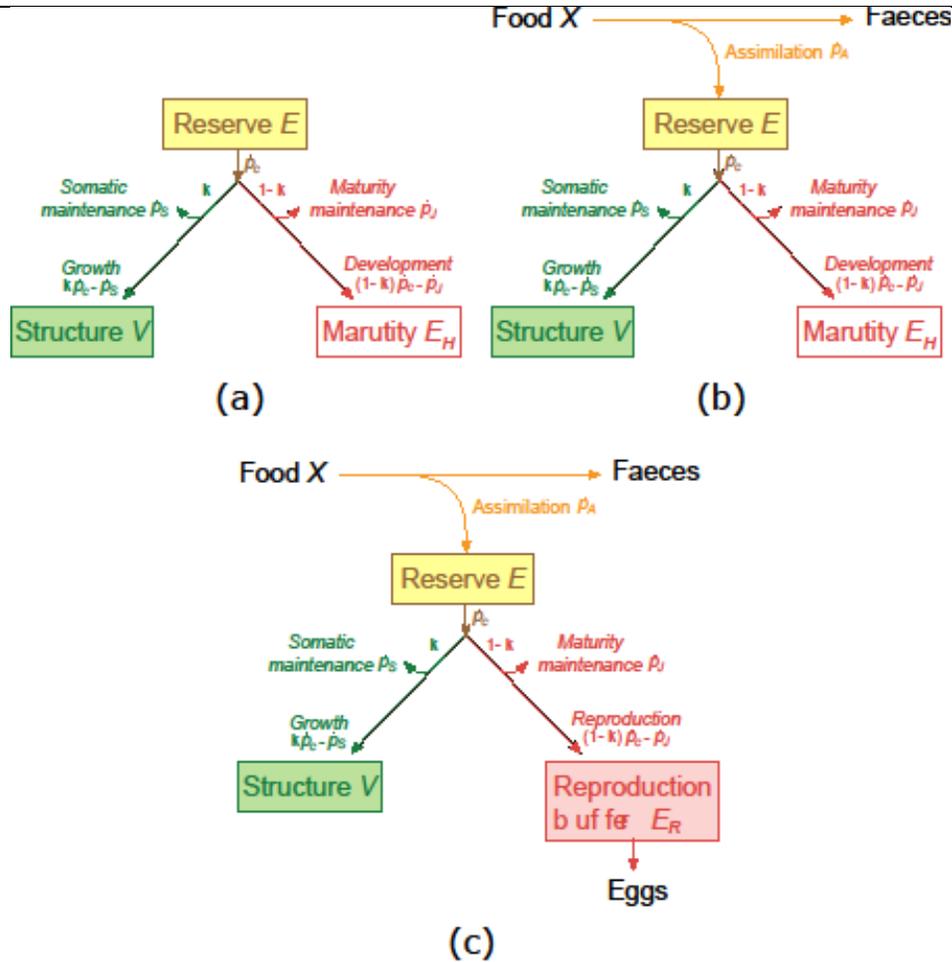


Figure 7: Schematic representation of the three life stages of the standard DEB model. (a) An embryo uses reserve to grow and develop. (b) At birth, a juvenile starts exogenous feeding, and (c) at puberty, an adult starts allocating energy to reproduction.

3.1.1. Methods

The DEB model:

The standard DEB model describes the entire life cycle of an organism through three life stages (Figure 7). This paragraph gives a short presentation of DEB theory; see Kooijman (2010) for more details.

Here, we introduce state variables and fluxes (Table 3) from a life cycle point of view. In DEB theory, life cycle is described in three stages, and the transition from one stage to the next depends on a state variable, called maturity E_H .

The organism does not feed during the first (*i.e.*, embryonic) life stage, so the flux for assimilation \dot{P}_A is zero. The organism uses the available energy in its reserve compartment (E), with a fixed allocation rate (κ), to grow in structure (V). A proportion κ of the mobilization flux \dot{P}_C goes to the structure (V) for its maintenance \dot{P}_S and its growth which thus equals $\kappa \dot{P}_C - \dot{P}_S$. What remains of the mobilization flux (*i.e.*, $(1 - \kappa) \dot{P}_C$) is allocated to maturity E_H for maintenance (\dot{P}_j) and maturity increase. The resultant increase in maturity is given by $(1 - \kappa) \dot{P}_C - \dot{P}_j$. The maintenance of the structure (\dot{P}_S) depends on temperature through the Arrhenius relationship ($c(T)$), and also on its surface and/or volume. The maintenance of maturity depends on temperature, with the same Arrhenius relationship ($c(T)$), and on the amount of maturity.

The second stage is the juvenile stage. It begins when the organism is able to feed exogenously, *i.e.*, when maturity has reached a fixed threshold (E_H^b). Therefore, the assimilation flux \dot{P}_A is no longer zero. The assimilation depends on temperature, environmental food condition ($f(X)$) and the structural surface of the organism. The assimilated energy supplies the reserve compartment from which energy is allocated to growth or maturation, still with the same κ allocation rule.

The organism enters the adult stage when maturity has reached a fixed amount of energy (E_H^p). From this moment, named puberty, energy that was previously allocated to maturity is now allocated to reproduction. Nevertheless, maturity maintenance continues, and the allocation rate to growth or maturity/reproduction is still the same.

The metabolic acceleration occurs between birth and a moment defined as metamorphosis (when maturity reaches a threshold value (E_H^j), before puberty) which might or might not correspond with changes in morphology.

Parameter estimation:

The parameters of the standard DEB model were estimated using the co-variation method (Lika et al., 2011). Parameter values are reported in Table 11. This method uses the simplex method to simultaneously minimize the weighted sum of squared deviations between model predictions and observations for a considerable number of data sets. Two types of data are used: univariate data and zero-variate data. Univariate data consist of sets of time-series observations, like growth versus time. The zero-variate data are composed of pseudo-data and real-data. Pseudo-data are parameter values that are supposed to be highly conserved among all the taxa, so that they serve as a kind of prior knowledge about the organism. Real data are empirical observations such as maximum length and weight at birth and/or puberty and/or death, lifetime, and number of eggs produced. A weight coefficient can be assigned to each uni-variate

data set, and both kinds of zero-variate data set. We assigned the same weight to every data set in the present study.

We accounted for sexual dimorphism by introducing different values (and therefore new parameters) for some maturity thresholds. We introduced sex-specific thresholds for metamorphosis (E_H^{jm}) and puberty (E_H^{pm}) for males that have different values than females. Another way to account for sexual dimorphism is to introduce sex-specific zoom factors such that males and females have different maximum assimilation rates ($\{P_{Am}^i\}$) and half-saturation ($K = \frac{\{J_{XAm}\} \mu_X}{\{E_m\}}$) coefficients. We did not opt for this solution because we are unaware of any evidence that feeding rate is sex-specific in walleye, and did not want to introduce a sex difference in the ability to compete for food because we intend to use this DEB model to describe the energetics of agents in an Individual-Based Model.

Table 11: Parameters of the standard DEB model for walleye (*Sander vitreus*).

Name	Notation	Dimension	Value
Primary parameters			
Volume-specific somatic maintenance rate	$[p_M]$	J.cm-3. d-1	41.2
Surface-area-specific somatic maintenance rate	$\{p_T\}$	J.cm-2. d-1	0
Volume-specific cost for structure	$[E_G]$	J.cm-3	5219.7
Energy conductance	\dot{v}	cm.d-1	0.0392
Fraction reserve used for growth + maintenance	κ	wd	0.4565
Maturity maintenance rate coefficient	$\dot{\kappa}_j$	d-1	0.002
Maturity threshold at hatching	U_H^h	J	4.37
Maturity threshold at birth	U_H^b	J	7.30
Maturity threshold at metamorphosis	U_H^j	J	138.6
Maturity threshold at metamorphosis for male	U_H^{jm}	J	80.06
Maturity threshold at puberty	U_H^p	J	505150
Maturity threshold at puberty for male	U_H^{pm}	J	130990

Fraction of the reproduction buffer fixed into eggs	κ_R	wd	0.95
Surface-area-specific searching rate	$\{F_m\}$	l.cm-2. d-1	6.5
Auxiliary and compound parameters			
Digestion efficiency of food to reserve	κ_X	wd	0.8
Arrhenius temperature	T_A	K	8000
Reference temperature	T_{ref}	K	293.15
Weibull aging acceleration	\dot{h}_a	l.d ⁻²	1.0399e-08
Gompertz stress coefficient	S_G	wd	0.0001
Zoom factor	z	wd	3.7391
Shape coefficient	δ_M	wd	0.1496

3.1.2. Results

Table 12: Real versus estimated data values used for parameter estimation of DEB model for Sander vitreus. Puberty is the start of investment into reproduction. To estimate age at puberty, we used the age at first reproduction minus the average value of spawning interval for males and females. We estimated length and weight at this age from literature growth curves.

Data (dimension)	Value	Source	Modeled
Age at hatching (d)	14	Nelson (1968)	14.92
Age at puberty for female (d)	730	Bozek et al. (2011)	713.4
Age at puberty for male (d)	547.5	Bozek et al. (2011)	528.3
Age at death (d)	7300	Bozek et al. (2011)	7300
Wet weight at birth (g)	0.031	Bozek et al. (2011)	0.0033
Wet weight at puberty for female (g)	134	Honsey et al. (2017)	157.8
Wet weight at puberty for male (g)	44	Honsey et al. (2017)	44.61
Wet weight at death for female (g)	2763	Honsey et al. (2017)	2799

Wet weight at death for male (g)	1605	Honsey et al. (2017)	1618
Length at hatching (cm)	0.65	Nelson (1968)	0.5918
Length at birth (cm)	0.9	Nelson (1968)	0.7011
Length at puberty for female (cm)	24	Bozek et al. (2011)	25.43
Length at puberty for male (cm)	16	Bozek et al. (2011)	16.69
Length at death for female (cm)	67	Bozek et al. (2011)	66.32
Length at death for male (cm)	54	Bozek et al. (2011)	55.24
Number of egg per day (#/d)	2055	Bozek et al. (2011)	883.2

Zero-variate data (Table 12) are accurately reproduced by the model. Puberty in DEB theory is defined as the start of investment in reproduction, whereas it is defined as the start of reproduction in the literature. Consequently, we estimated the age at puberty by subtracting the average value of spawning interval for males and females from their respective age at first reproduction. We estimated length and weight at puberty based on published growth curves (Figures 8, 9 and 10).

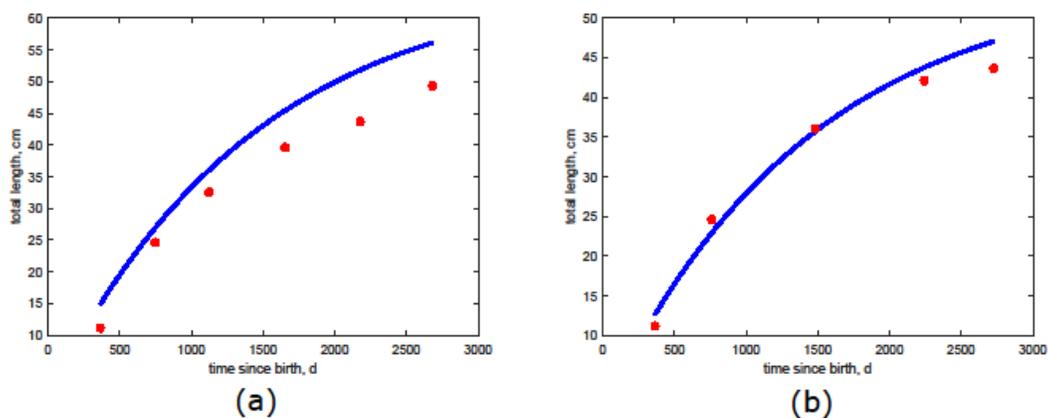


Figure 8: Model outputs versus length data for female (a) and male (b) *Sander vitreus*. Model outputs are the blue lines and data are the red dots. Data are extracted from Colby et al. (1979).

Univariate data include data on length over time (Figures 8 and 9), weight versus length (Figure 10), eggs versus length (Figure 11) and incubation time versus temperature (Figure 12).

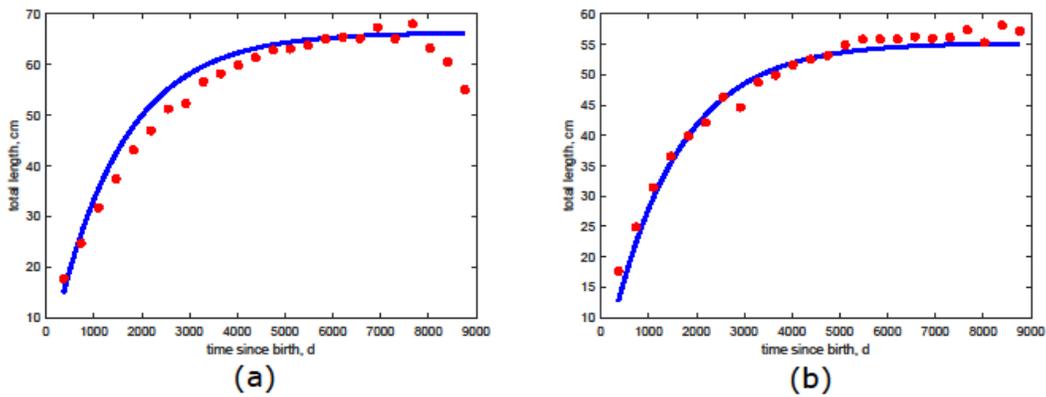


Figure 9: Model outputs versus length data for female (a) and male (b) *Sander vitreus*. Model outputs are the blue lines and data are the red dots. Data are extracted from Honsey et al. (2017).

The DEB model reproduced all the zero-variate data well (Table 5). Walleye exhibits sexual dimorphism. Female walleye grow larger in length and weight than male walleye, and start reproducing later. This is also accounted for in the model, and was accurately reproduced both for length (Figures 8 and 9) and weight (Figure 10).

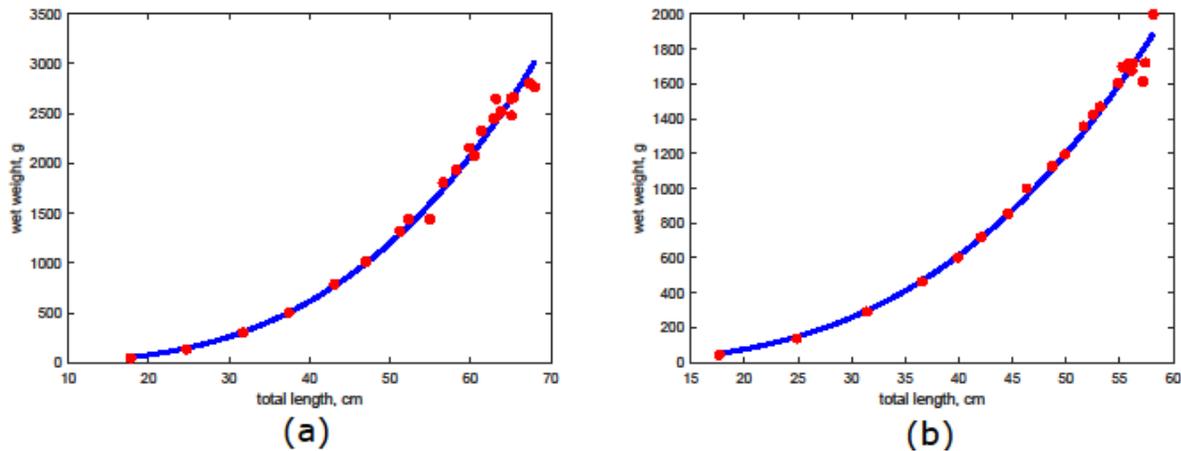


Figure 10: Comparison of model outputs and length versus weight data for female (a) and male (b) *Sander vitreus*. Model outputs are the blue lines and data are the red dots. Data are extracted from Honsey et al. (2017).

Female reproduction (egg number) as a function of length is also well reproduced by the model. Figure 11 shows data on reproduction at two food and temperature conditions in Lake Erie that are also well reproduced. Incubation time (time to hatch) as a function of temperature (Figure 12) is accurately

reproduced. The accurate reproduction of these data at different food and temperature conditions validates the realistic behavior of the model in different modeling contexts.

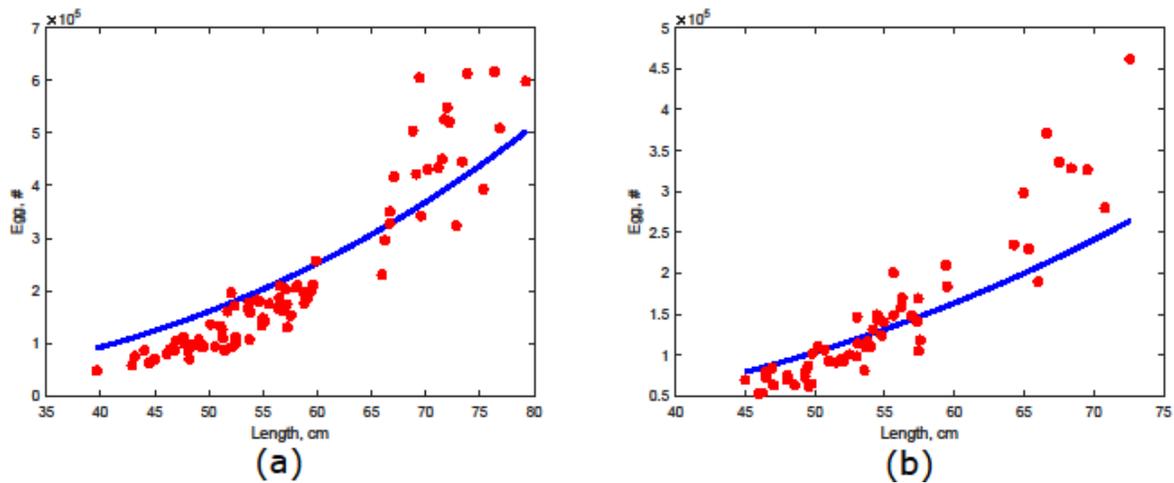


Figure 11: Comparison of model outputs and egg versus length data for East Erie Lake (a) and West Erie Lake (b) for *Sander vitreus*. Model outputs are the blue lines and data are the red dots. Data are extracted from Wolfert, (1969).

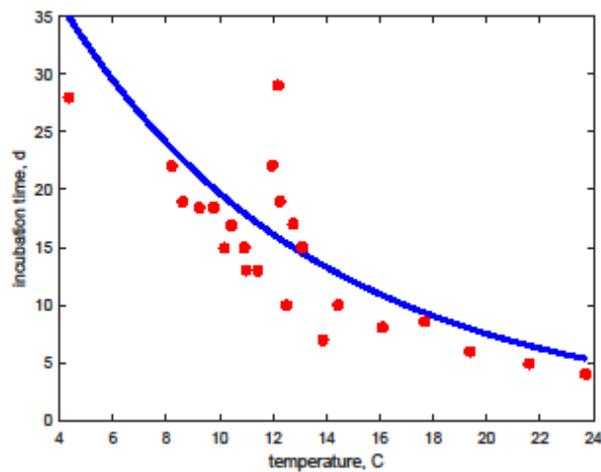


Figure 12: Comparison of model outputs and incubation time versus temperature data for *Sander vitreus*. Model outputs are the blue lines and data are the red dots. Data are extracted from Colby et al. (1979).

3.2. IBM calibration

We used walleye population data for Lake Erie from Nate et al. (2011) for Age-0 fish density (Figure 13), Age-4 and older fish density (Figure 14), PSD (Figure 15). Based on results showing that food-controlled populations exhibit a smaller population-level response to stressors than predation-controlled populations (Vaugeois et al., 2020), we selected high values for the intrinsic growth rate a_e ($J.J^{-1}.d^{-1}$) and the carrying capacities of the two food items, K_{E1} and K_{E2} ($J.m^{-2}$). a_e was fixed to 0.8, K_{E1} and K_{E2} to 50 and 400 respectively.

Our work took into account the uncertainty of the change kinetic of the individual-level effects in a varying CECs exposure regime. To do so, we established 3 toxicokinetic treatments for each of the agricultural and urban mixture exposure scenarios. In the first treatment, we used the last 30 days of exposure to calculate the average exposure-level of the organism at the moment of the reproduction. In the second and third treatments, we respectively used the last 15 and the last 5 days of exposure. Considering different time periods to calculate the average exposure-level, and thus the associated individual-level effect, resulted in different values at the moment of reproduction between the different treatments. As a consequence, we had to calibrate the model differently for each mixture type, and for each treatment for the urban mixture scenario. The values for each treatment and mixture type are reported in the Table 13, and discussed below.

Table 13: Predation related parameters for all Agricultural, Urban and intermediate mixture type scenarios.

Parameter	Agricultural mixture	Urban mixture	Urban mixture	Urban mixture	Intermediate mixture	Intermediate mixture	Intermediate mixture
		30 days	15 days	5 days	30 days	15 days	5 days
Annual cumulative egg and larvae survival rate to predation (wd)	0.00005	0.000055	0.000055	0.000058	0.000055	0.000055	0.000055
Annual cumulative juvenile survival to predation (wd)	0.35	0.35	0.3675	0.38	0.35	0.3675	0.3675
Annual cumulative adult survival rate to predation (wd)	0.7	0.735	0.735	0.735	0.735	0.735	0.735

Bozek et al. (2011) reported that survival from egg to age 1 is in the order of 0.01%. Consequently, we calibrated the model to have a similar survival rate from egg to the end of the larval stage. The annual egg and larvae survival rate ranges from 0.05% to 0.058%. This is in accordance with the lowest egg survival rate (7%) reported in Erie Lake in Roseman et al. (1996) multiplied by the hatching rate (78%) reported in Malison et al. (1990) and the daily survival rate of larvae of 0.85 reported in Mion et al. (1998). Juvenile cumulative annual survival rate ranges from 0.35 to 0.38, which is lower than the cumulative annual survival rate reported in Hayden et al. (2018) for older individual (0.6 to 0.7 for age 2 and older individuals). The cumulative annual adult survival rate ranges from 0.7 to 0.735 in accordance with the values reported in Hayden et al. (2018) (0.64 to 0.77 for age 5 and older).

Age-0 fish density (Figure [13](#)), age-4 and older fish density (Figure [14](#)), and PSD (Figure [15](#)) were all similar for all the toxicokinetic scenarios, and for both the agricultural and urban exposures.

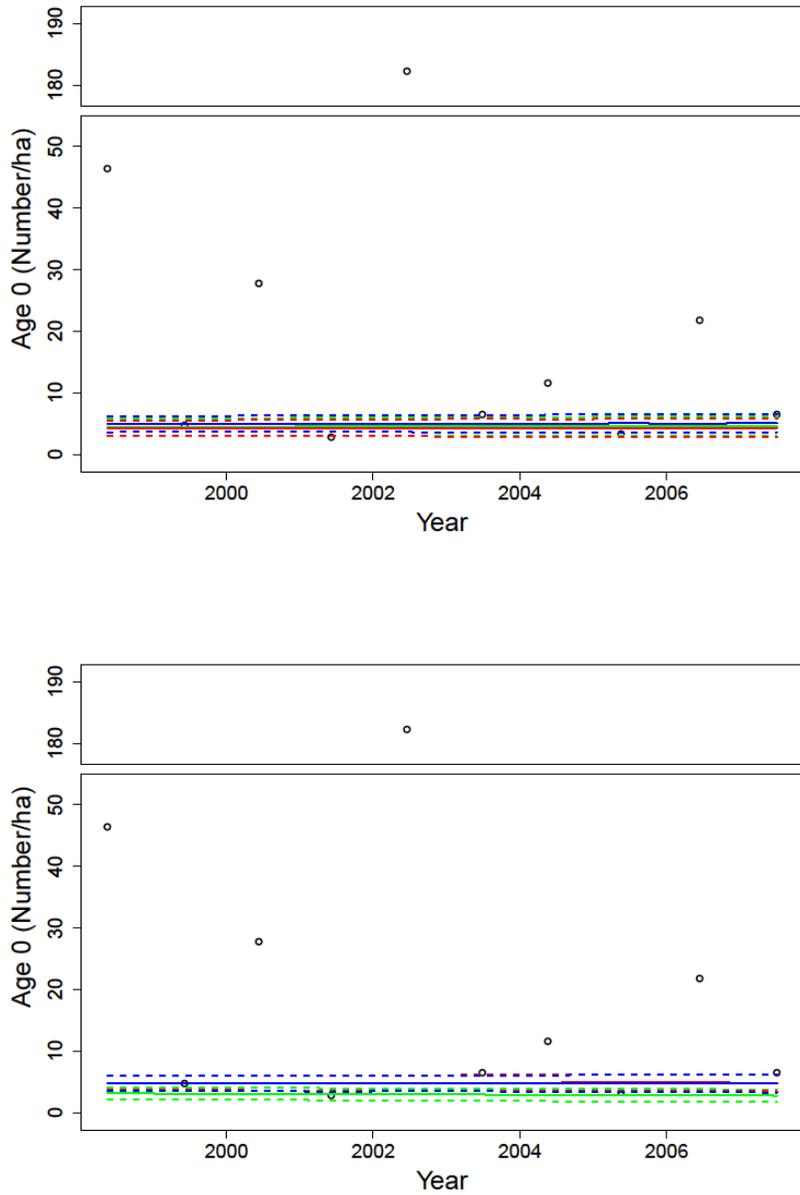


Figure 13: Density (number per hectare) of age 0 walleye in Lake Erie. Dots are data from (Nate et al., 2011). The continuous lines are the yearly average for 400 replicates of the agricultural (top panel) and urban (bottom panel) mixture simulations. Dotted lines are standard deviation in the 400 replicates. Red lines are for the 30 days treatment, Green lines for the 15 days treatments, and blue lines for the 5 days treatment.

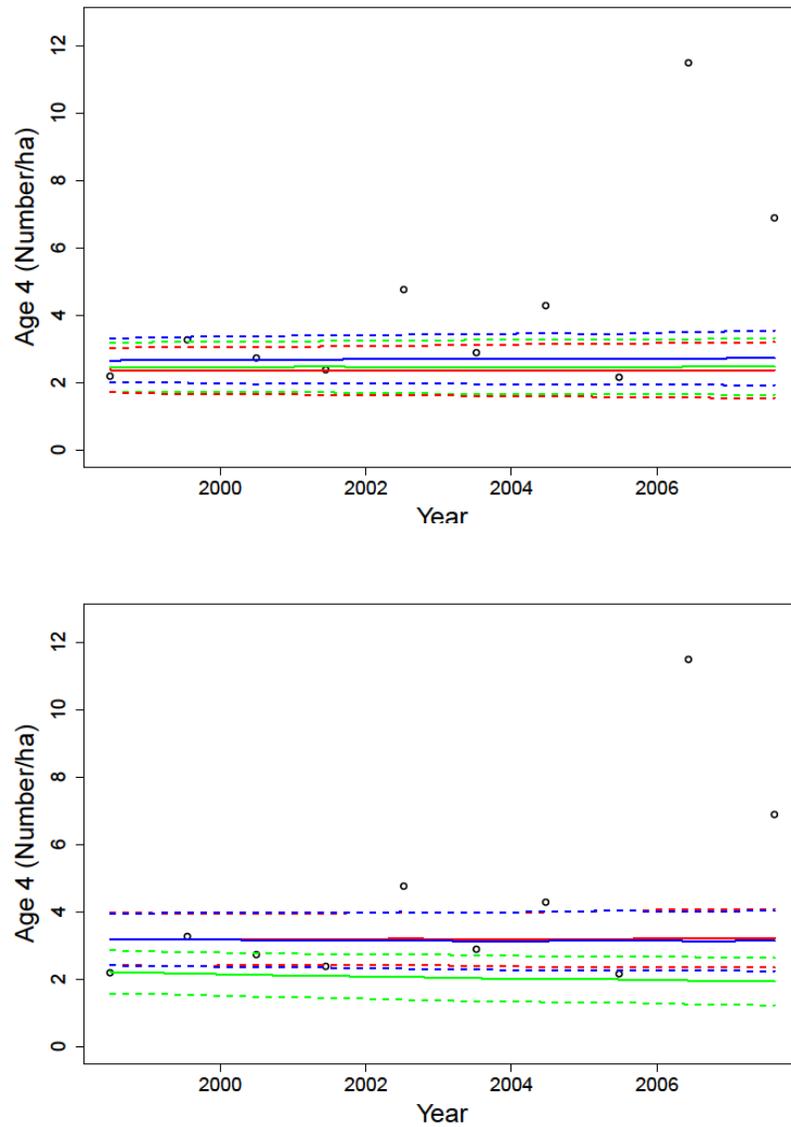


Figure 14: Density (number per hectare) of age 4 and older walleye in Lake Erie. Dots are data from (Nate et al., 2011). The continuous lines are the yearly average for 400 replicates of the agricultural (top panel) and urban (bottom panel) mixture simulations. Dotted lines are standard deviation in the 400 replicates. Red lines are for the 30 days treatment, Green lines for the 15 days treatments, and blue lines for the 5 days treatment.

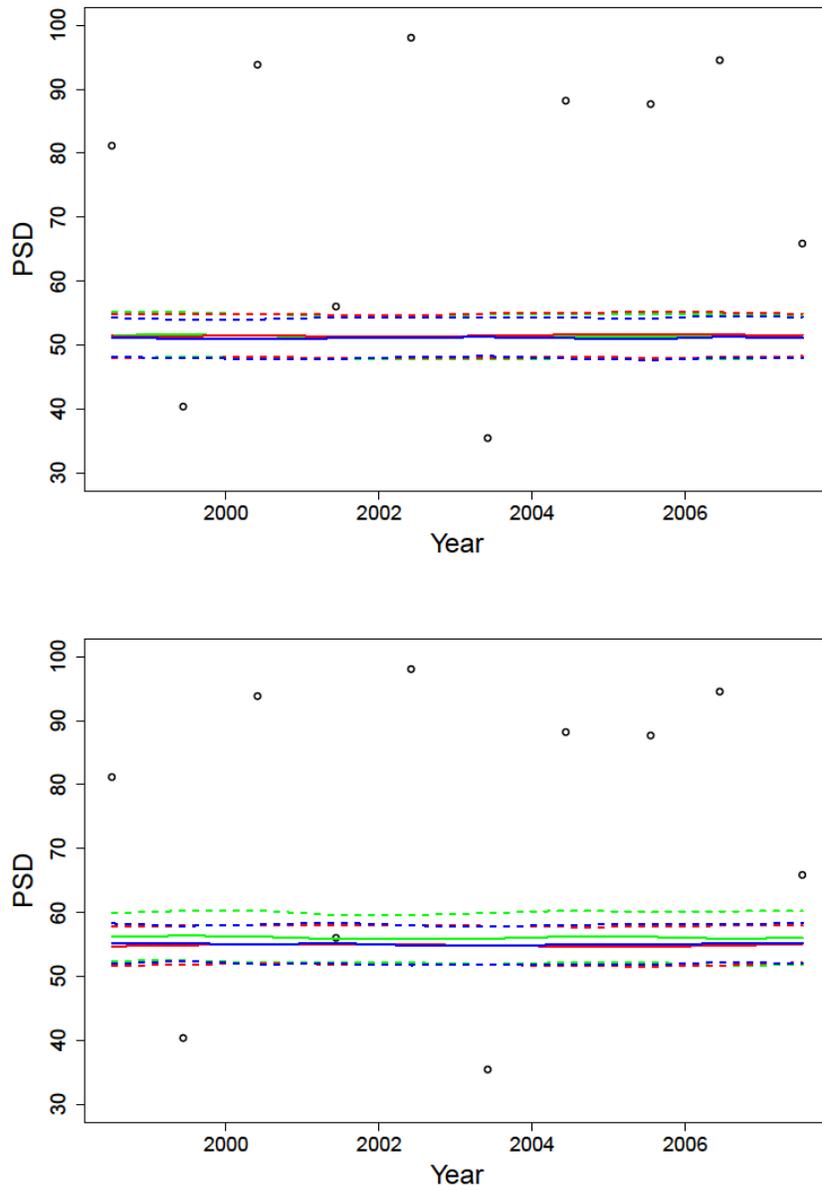


Figure 15: Proportional Stock Density for walleye in Lake Erie. Dots are data from (Nate et al., 2011). The continuous lines are the yearly average for 400 replicates of the agricultural (top panel) and urban (bottom panel) mixture simulations. Dotted lines are standard deviation in the 400 replicates. Red lines are for the 30 days treatment, Green lines for the 15 days treatments, and blue lines for the 5 days treatment.

4. Conceptual model evaluation

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

Summary:

Consideration of modeled metabolic processes was based on Dynamic Energy Budget theory. Fish movement, reproduction site selection and fidelity to this site were based on literature data. Effects of CECs on walleye were based on published results of effects on fathead minnow. Levels of exposure were based on literature data.

The conceptual model is based on DEB theory (see section [3.1.1](#)), which postulates how resources are assimilated and allocated to metabolic processes. It is based on first principles of conservation of energy, matter, isotopes and time, and follows strict assumptions about the way in which energy fluxes are distributed in the organism. This model was carefully parametrized for walleye based on published data (section [3.1](#)). The onset of adult migration into the river, reproduction site selection, and reproduction site fidelity were based on published observations (see sections [2.8.3](#) and [2.12.2](#), respectively). Effects of CECs on walleye were based on published data on fathead minnow (we discuss this point in the main paper), and exposure level per river zone were based on published data (see section [2.13](#)). The scheduling of processes and events is described in section [2.4](#).

5. Implementation verification

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

Summary:

Model implementation was verified in a series of tests to ensure that the code reproduced the concepts described in sections [2.4](#) and [2.5](#). Verification was performed using modeling platform tools for syntax checking, in addition to visual testing, print statements, stress tests, test programs, and code reimplementation.

Model code was tested to verify that the model behaves as expected and as planned. The model was implemented in Java, and parts were re-implemented using Matlab (MATLAB R2016b) or R (R Core Team 2017). All of these languages offer several tools that enable the developer to check whether the implemented syntax is correct.

Implementation testing was done on several levels:

1. Syntax checking. Syntax errors such as forgetting a bracket are immediately picked up by the software, and must be corrected before simulations are allowed to proceed. Run-time errors are not syntax errors, but represent events that the software cannot deal with. This, for instance, includes divisions by zero or producing numbers that are too large for storing. Even though run-time errors cannot directly pinpoint to the problem, they offer helpful directions and explanations of the issue.
2. Visual testing of model outputs. Visual testing was used to identify errors that are be unlikely to be detected soon, if ever, via other methods. Individual energy fluxes and properties (e.g., length, number of eggs, reproduction period, and migration pattern) and overall population dynamics have all been monitored to determine that the model behaves as expected. For instance, modeled fluxes have been controlled for equilibrium, the energy entering the organism being equal to the energy used and excreted by the organism. Food levels have been

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- adjusted to avoid frequent extinctions, and recruitment has been adjusted to avoid the death of too many adults by starvation.
3. **Print statements.** Print statements allowed for a visual check and manual calculation of the correct functioning of all sub-models. We programmed the model to print the value of some variables at different times to check that the model was behaving as expected. Basic examples are: writing the number of agents at every time step to check that they are actually dying and leaving the model; writing some particular energy values (such as energy at birth); writing the time of a specific event, *e.g.*, reproduction. Print statements were also used to locate issues such that they would have a role of markers in the code, *e.g.* if not printed, that meant that the code lines were not reached or a particular error was (not) made.
 4. **Stress tests.** Stress tests were performed using extreme values of parameters and comparing simulation outputs to expectations. For example, food availability or temperature were changed to study both individual- and population-level dynamics; reproduction-related parameters were shut off to check population dynamics.
 5. **Test programs.** In some cases, a separate, short program under simplified conditions was written to test a particular algorithm or procedure. For instance, the temperature implementation and calculation of the shape correction factor were initially developed in a secondary program.
 6. **Simulation experiments.** Several controlled simulation experiments were performed in which the model or its parts were simplified so that the outcome of each experiment could be predicted and verified. This includes, for example, the different mortality submodels.
 7. **Code reviews.** The code was peer-reviewed, *i.e.*, it was thoroughly compared with the written formulation of the model by one other scientist and with published DEB-IBMs.
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6. Model output verification

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

Summary:

Here we summarize how well the model recreates the individual-level input data. Population-level outputs was already evaluated in section [3.2](#). We also checked that the temperature input data were correctly implemented.

6.1. Individual scale

The Table [14](#) shows how the DEB-IBM reproduces the individual-level data used for the parametrization of the DEB model detailed in section [3.1](#). All data are correctly simulated. Female growth (Figure [16](#)) as well as male growth (Figure [17](#)) are also in accordance with the literature (section [3.1](#)).

Table 14: Modeled data with the IBM versus modeled data during the parameter estimation of DEB model.

Data (dimension)	Modeled with IBM	Modeled with DEB model	Percent difference (%)
Age at hatching (d)	17	14.92	12.2
Age at puberty for female (d)	736	713.4	3.1
Age at puberty for male (d)	545	528.3	3.1
Age at death (d)	7383	7300	1.1
Wet weight at birth (g)	0.0034	0.0033	3
Wet weight at puberty for female (g)	156.5	157.8	0.8
Wet weight at puberty for male (g)	44.38	44.61	0.5
Wet weight at death for female (g)	2804	2799	0.2

Wet weight at death for male (g)	1664	1618	2.8
Length at hatching (cm)	0.62	0.5918	4.5
Length at birth (cm)	0.72	0.7011	2.6
Length at puberty for female (cm)	25.36	25.43	2.8
Length at puberty for male (cm)	16.66	16.69	1.4
Length at death for female (cm)	65.89	66.32	0.7
Length at death for male (cm)	55.63	55.24	0.7
Number of egg per day (#/d)	912	883.2	3.6

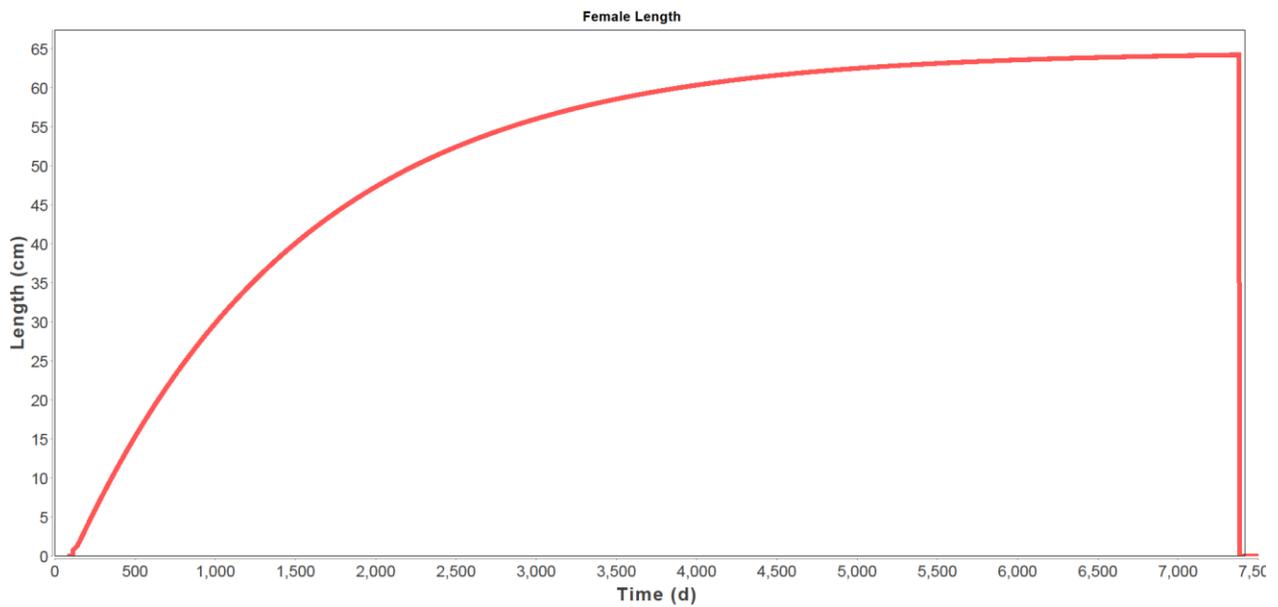


Figure 16: DEB-IBM output on female growth as function of time.

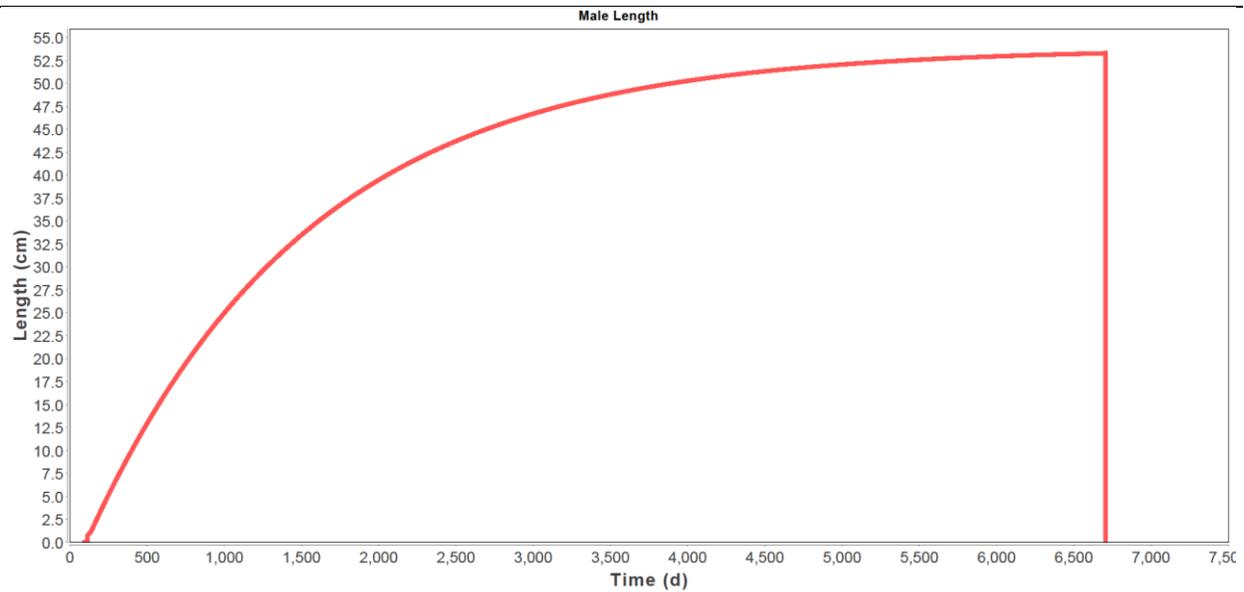


Figure 17: DEB-IBM output on male growth as function of time.

6.2. Population scale

Section [3.2](#) describes how we used population-level model output to calibrate our simulations. As showed in the Figures [13](#), [14](#) and [15](#), our population-level outputs are consistent with published data. The modeled spawning site fidelity rate (Figure [18](#)) is in accordance with the published value that was used for calibration (70% probability; Hayden et al. (2018)). Reproduction occurs from site 6 to 10, with a larger frequency at site 6 and 7 (Figure [19](#)), in accordance with observed eggs densities in the Maumee River (Schmidt 2016).

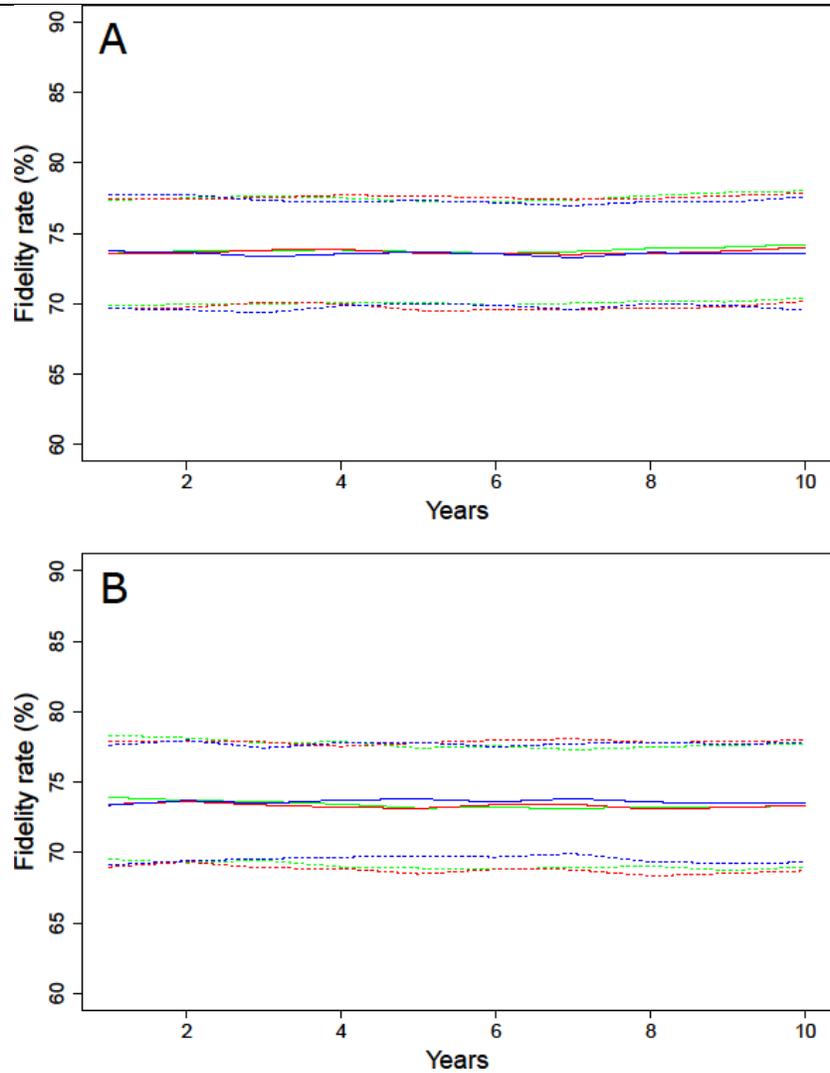


Figure 18: Spawning site fidelity rate. The continuous lines are the yearly average for 400 replicates of the urban (panel A) and agricultural (panel B) mixture simulations. Dotted lines are standard deviation in the 400 replicates. Red lines are for the 30 days treatment, green lines for the 15 days treatments, and blue lines for the 5 days treatment

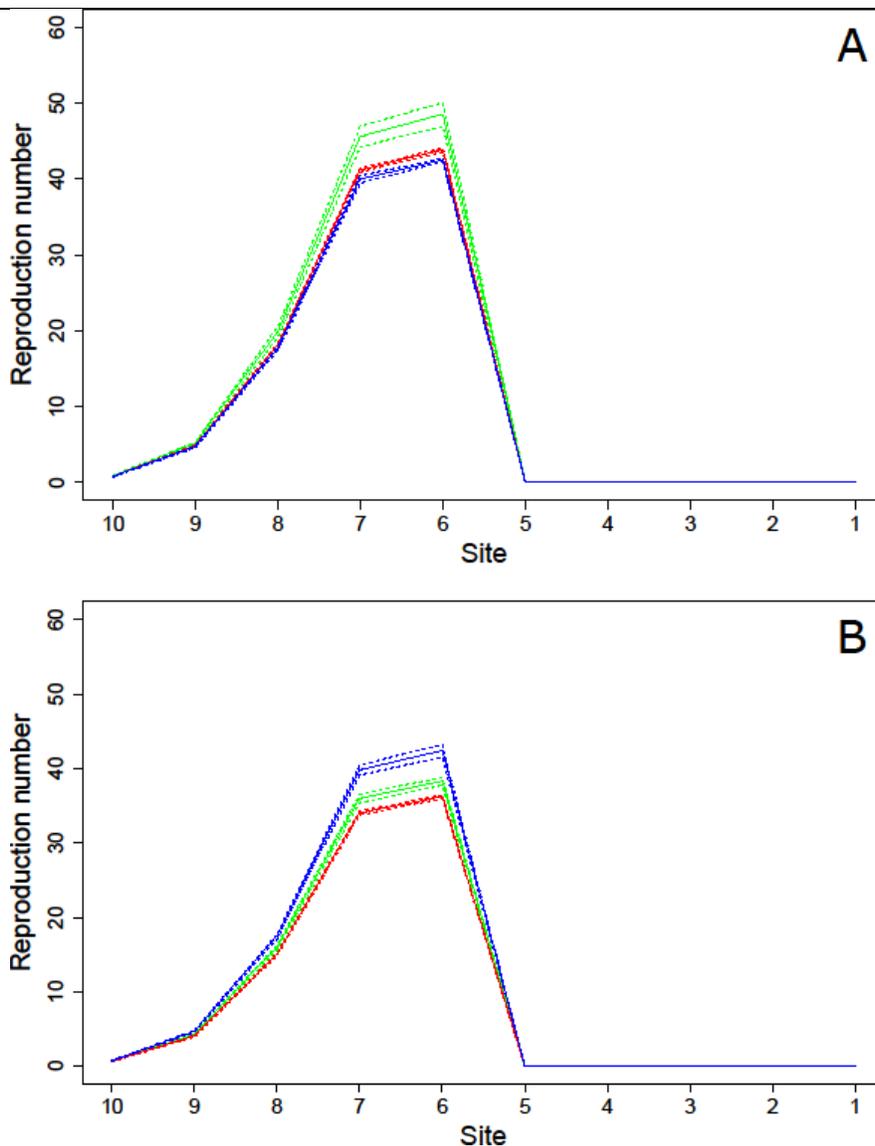


Figure 19: Reproduction per river site. The continuous lines are the yearly average for 400 replicates of the urban (panel A) and agricultural (panel B) mixture simulations. Dotted lines are standard deviation in the 400 replicates. Red lines are for the 30 days treatment, green lines for the 15 days treatments, and blue lines for the 5 days treatment

6.3. Toxicokinetic approximation

We implemented a TK sub model to assess and compare the goodness of our toxicokinetic approximation. We used the following, one-compartment TK model (Landrum et al., 1992):

$$\frac{dC_{Int}}{dx} = k_u \dot{C}_{Ext} - k_e \dot{C}_{Int},$$

where C_{Int} is the internal concentration (amount/mass), C_{Env} is the concentration in the water (amount/volume), and k_u in and k_e out are the uptake rate constant (volume/mass/time) and the elimination rate constant (volume/mass/time), respectively. Under the simplifying assumption that $k_u = k_e$, the model can be write as:

$$\frac{dC_{Int}}{dx} = k_a \dot{(C_{Ext} - C_{Int})},$$

where k_a is an adjustment coefficient (volume/mass/time) describing how quickly equilibrium between environmental and internal concentrations is reached. Dilution by growth was not accounted for in the model because the impacted organisms were adults. In our model, we associated locations to different mixture levels and types, and used laboratory data to link exposure levels to individual-level effects. However, we do not have data on internal concentration of toxicants in fish, and the stoichiometry of chemical in the different levels of mixture was not always constant. Consequently, we hypothesized that effect level was linearly proportional to exposure level.

We simulated the effectiveness of the whole watershed mitigation strategy and the single site mitigation strategy for sites 7 and 8, for the 3 toxicokinetic scenarios (fast, moderate and slow) under urban exposure. For fast toxicokinetics, we used a k_a value of 0.35. For moderate and slow, we used values of 0.15 and 0.04, respectively. Figure [20](#) shows that our method to represent toxicokinetic is a good approximation of a one-compartment TK model with identical uptake and elimination rate.

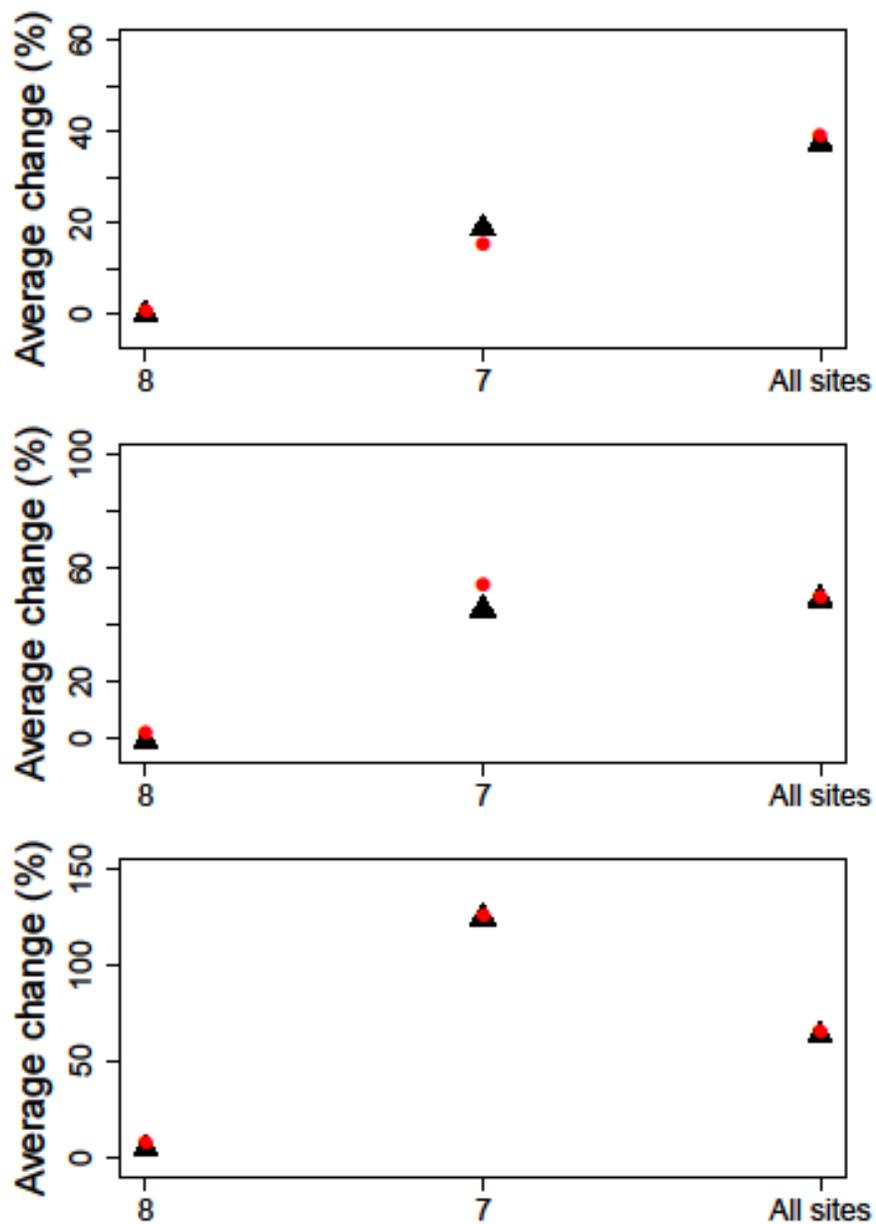


Figure 20: Mitigation effectiveness simulated with the approximation method presented in this study (black triangles) versus mitigation effectiveness simulated with the one-compartment TK model (red circles) for slow (upper panel), moderate (middle panel), and fast (lower panel) toxicokinetics.

7. Model analysis

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

Summary:

In this section, we justify the selection of 400 replicates and present the results of sensitivity analysis.

7.1. Number of replicates

We selected the number of replicates to be 400 because the value of the average population size over the last five years prior to start of mitigation was stable from 300 to 400 replicates (Figure 21).

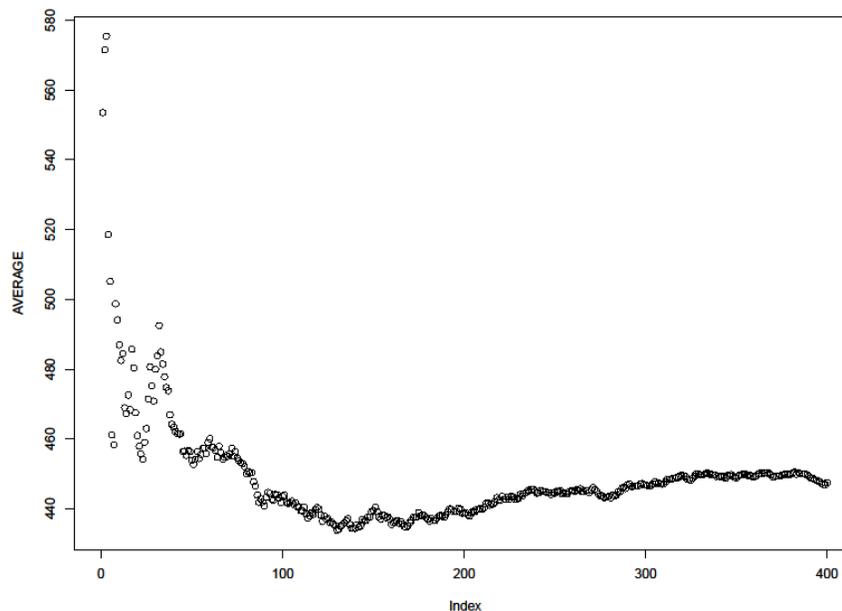


Figure 21: Average population size over the last five years prior to start of mitigation (y-axis) versus number of replicates (x-axis).

7.2. Sensitivity analysis

The aim of our study was to estimate the effectiveness of two mitigation strategies under multiple scenarios. In this section, we present the results of a sensitivity analysis that considered a $\pm 10\%$ variation of DEB parameter values. The changes in effectiveness of the whole watershed was calculated as

$$\Delta Obs = \frac{\overline{Obs} - \overline{Obs_{ref}}}{\overline{Obs_{ref}}} * 100,$$

where $\overline{Obs_{ref}}$ is the average effectiveness of whole watershed mitigation of 400 replicates with the original set of parameters, and \overline{Obs} is the average effectiveness of whole watershed mitigation of 400 replicates with a modified set of parameters ($\pm 10\%$ on the value of one parameter). Both were run under the agricultural mixture exposure with fast toxicokinetics. This analysis of sensitivity incorporates both the sensitivity of population dynamics and the sensitivity of the response to stressor. Results show that effectiveness of whole watershed mitigation is sensitive to changes in energetic parameters, especially when increasing z , \dot{v} , κ , $[E_G]$, E_H^p , E_H^{pm} and T_A ; or decreasing κ , $[P_M]$, $[E_G]$, E_H^b and E_H^j . κ is the most sensitive parameter which is normal because it is strongly correlated with eggs production and, consequently, to population recruitment.

Table 145: Sensitivity analysis of whole watershed mitigation effectiveness for $\pm 10\%$ variation of DEB parameters. $\Delta Effectiveness$ is expressed as a percentage difference from the mitigation effectiveness (12.88%) estimated in the study.

Symbol	Values	$\pm 10\%$ values	$\Delta Effectiveness$ (%)
z	3.739	4.113; 3.365	-35.14; 14.99
$\{F_m\}$	6.5	7.15; 5.85	20.04; 5.13
\dot{v}	0.03923	0.04315; 0.03530	51.38; 19.34
κ	0.4565	0.5021; 0.4108	-45; -68.4

$[P_M]$	41.199	45.319; 37.079	9.54; 41.19
$[E_G]$	5220	5740; 4700	-28.25; 29.79
E_H^h	4.3679	4.805; 3.931	7.51; -14.82
E_H^b	7.299	8.028; 6.569	5.42; -36.98
E_H^j	139	152; 125	-4.37; -30.39
E_H^p	505000	556000; 455000	28.81; -3.98
E_H^{jm}	80.059	88.065; 72.053	-5.31; 15.03
E_H^{pm}	131000	144000; 118000	32.51; -4.53
δ_M	0.1495	0.1645; 0.1346	17.25; 14.96
T_A	8000	8800; 7200	-20.23; 5.88

8. Model output corroboration

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

Summary:

Our model outputs regarding the efficiency of the different mitigation strategies have not been compared to independent data. Model outputs on individual growth and reproduction, and outputs on population structure and density, were all realistic compared to literature data.

Our model is based on the strong assumptions of DEB theory, and on published data from multiple individual- and population-level studies. In this study, we proceeded to a comparative assessment of different management strategies. We aimed at identifying which data are the most important to consider for different management strategies. As such, we were more interested in the qualitative differences than in the quantitative differences. Nevertheless, the population density observed during recovery are realistic when compared to independent historical stock of walleye in the Erie Lake (Dippold et al., 2020).

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