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Dietary bioaccumulation of persistent organic pollutants in the common sole *Solea solea* in the context of global change. Part 2: Sensitivity of juvenile growth and contamination to toxicokinetic parameters uncertainty and environmental conditions variability in estuaries

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Abstract :

The amount of potentially toxic chemicals in a fish depends on various environmental factors, such as temperature and feeding ecology, which can be affected by Global Changes (GC). The main objective of the present work was to study the relative influence of temperature, food quality and food availability on the growth and contamination of juveniles of common sole (Solea solea), a marine flatfish species known to be a relevant indicator of the nursery quality. It focuses on two Persistent Organic Pollutants (CB153 and L-PFOS) of legacy and emerging concern, respectively. To achieve this, we used a toxicokinetic (TK) model in which toxicant flows are mechanistically predicted using a bioenergetic model based on the Dynamic Energy Budget (DEB) theory. This modelling framework was applied to juvenile sole from the Gironde estuary (SW France) and allows accounting for the influence of environmental conditions on fish biological processes involved in toxicant fluxes. To compare their respective influence on model predictions of age, length, and contamination at puberty, we included in a global sensitivity analysis: (1) environmental variability gathered from literature for this particular estuary and (2) TK parameters (i.e. assimilation efficiency AE and elimination rate) variability and uncertainty gathered from literature about each contaminant but for different fish species and experimental conditions. Then, model predictions were confronted to fish contamination measurements from the Gironde Estuary with different combinations of TK parameter values from literature. Results highlighted a key role of diet composition on fish contamination and growth while water temperature only affected growth. It stressed the need to focus on GC impact on benthic communities and their consequences on juvenile fish diet for future work on GC scenarios. Furthermore, for both chemical, the range of variability of TK parameters from experiments led to underestimated fish contaminations. The best model fits were obtained using TK parameter values from model applications: from Mounier et al. (n.d.) for CB153 (Solea solea, experiment, AE=0.8 and =0

d−1) and from de Vos et al. (2008) for PFOS (food chain of the Western Scheldt estuary, The Netherlands, AE=0.8 and =0.8 10−2.d−1).

Highlights

► Sole DEB model is coupled with a one-compartment TK model. ► Temperature, diet, and prey contamination are highly variable in estuaries. ► Juvenile sole growth and contamination are sensitive to these factors. ► In particular, diet composition is the major influencing environmental factor. ► Uncertainty in TK parameters has a strong influence on sole contamination variance.

Keywords : Gironde estuary, Solea solea, DEB model, TK model, CB153, PFOS, sensitivity analysis

1. Introduction

Bioaccumulation is a fundamental process in environmental toxicology because it controls the amount of potential toxicants in individual organisms (Arnot and Gobas, 2004). Thus, predicting chemical body burdens is important to assess ecological adverse effects (van der Oost et al., 2003). The observed contamination levels of organisms are the result of different contaminants inflows and outflows related to 4 main processes: uptake, internal distribution, biotransformation and elimination (Ashauer and Escher, 2010). These fluxes themselves depend on several factors (Ashauer and Escher, 2010; Grech et al., 2017): (1) the contaminants physicochemical properties and structure, (2) the metabolic capacities of the species in question (feeding rate, respiration and biotransformation capacity) and (3) the individuals physiological state depending on their life stage and environmental conditions they have experienced (e.g., environmental contamination, temperature or diet). Disentangling and quantifying the relative importance of chemical, environmental and physiological factors underlying this observed variability of individual contamination levels remains a major challenge that is difficult to address by conventional statistical approaches.

In this context, the use of a mechanistic framework for modelling toxicokinetic (TK) processes is required to predict the evolution of toxicants bioaccumulation dynamics within the frame of Global Changes. More specifically, there is a need to develop mechanistic models disentangling the relative effect of ecological, physiological and biochemical characteristics, and environmental conditions on internal individual concentrations (Grech et al., 2017). Mechanistic toxicokinetic (TK) models aims at predicting organisms' contamination by modelling uptake and clearance contaminants flows according to biological flows. In most cases, these biological flows are considered to be constant and predicted organisms' contamination is given at steady state. This approach is the simplest one and is useful to compare bioaccumulation between chemicals or species, but it is not adapted to fluctuating environmental conditions (Ashauer et al., 2006). To address this issue, some TK models have been developed within the conceptual framework of the Dynamic Energy Budget (DEB) theory (Kooijman, 2010) to predict consequences of environmental changes (e.g., temperature, food quality or food availability) on biological processes that control chemical fluxes (see TK models using sub-model based on DEB theory: Bodiguel et al., 2009 & Eichinger et al., 2010 for one-compartment TK models, and Grech et al., 2019 for a physiologically-based toxicokinetic model). The implementation of a DEB-TK model was of interest to study the influence of the environment on the internal concentrations to implement, in perspective, a DEBtox approach linking contamination levels and potential adverse effects at the individual level (DEBtox models, see Jager and Zimmer, 2012; Kooijman and Bedaux, 1996). One of the main strengths of the DEB theory is that it allows the modelling of toxic effects on growth, reproduction, and survival, in a consistent and well-documented framework (see for instance Baas et al., 2018, for a review on the use of DEB models in ecological risk assessment).

Persistent Organic Pollutants (POPs) are of particular interest when studying bioaccumulation as they are characterised by their persistence in the environment, their toxicity, and their high bioaccumulative and long-range transport potentials. Polychlorinated biphenyls (PCBs) are compounds from a historical family of POPs. Banned decades ago, they are still found in all environmental compartments and their bioaccumulation has long been studied. Contrary to PCBs, Perfluoroalkylated Substances (PFASs) are of emerging interest and their ecodynamics is still relatively poorly known, especially in aquatic environments (Houde et al., 2006; Munoz et al., 2017a; Xiao, 2017). A better understanding of contaminant transfer processes in aquatic food webs, and their controlling factors, is required to better assess the environmental and health risks associated with the presence of these xenobiotics.

Among hydrosystems, coastal and estuarine ecosystems contribute greatly to the economic importance of coastal marine environments (Costanza et al., 1997). For instance, numerous marine fish species spend their juvenile phase in estuarine nursery grounds (Beck et al., 2001; Able, 2005).

This phase of their life cycle during which the individuals reach puberty (i.e., defined as the start of energy allocation to reproduction) is highly critical for the fitness of the population (Beck et al., 2001; Able, 2005; Rochette et al., 2010). However, physicochemical factors of estuarine essential habitats are naturally highly variable (e.g., Elliott & Hemingway, 2002; Lobry et al., 2003) and also particularly affected by anthropogenic pollutions, especially POPs (e.g., Budzinski et al., 1997; Matthiessen and Law, 2002; Munoz et al., 2019). Both stress sources can affect juvenile survival, growth and health (Gilliers et al., 2004) and consequently population dynamics. Organic contamination has already been related to nursery dysfunction (e.g., Courrat et al., 2009; Gilliers et al., 2006a, 2006b). In particular, growth rates and abundance of juvenile common sole (*Solea solea* L.) from several nursery areas along the French coast were found to be highly correlated with their level of chemical pressure (Amara et al., 2007; Gilliers et al., 2006b). The common sole is thus considered as a relevant model species to study the quality of coastal and estuarine nursery areas in Western Europe.

The Gironde estuary (SW French Atlantic coast) appears to be a relevant case study to analyse the sensitivity of POPs bioaccumulation in juvenile common sole to several GC factors in nursery grounds. Indeed, the question of interactions between environmental changes and contaminations is highly topical in this particular area for at least three reasons. First, it is one of the largest European estuaries (Lobry et al., 2003), and thus, one of the main nursery ground for the Atlantic sole stock, which is one of the most economically important fish stock for the Bay of Biscay (Le Pape et al., 2003). Second, abiotic and biotic contamination has been studied for several years for PCBs (Bodin et al., 2014; Lauzent, 2018; Tapie et al., 2011) and more recently for PFASs (Munoz et al., 2017b, 2017a). Third, significant changes in the abundance of flatfish populations (Hermant et al., 2010; Pasquaud et al., 2012) and in the structure and functioning of the whole food web (Chevillot et al., 2016; Chevillot et al. 2019) in relation with strong modifications of physicochemical conditions (warming and salinization) were recently highlighted (Chaalali et al., 2013a).

In essence, the analysis in the present paper aims at determining which factors affected by GC have the highest influence on fish contamination, so as to better identify which ones are of particular interest to study future environmental changes. For this, we used a common sole DEB model (Mounier et al., submitted, this special issue) coupled with a one-compartment TK model to account for the influence of environmental conditions on biological flows, and thus on contaminant flows. Among these environmental conditions, water temperature (Chaalali et al., 2013a) and prey availability (Chevillot et al., 2019) are already affected by local and global modifications, and the composition of the sole diet is known to fluctuate with size, season and prey availability (Ballutaud et al., 2019; Pasquaud, 2006). Also, contamination of the environment and thus of prey is expected to change with the management of pollutant sources. The first objective was therefore to describe the sensitivity of juvenile sole growth and POP contamination to the highly variable environmental conditions of estuaries by means of a sensitivity analysis on DEB-TK.

In our study, we focused on CB153 (2,2',4,4',5,5' hexachlorobiphenyl) and L-PFOS (linear isomer of perfluorooctane sulfonate) as these compounds are the major ones in the natural environment for PCBs and PFASs, respectively. In addition to environmental variability, we included TK parameters variability and uncertainty in the sensitivity analysis on fish contamination. Indeed, TK parameters estimated values are also known to be highly variable between studies (e.g., for PCBs Kobayashi et al., 2011), which also complicates the prediction of fish contamination. Moreover, the uncertainty in these parameters for PFASs is high due to the scarce number of related studies. Finally, we compared DEB-TK predictions of fish contamination by CB153 and L-PFOS to measurements in juvenile sole from the Gironde estuary. This allowed assessing the realism of environmental and TK parameters used in modelling scenarios.

2. Materials and methods

2.1. General framework of the study

The general framework of this study relies on the coupling between a Dynamic Energy Budget (DEB) model and a toxicokinetic (TK) model on which a global sensitivity analysis (SA) was conducted to highlight to which TK parameters and environmental inputs of the DEB-TK affected by GC, model outputs of fish growth and contamination are the most sensitive.

The general articulation between data, model inputs, model coupling and model outputs used in the present paper is presented in Figure 1.

We studied the sensitivity of 4 model outputs: age at puberty, length at puberty, and internal contamination of fish when reaching puberty, for each of the two contaminants (i.e. CB153 and L-PFOS). As some DEB parameters differed between sexes in the model used (i.e. maximum food assimilation rate and maturation threshold at puberty, see Mounier et al., submitted, this special issue), especially concerning food ingestion, and thus growth and contaminant ingestion, we differentiated these 4 predictions by sex, which led to 8 model outputs. We focused on the puberty stage considering that the growth phase in nursery grounds lasts until puberty, which may be the trigger event for fish to leave nursery grounds.

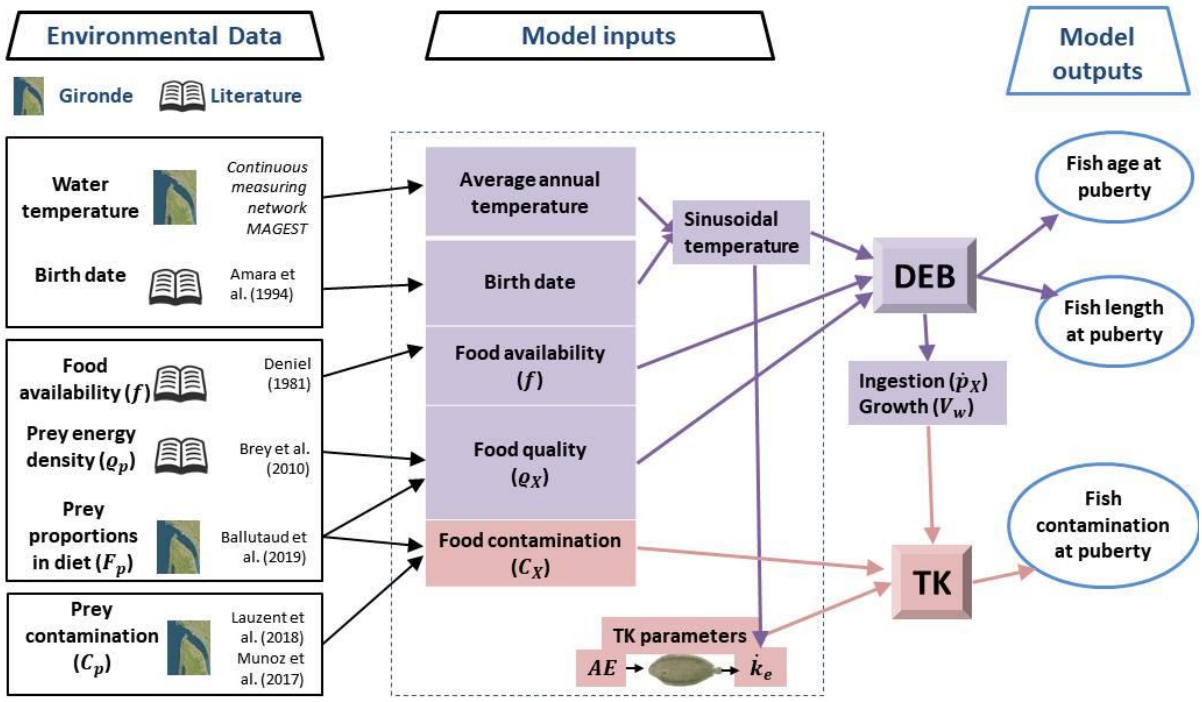

Figure 1 – Synoptic diagram of the general articulation between data, model inputs, model coupling and model outputs used in the present paper.

We used the most recent version of DEB model on *Solea solea* developed by Mounier et al. (submitted, this special issue) to study bioaccumulation under experimental and *in situ* conditions. The DEB parameters were calibrated for each sex of *S. solea* using the latest method for DEB parameters

estimation and a broad compilation of data from literature. For details on structure, parameters and calibration of the DEB model, we encourage the interested reader to refer to Mounier et al. (submitted, this special issue). In this materials and methods section, we only present the TK model developed considering both uptake and elimination fluxes, and how it relates with this DEB model. TK parameters and the environmental forcings of the DEB-TK model are listed.

To perform the sensitivity analysis of the DEB-TK model predictions, we have to know the range of variability associated to each model input (i.e., environmental inputs and TK parameters). To determine these ranges, environmental data from the Gironde estuary was gathered, when available, from previous field-based studies (see section 2.3). Our strategy to go from raw observations to simulation characteristics for model inputs is presented in section 2.4. Next, the principles of the global sensitivity analysis (SA) are presented. As the variability of the food contamination input relies on both diet composition and preys contamination variabilities, a complementary variance analysis was conducted on food contamination to disentangle the relative influence of these factors. For that purpose, a nominal value and a range of variability were defined for diet and prey contaminations.

On a final step, model predictions were compared with measurements of CB153 and L-PFOS contaminations in sole individuals from the Gironde estuary.

2.2. Toxicokinetic model

General principles

The mechanistic TK model presented below is a one-compartment kinetic model similar to the one presented by Arnot and Gobas (2004), who related bioaccumulation in an aquatic organism to 6 major routes of chemical uptake and elimination: dietary uptake, gill uptake, gill elimination, metabolic transformation, faecal egestion and growth dilution. The fundamental interest of this DEB-TK model is to consider non-constancy of these different chemical fluxes. We used the DEB theory (Kooijman, 2010) to predict the variation of chemical fluxes due to environmentally induced variations of metabolic activity, ingestion and growth dynamics. In the present model, no retroaction of contamination level on DEB parameters is implemented (i.e. no sub-lethal effects of the level of contamination are applied on fish metabolism). Furthermore, as we focus on the juvenile phase, the reproduction and thus the transfer to the gametes are not accounted for.

Model characteristics and equations

A more detailed version of TK equation is provided in the supplementary material (Appendix A). This DEB-TK model only considers dietary uptake, where food is a mix of different prey. Dietary uptake (Q_{in} in ng of contaminant) was related to food contamination (C_X in ng g_{food}^{-1} dw), dynamic ingestion rate predicted by the DEB model ($\dot{p}_X/\varrho_X$ in g_{food} dw per day, with $\dot{p}_X$ the food ingestion flux in J.d^{-1} and ϱ_X the food energy density in J.g_{food}^{-1}) and assimilation efficiency of chemical from food (AE in ng of chemical assimilated per ng of chemical ingested). AE is the TK parameter that describes the proportion of the chemicals ingested with food that is assimilated by the fish. This approach was used in Bodiguel et al. (2009) and Eichinger et al. (2010). In this approach, contaminants in the faeces represent the non-assimilated part of ingested contaminants.

Contaminant elimination was considered using a second TK parameter, the elimination rate ($\dot{k}_e$, in d^{-1}), that quantifies gill elimination, metabolic transformation, and faecal elimination (i.e., due to the chemical partition between the organism and the digested food in guts). We assumed first order elimination kinetics (i.e., no saturation). Also, as well as other metabolic rates, elimination rate is supposed to be affected by temperature (see Kooijman et al., 2009 for general theory, and Borgå et al., 2010 for an application of this principle to the study of climate change impacts on bioaccumulation in a food web). Thus, $\dot{k}_e$was defined as the daily diminution of the contaminant concentration in fish

(c in ng.cm^{-3}) at the reference temperature (T_{ref} =293 K²). It was then corrected by the actual temperature (T) following the same Arrhenius temperature correction factor as for all the DEB energetic fluxes (cT, dimensionless see Mounier et al., submitted, this special issue) following this equation:

$$cT = \exp\left(\frac{T_A}{T_{ref}} - \frac{T_A}{T}\right) \times \frac{1 + \exp\left(\frac{T_{AL}}{T_{ref}} - \frac{T_{AL}}{T_L}\right) + \exp\left(\frac{T_{AH}}{T_H} - \frac{T_{AH}}{T_{ref}}\right)}{1 + \exp\left(\frac{T_{AL}}{T} - \frac{T_{AL}}{T_L}\right) + \exp\left(\frac{T_{AH}}{T_H} - \frac{T_{AH}}{T}\right)}$$

With the temperature correction parameters T_A=5119 K, T_{AL}=50 000 K, T_L=276 K, T_H=303 K and T_{AH}=100 000 K.

Fish internal concentration is expressed per unit of somatic volume (V_w in cm^3). V_w is the sum of the structural volume (V) and the reserve volume (V_E) computed from the DEB model (with $V_E = E/(\varrho_E \times d_V)$, which assumes that densities of reserve and structure are equal).

The equation describing the evolution of the fish internal concentration (c in ng.cm^{-3}) from ingestion of contaminated food, growth dilution and elimination is:

$$\frac{dc}{dt} = \frac{AE \cdot \frac{\dot{p}_X}{\varrho_X} \cdot C_X}{V_w} - \frac{1}{V_w} \cdot \frac{dV_w}{dt} \cdot c - \dot{k}_e \cdot cT \cdot c$$

Chemical body burden (Q in ng) can be thus calculated as the product of c and V_w. Contaminant mass concentrations in fish (C_w in ng g_{fish}^{-1} ww) can be calculated from Q and corresponding total weight predicted by the DEB model (W_w).

Model parameters and forcings

The DEB model from Mounier et al. (submitted, this special issue) is used to predict fish growth (in volume V_w and weight W_w) and temperature correction factor (cT). Even though DEB parameters are individual-specific, the sets of estimates are quite homogeneous at the population level as the individuals are genetically close (Kooijman, 2010). Thus, DEB parameters were considered to be constant between individuals in our work on soles from a single study site.

On the contrary, TK parameters depend on many chemical, biological and environmental factors. However, the way in which these factors influence TK parameters is not always well known, especially for compounds of emerging interest such as PFASs (Borgå et al., 2004). They first depend on the affinity of the chemical to different biomolecules, which relies on its physicochemical properties and its structure (see for instance Ng and Hungerbuhler, 2014 for PFASs; and Arnot and Gobas, 2003, for hydrophobic chemicals such as PCBs). In relation to this chemical properties, TK parameters also depend on fish characteristics, such as fish lipid content or fish biotransformation capacity (Borgå et al., 2004).The assimilation efficiency (AE) also depends on diet assimilation efficiency (Gobas et al., 1999) and especially on the assimilation of the lipid part of the food for PCBs (Kobayashi et al., 2011) and probably for PFASs too (de Vos et al., 2008). Consequently, several sets of empirical values for different fish species are available in the literature (see 2.4.5 for details). In the present work, the variability and uncertainty in the values of the two TK parameters presented above (i.e., AE and $\dot{k}_e$) will be considered only for the studied compounds (i.e., CB153 and L-PFOS).

DEB-TK environmental forcings are temperature (i.e., T, in Kelvin), food availability (i.e., f, the scaled function response from DEB theory, dimensionless), food quality (i.e., ϱ_X, the food energy density, in J.g_{food}^{-1}) and food contamination (i.e., C_X in ng.g_{food}^{-1}). Each environmental forcing can be either constant or dynamic.

2.3. Study site and environmental data

2.3.1. The Gironde estuary

Located on the French Atlantic coast, in SW France, the Gironde estuary (see Figure B1 in supplementary material) is the largest estuary in Western Europe (Lobry et al., 2003). Recent ecological assessments led to conclude that it is in a poor ecological status (Courrat et al., 2009; Delpech et al., 2010) in relation, in particular, with global contamination (Courrat et al., 2009; Gilliers et al., 2006b). Consequently, the bioaccumulation, the trophic magnification and the toxicity potential of several POPs are studied there (Munoz et al., 2017a; Tapie et al., 2011).

2.3.2. Water temperature

Seasonal and inter-annual water temperature data were provided by the high-frequency monitoring program of the Gironde fluvial-estuarine system (MArel Gironde ESTuary, MAGEST, http://www.magest.u-bordeaux1.fr/). We used mean daily temperature measured in the central zone of the estuary (see map in Figure B1). We selected 5 years with a limited number of missing data to be able to compute representative mean annual temperature (see Figure B2).

2.3.3. Diet composition

The juvenile common sole diet composition and associated variability were obtained from ESCROC mixing model estimations for the Gironde estuarine food web (Ballutaud et al., 2019). Five preys were identified in sole diet. As a nominal "value", we used the median values of proportions among the different sets of solutions (i.e., 150,000 solutions of possible diet composition), standardized to sum to 1 (52.8% of Gammarids, 14.6% of brown shrimp, 13.5% of *Nereis*, 11.2% of white shrimp and 7.9% of crab – see Figure B3).

2.3.4. Juvenile sole and preys contamination

Preys contamination data (C_p, ng.g_{prey}^{-1} dw) from the Gironde estuary used in this study came from Lauzent (2018) for CB153 and Munoz et al. (2017a) for L-PFOS (see Munoz, 2015 and Munoz et al., 2017a for details on sample collections, 3 samples per prey species). Common sole samples (from 46 juveniles) were collected several years after in the mesohaline zone of the Gironde estuary (see map in Figure B1). All fish samples were weighed and measured. Their average total length was 15.7 cm (min-max = 8.4-26.5 cm) and their average weight was 42.5 g (min-max: 4.9-165.5 g). The sample preparation and detailed analytical procedure for PCBs and PFASs were published previously (Lauzent, 2018; Munoz et al., 2017a; Thompson and Budzinski, 2000).

Only 3 samples were measured for each prey, thus the distributions of prey contamination are unknown. The nominal value for contamination of a given prey was therefore set as the mid-range (i.e., the average of the largest and smallest values) of observed contamination level The range thresholds were set as the minimum and maximum observed values (data summary is provided in section 2.4.6, Table 1 and detailed data is represented in Figure B4).

2.4. Model inputs computation and associated uncertainty

As environmental conditions are highly variable in space and time in a macrotidal estuary such as the Gironde, we chose to simplify analyses by setting model simulations with constant environmental forcing variables except for temperature, which was modelled as a sinusoid function. We assumed that virtual fish were born uncontaminated. In this section, we presented, for each model input, (1) how it was computed from environmental data and (2) its associated uncertainty. The uncertainty was defined by estimating a range of values (i.e., a minimum and a maximum) for each model input. Due to the low number of samples in the datasets used (presented section 2.3), uniform distributions

between these ranges were associated with their respective model inputs. The model inputs and their associated uncertainty are summarised in Table 2 (section 2.4.6).

2.4.1. Average annual temperature ("temp") and birth date ("birth")

For modelling purpose, the daily temperature dynamics $T(d)$ was represented by a sinusoid to account for seasonal variations:

$$T(d) = \hat{T} + A \times sin\left(\frac{2\pi}{365} \times (d + \varphi)\right) \quad \text{Eq. 1}$$

with $\hat{T}$ the average annual temperature, A the amplitude and φ the phase expressed in days.

$\hat{T}$ was computed for each year selected from the temperature dataset listed in the section 2.3.2. The amplitude A was fixed to 9°C (i.e., the approximated mean amplitude value observed in the Gironde estuary temperature time series in section 2.3.2).

φ value was used to model the influence of temperature life history related to the settlement date on DEB-TK predictions. To reproduce the phase shift necessary to make d=0 corresponding to the 1st of January, φ had to be equal to 240 days. Thus, for a given fish, φ was calculated as 240 plus the day of the year at birth, within the spawning season.

The temperature conditions experienced by an individual during its nursery phase depend on both the year of birth and the settlement date. They thus can be variable at the annual (year of birth) and seasonal (settlement date) levels. Indeed, average annual temperature can vary by several degrees in the Gironde estuary (see 2.3.2 and Table 2 in 2.4.6). Inter-annual variability is obtained by considering $\hat{T}$ variations between years using *in situ* data presented above. Minimum and maximum values of $\hat{T}$ were respectively 14.7°C and 16.3°C.

Also, the common sole is a batch spawner with a large spawning season in the Bay of Biscay (Deniel, 1990). Thus, the environmental conditions encountered in the estuary by the individuals from the earlier and the later batches may also differ. In our case, the spawning season is known to last for several months (i.e., from early December to late March), with a peak in late January and early February (Amara et al., 1994). Consequently, birth date range was December 1 (i.e., 335th day of the year) – March 31 (i.e., 90th day of the year). As a simplification, we assumed that larval drift duration was the same during all the spawning season. See supplementary material (Appendix C, Figure C1) for a graphical representation of birth date influence on temperature sinusoid experienced in the estuary after settlement.

2.4.2. Food availability ("avail")

The DEB parameter used to describe food availability is the "scaled functional response", hereafter symbolized f. f is considered constant over life and its value can be approximated by dividing the asymptotic length observed in the studied environment (Linf) by the theoretical maximal length that an animal can attain if food is not limited (Lmax) (Kooijman, 2010). In the absence of age–length relationship for the studied population from the Gironde estuary, it was not possible, however, to estimate f in our case study. We thus assumed that f was similar to the one for the Douarnenez Bay's population (Brittany, NW French coast) for which a large set of age–length data were available.

The food availability encountered all over the juvenile period in the estuary may differ from one individual to another, depending, for instance, on their different locations in the estuary during this period. Thus, to obtain the range of f values, we divided the minimum (41 cm) and maximum (47 cm) total lengths of fully grown males (over 15 years old, n=8) from Douarnenez Bay (Deniel, 1981) by the

total length of the largest one ever observed (75 cm, male, http://www.fishbase.org). Thus, f was supposed to be between 0.547 and 0.627.

2.4.3. Food quality ("quality")

The DEB parameter used to describe food quality is the food energy density ϱ_X ($J.g_{food}^{-1}$ dw). It is a combination of diet composition and prey energy density. ϱ_X was computed for each diet composition solution from the corresponding dry mass proportion of preys F_p in the diet (see section 2.3.3) and from dry energy density of each prey species ϱ_p ($J.g_{prey}^{-1}$ dw), as follows:

$$\varrho_X = \sum_{p=1}^{5} (\varrho_p F_p) \qquad \text{Eq. 2}$$

As ϱ_p values were not reported in literature for the Gironde estuary case study, we used values of corresponding species from a databank of conversion factors updated in 2012 (Brey, 2001; Brey et al., 2010): 15,770 $J.g^{-1}$ dw for Gammarids, 17,396 $J.g^{-1}$ dw for brown shrimp, 17,359 $J.g^{-1}$ dw for *Nereis*, 19,319 for white shrimp and 11,887 $J.g^{-1}$ dw for crab.

ϱ_p was considered constant but diet composition was variable. Indeed, diet composition can modulate food quality as the different preys do not provide the same energy. ϱ_X range was fixed to the minimum and maximum values computed from the results of ϱ_X for all diet composition solutions provided by ESCROC (n=150,000). ϱ_X estimates ranged from 14,047 to 18,034 $J.g_{food}^{-1}$ dw.

2.4.4. Food contamination ("contam")

Food contamination level C_X ($ng.g_{food}^{-1}$ dw) is a combination of diet composition and prey contamination. It was computed using the formula:

$$C_X = \sum_{p=1}^{5} (C_p F_p) \qquad \text{Eq. 3}$$

where C_p is the concentration in the prey p ($ng.g_{prey}^{-1}$ dw) and F_p is the dry mass proportion of prey p in the diet.

Diet composition can also modulate food contamination as the different preys do not contain the same amount of contaminant (see 2.3.4). Thus, we computed C_X for each diet composition solution (n=150,000, see section 2.3.3) with either the minima or the maxima contamination observed for each prey (see section 2.3.4 for preys contamination). The lower and upper boundaries for food contamination were fixed to the minimum and maximum C_X values computed, respectively (i.e., 3.3-24.5 $ng.g^{-1}$ dw for CB153 and 6.2-79.3 $ng.g^{-1}$ dw for L-PFOS).

2.4.5. TK parameters (AE and $\dot{k}_e$)

TK parameters input values and associated variability were gathered from literature (Kobayashi et al. (2011), Fisk et al. (1998), and Buckman et al. (2004) for CB153, and Hassell et al. (2019), Goeritz et al. (2013), and Martin et al. (2003) for the PFOS) for several fish species, because no specific data's on sole were found.

For assimilation efficiency (AE), estimates for PCBs were compiled by Kobayashi et al. (2011) and were ranging from 0.26 to 1 for CB153. Most previous estimates of fish TK parameters for PFOS were estimated at the carcass level and reported high but non-realistic estimates for AE (i.e., AE >100%

from Martin et al., 2003a). Thus, by default, we retained 1 as the higher value of the range. The lower bound was provided by Hassell et al. (2019) for L-PFOS, at the whole body level. It was computed as the estimate minus 1.96 times the associated standard error. This led to a range of AE values from 0.53 to 1 for the L-PFOS.

The elimination rate ($\dot{k}_e$) values were compiled from Buckman et al. (2004) and Fisk et al. (1998) for CB153, and Goeritz et al. (2013), Hassell et al. (2019), and Martin et al. (2003) for PFOS. A range for $\dot{k}_e$ was calculated using the estimate provided by the authors ±1.96 times the associated standard error, when the latter was provided. These different $\dot{k}_e$ values were obtained under different temperature conditions, varying from 8 to 17.5°C depending on the studies. Hence, to be compared with each other, the estimates from the different sources were corrected to be given at 20°C (i.e., the reference temperature for the Arrhenius correction, see temperature correction parameter estimates from Mounier et al., submitted, this special issue). We considered the minimum and maximum values estimated at 20°C as the range of variation of $\dot{k}_e$ (i.e., [0.45 – 2.24] for CB153 and [5.22 – 11.28] for PFOS, all in $10^{-2}.d^{-1}$).

2.4.6. Summary of model input data

Model input nominal values and ranges are summarized in Table 1 for preys characteristics. The ranges of variation of other environmental variables and TK parameters are given in Table 2.

Table 1 - Summary of the nominal values for prey input variables and associated range [min; max] for prey contamination (C_p). See text for details. WS: White shrimp, BS: Brown shrimp, Gam: Gammarids, Hed: ragworm, Cra: shore crab.

Description	WS	BS	Gam	Hed	Crab	Ref
Mass proportion in diet (%)	11.2	14.6	52.8	13.5	7.9	Ballutaud et al., 2019
Energy density ($J.g^{-1}$ dw)	19,319	17,396	15,770	17,359	11,887	Brey et al., 2010
CB153 ($ng.g^{-1}$ dw)	24.0 [21.3; 26.6]	3.7 [0.6; 6.8]	15.6 [8.4; 22.7]	5.3 [4.1; 6.4]	9.6 [6.2; 12.9]	Lauzent, 2018
L-PFOS ($ng.g^{-1}$ dw)	8.4 [4.6; 12.2]	25.9 [15.8; 36.0]	11.5 [8.6; 14.5]	68.7 [11.5; 125.9]	6.6 [5.6; 7.5]	Munoz et al., 2017a

Table 2 - Summary of inputs variability included in the sensitivity analyses.

Description	Symbol	Unity	Min - Max
Average annual temperature (temp)	$\hat{T}$	°C	14.7 – 16.3
Day of the year at birth (birth)	d_b	d	335 – 90
Food availability (avail)	f	-	0.547 – 0.627
Food energy density (quality)	ϱ_X	$J.g^{-1}$ dw	14,047 – 18,034
Food contamination (contam)	C_X	$ng.g^{-1}$ dw	CB153: 3.3 – 24.5 L-PFOS: 6.2 – 79.3
Assimilation efficiency of contaminant	AE	-	CB153: 0.26 – 1 PFOS: 0.53 – 1
Elimination rate at 20°C	$\dot{k}_e$	$10^{-2}.d^{-1}$	CB153: 0.45 – 2.24 PFOS: 5.22 – 11.28

2.5. Sensitivity analyses

2.5.1. Global sensitivity analysis

General principle

A global sensitivity analysis was implemented to assess which were the inputs whose variability mainly explains the outputs variability. It also allows detecting interactions between model inputs and provides sensitivity results considering the entire input space.

This global sensitivity analysis was performed using the variance-based Sobol' method (Saltelli et al., 2010). It is a model independent method that allows estimating, within a probabilistic framework, the contribution of each model input variance, and of their interactions, to the unconditional variance of a model output. Sobol' first order indice (Si) quantifies the sensitivity of a model output variance to the main effect of a model input. It thus measures the effect of varying this particular input alone considering variations in other input parameters. By construction, Si indices sum to 1 for a given model output. The more a Si value is close to 1 for a particular input parameter, the more sensitive is the model output variance to this input variance.

The Sobol' total index (STi) considers the contribution to the output variance of all variance caused by a given input and its interactions. Thus, the difference between Si and STi values for a given input-output couple provide information about the sensitivity of the output variance to interactions of the given input with all the other inputs combined.

Computation

To estimate both Si and STi indices at the same time we used Jansen estimators (Jansen, 1999) with improved formulas from Saltelli et al. (2010) computed using the "soboljansen" function from R package "sensitivity" (Iooss et al., 2019). This function computes the Monte Carlo estimation of the Sobol' indices using two independent input matrices with n rows (the random sample size, n = 10,000) and p columns (the number of inputs ; p = 4 for growth outputs - i.e., "birth", "temp", "avail", "quality" ; p = 7 for contamination outputs – i.e., idem + "Contam", "AE", "ke"). In both matrices, every row represents a possible set of input values for the DEB-TK model. To build these matrices, we optimised model inputs combinations using scrambled Sobol' sequences (i.e., quasi-random low-discrepancy sequences with both Owen and Faure-Tezuka type of scrambling) computed using the "sobol" function from the R package "randtoolbox" (Dutang and Savicky, 2009). Each model inputs values were transposed from 0 to 1 sampling to their respective ranges defined in the section 2.4. These lower and upper limits (Erreur ! Source du renvoi introuvable.) were defined either to cover the variability of environmental conditions observed in the Gironde estuary or to cover the uncertainty in TK parameter values.In order to compute Sobol' indices, outputs are predicted for each row of the matrices and returned by the function. Each row corresponds to one fish simulated with a constant value for each model input, given in the matrix. To assess confidence intervals on the estimation of Sobol' indices, bootstrapping with resampling was used within the "soboljansen" function. The n samples used for the model evaluations were 250 times sampled with replacement, whereby, for each resampling the function computes Sobol' indices to obtain the 95% confidence intervals for Si and STi values.

2.5.2. Complementary variance analysis on food contamination

Food contamination variability used as a model input to calculate the Sobol' indices is actually a compound variable (see 2.4.4). Its variability mixes variabilities of the diet composition and the individual contaminations of each of the 5 preys (see 2.3.3 and 2.3.4 respectively). To disentangle the relative influence of the contamination of each prey on the contamination of sole, a complementary

analysis was thus required. For this particular complementary analysis, we introduced 6 dummy variables:

- the first dummy variable is set to 1 to indicate that the diet composition is variable, while a -1 indicates that the diet composition is fixed to its nominal value;
- the 5 other dummy variables correspond to each of the 5 preys: a -1 indicates that the corresponding prey contamination is set to its nominal value while a 1 indicates that it is variable.

To explore the effects (main and interactions) of each of these 6 sources of variability, we generated an orthogonal fractional factorial 2-level design of resolution V using the "FrF2" function from the eponym R package (Grömping, 2014), with the 6 dummy variables as factor of the design. It permits to obtain the smallest necessary experimental design (i.e., smallest number of factors combination to be computed) which was here composed of 32 runs (instead of 64 for the full factorial design). Each "experiment is composed of a particular combination of the different 2-level factors (i.e., "-1" or "1" values for the 6 factors).

For each experiment, the model was run with 50,000 different sets of parameters values according to the following rule:

- the value of a parameter was set to its nominal value for the 50,000 runs if the corresponding dummy variable equals -1

- if the corresponding dummy variable equal 1, then 50,000 values were uniformly drawn between min and max values for contamination of species, while 50,000 diet compositions were randomly sampled from the posterior distribution (see section 2.3.3) for diet composition.

Finally, from these model predictions, a variance analysis was carried out to assess the contribution of the different considered environmental variables and their interactions to food contamination variance.

2.6. Model predictions vs *in situ* measurements

Finally, model predictions were compared to *in situ* measurements following two steps.

As a first step, we graphically compared contamination levels measured in fish from the Gironde estuary (see 2.3.4) with distribution of DEB-TK predictions of contamination at puberty computed for the purpose of the Sobol' indices estimations. By doing this, we were able to compare variability of field concentrations with the variability of predicted concentrations due to variability and uncertainty of model inputs (i.e., environmental variables and TK parameters). For comparison purpose with measurements, model predictions of contamination at puberty were associated with the predicted range of length at puberty from the same analysis.

On a second step, we addressed model predictions with different scenarios of fixed values of TK parameters:

- a "worst case" scenario of chemical bioaccumulation with TK parameters classically used in ecological risk assessment models (AE=1 and $\dot{k}_e$=0),
- two scenarios from experimental estimates:
    - from Goeritz et al. (2013) for the PFOS estimated for the rainbow trout: AE=0.721 and $\dot{k}_e$=5.8 10^{-2}.d^{-1} at 20°C;
    - from Mounier et al. (submitted, this special issue) for the CB153, applied to the common sole: AE=0.8 and $\dot{k}_e$=0.d^{-1};

- a scenario from de Vos et al. (2008) who explored the behaviour of PFOS uptake and elimination using the bioaccumulation model OMEGA: AE=0.8 (i.e., uptake "comparable to moderately hydrophobic compounds") and $\dot{k}_e$=0.8 10^{-2}.d^{-1} (i.e., elimination "best described by elimination kinetics of metals", non-specified temperature, value applied directly);

For these scenarios, as TK parameters were fixed the variability considered only relied on environmental forcings variability. Practically, we built matrices in the same way as for the Sobol' method (each line or sample corresponded to a possible combination of input variables). We computed contamination predictions at puberty for these samples and confronted them with data in the same way as presented in the first paragraph.

For each step, model fit was assessed comparing (1) the minimums and maximums values of predictions and measurements, and (2) the median of predictions (i.e., the distribution reflecting notably the diet composition distribution and its consequences on food contamination) with the average value of all measurements (i.e., regardless of fish size).

2.7. Implementation

Sensitivity analyses and DEB-TK simulations were implemented using R language (R core team, 2017) version 3.6.1 and the integrated development environment (IDE) R-studio version 1.2.5019.

3. Results

3.1. Sensitivity analysis

No major influence of sex was found in the global analysis. Results are thus only presented here for females. Detailed results for each sex can be found in supplementary material (Appendix D, Table D1).

Si and STi estimates for biological outputs (Figure 2) were very close (Si/STi > 0.9), which indicates little interactions between model inputs. The main contributor to age and length variance was the variability in food quality (Si=0.68) and, to a much lesser extent, in food availability (Si=0.2). By contrast, age at puberty was slightly sensitive to average annual temperature (Si=0.09) and nearly not affected by birth date (Si<0.02).

Global sensitivity of contamination predictions to environmental inputs variability were similar for CB153 and L-PFOS and close to zero, apart from food contamination (Si and STi <0.01, see Figure 2). Food contamination was the major contributor to fish contamination variance (Si=0.38 and 0.7 for CB153 and L-PFOS, respectively). For CB153, food contamination was closely followed by the two TK parameters (Si=0.26 and 0.23 for $\dot{k}_e$ and AE, respectively). In contrast, the influence of food contamination is much higher than TK parameters for L-PFOS (Si=0.14 and 0.09 for $\dot{k}_e$ and AE, respectively). Nevertheless, for both chemical, the influence of $\dot{k}_e$ variability was higher than the influence of AE variability. For both these influent inputs and both chemicals, STi values were different from Si values (Si/STi around 0.75), indicating interactions between inputs.

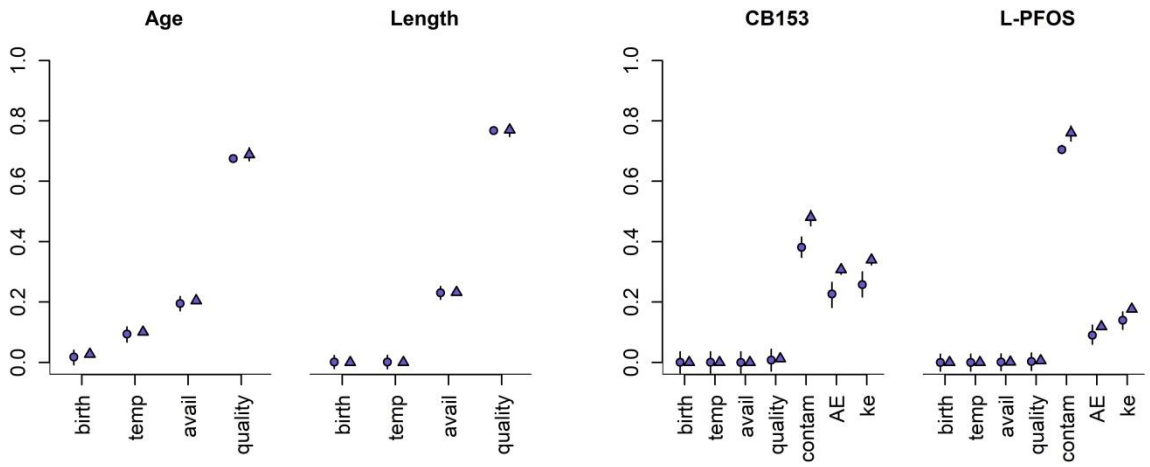

Figure 2 - Sobol's first order indices (Si, main effect in circles) and Sobol's total indices (STi, total effect in triangles) estimated at puberty for female for each model ouput. See detailed values in supplementary material (Appendix D, Table D1).

The distributions predicted for each output are presented in Figure 3. Considering the range of environmental variability accounted in this study, age at puberty, predicted for the purpose of the computation of Sobol' indices, varied by one year (i.e., between 1.6 to 2.7 years old), with a median value of 2.2 years old. Estimates for length at puberty varied from 20.9 to 22.3 cm, with a median value of 21.7 cm. When considering both environmental and TK parameters variability, contamination levels in fish varied by a factor 54 to 124 for L-PFOS and CB153, respectively (between 0.1 and 5.4 $ng.g^{-1}$ ww and between 0.1 and 12.4 $ng.g^{-1}$ ww, respectively). Contrary to biological outputs, the median of estimated values for contaminations outputs (1.9 and 1.4 $ng.g^{-1}$ ww for CB153 and L-PFOS respectively) were close to the minimal values.

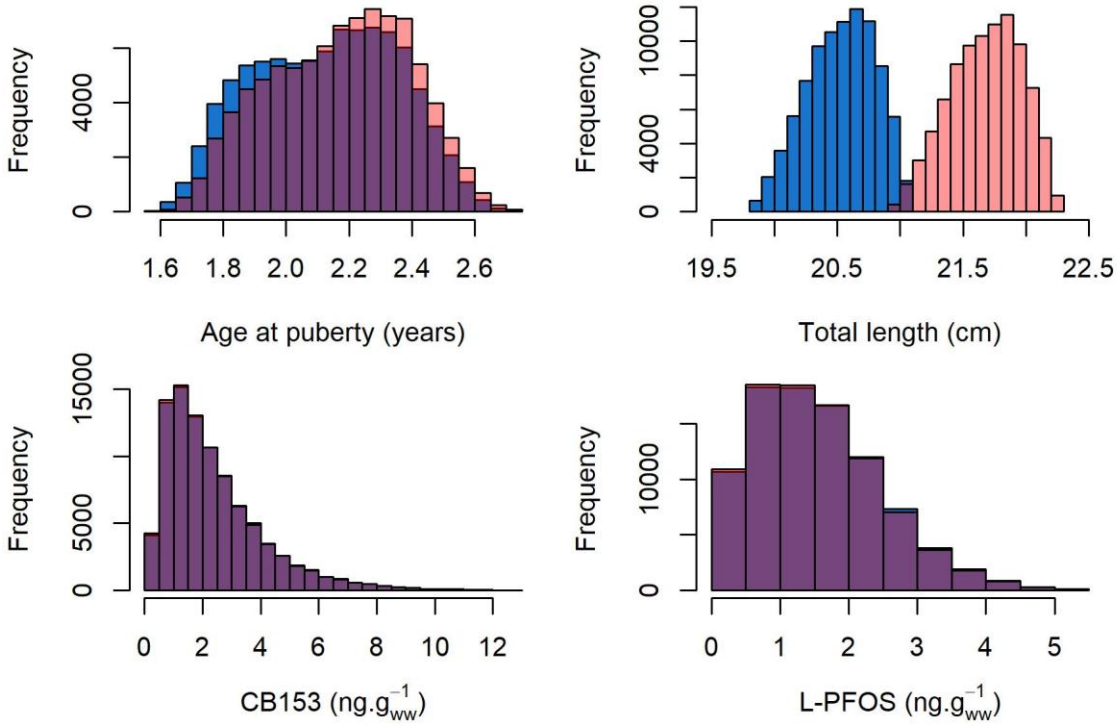

Figure 3 - Model outputs distributions computed for Sobol' indices estimations. Male distribution is in blue and female distribution is in transparent red.

3.2. Variance analysis on food contamination

Since food contamination is one of the main factor influencing the model outputs, it was crucial to disentangle the relative effect of diet composition and respective prey contaminations (Figure 4). Almost all the variance (>90%) in food contamination was induced by only two factors. Unsurprisingly, the variability in diet composition explained 39% and 50% of food contamination variance for CB153 and L-PFOS, respectively. For CB153, the variability of contamination levels in Gammarids (the main prey of sole juveniles) explained almost all the remaining variance (57%) whereas for L-PFOS it was *Nereis* (i.e., *Nereis diversicolor*, the most contaminated prey species for this contaminant) (45%). The influence of the other factors was therefore considered as negligible. The residual variance, that could be associated to interactions, was also negligible (<5%).

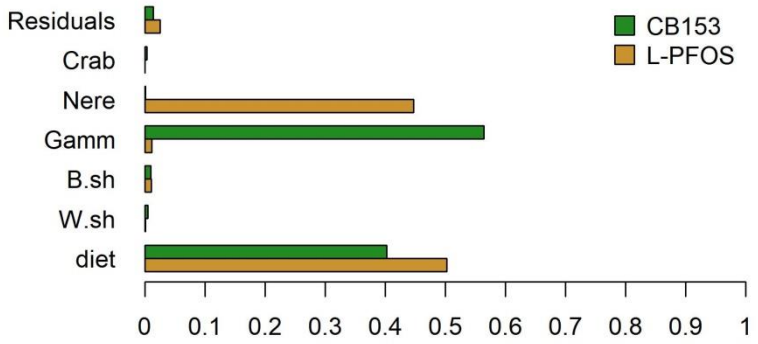

Figure 4 - Proportions of total variance (x-axis) from ANOVA on food contamination variance induced by model inputs variability (y-axis) for CB153 and L-PFOS.

3.3. Data comparison to model predictions

When considering environmental and TK parameters variability fish contamination levels were underestimated for both chemicals compared to *in situ* measurements (Figure 5 and Table 1). Levels were underestimated by a factor 3.5 for L-PFOS and 3.9 for CB153. The maximum values were less underestimated for CB153 (factor 1.5) than for L-PFOS (factor 2.4). The minimums were much more underestimated than the maximums (i.e., by a factor 9 and 18 for L-PFOS and CB153, respectively).

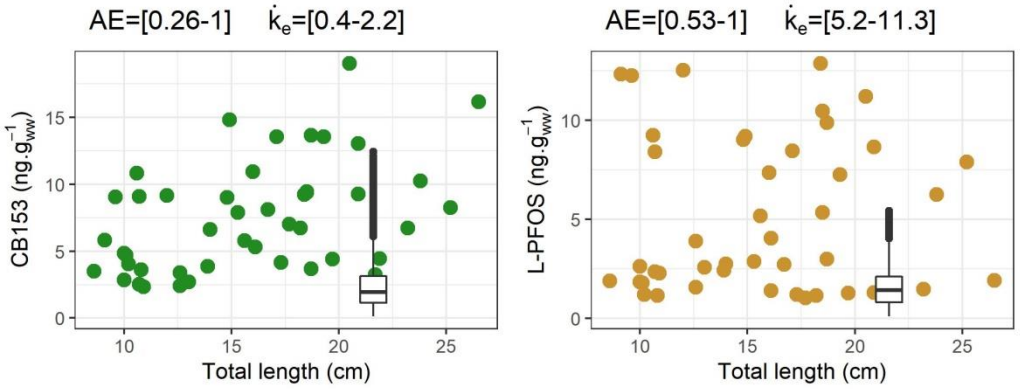

Figure 5 - Fish contamination predictions (ng.g^{-1} ww) for CB153 (on the left) and L-PFOS (on the right) considering environmental and TK parameters variability (boxplot) and Gironde estuary measurements (points). $\dot{k}_e$ values are given in 10^{-2}.d^{-1} at 20°C.

With the worst case scenario (Figure 6 - A), the distributions of the model predictions for CB153 and the observations were similar (Table 1) even though the upper part of the contamination distribution was higher than the highest measurement. On the contrary, L-PFOS contamination was overestimated by a factor 10 (Table 1).

For the experiments scenarios (Figure 6 – B), predicted contamination level and range of variability with TK parameters used by Mounier et al. (submitted, this special issue) were consistent with observations for CB153. For L-PFOS, predictions with the estimates from Goeritz et al. (2013) underestimated both level and range of contamination.

Finally, de Vos et al. (2008) scenario (Figure 6 - C) produced the best model fit for L-PFOS, with an overestimation of contamination by a factor 2 for both mean level and range of variability.

Table 1 - Comparison of predicted distributions for the different scenarios of TK estimates (median [min-max]) with the observed distributions (mean [min-max]).

	CB153	PFOS
Observations	7.47 [2.33-19.03]	4.96 [1.04-12.85]
Predictions with variability on all inputs	1.93 [0.13-12.41]	1.42 [0.11-5.41]
Worst case scenario	13.85 [2.65-32.99]	42.67 [4.95-106.94]
Experiments scenario	11.08 [2.12-26.4]	2.08 [0.28-4.25]
de Vos et al. (2008) scenario		10.87 [2.06-25.78]

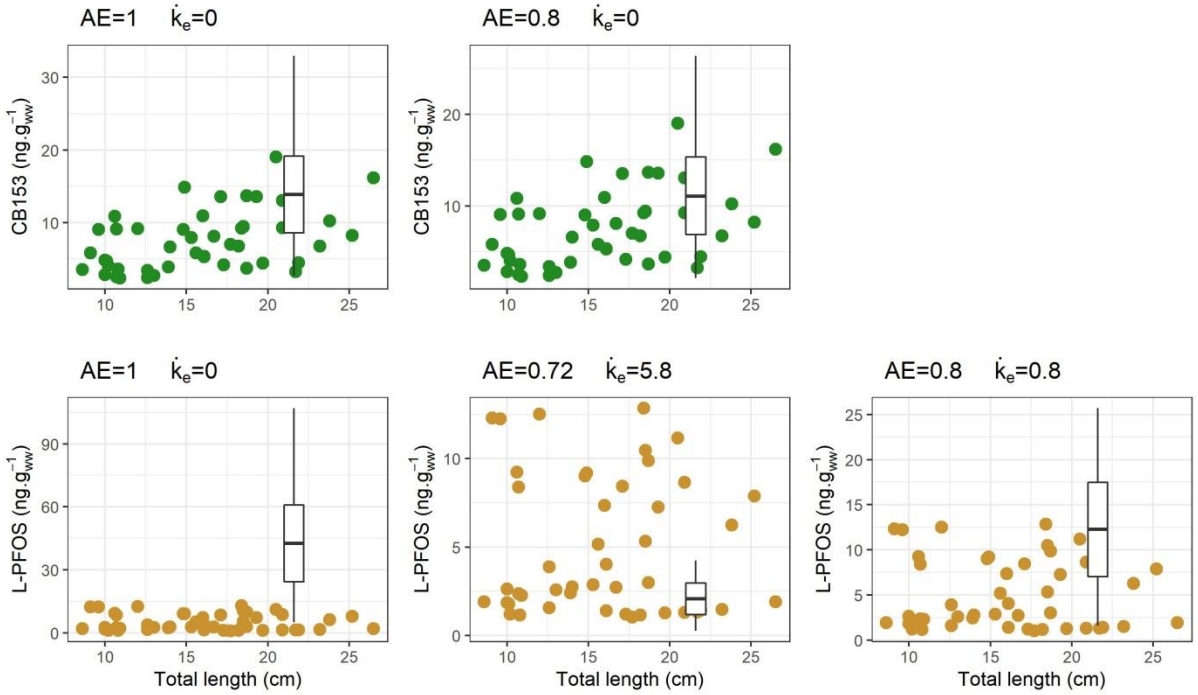

Figure 6 - Fish contamination predictions (ng.g^{-1} ww) considering environmental variability and the different scenarios of fixed TK parameters and (boxplot) compared to the measurements from the Gironde estuary (points) for CB153 and L-PFOS. (A) the worst case scenario, (B) scenarios from experimental estimates, and (C) scenario from de Vos et al. (2008). TK values are given for each scenario on each panel. $\dot{k}_e$ values are given in 10^{-2}.d^{-1} at 20°C.

4. Discussion

4.1. Main goals and outcomes

The first aim of this study was to prioritize the influence of the environmental factors involved in Global Change on the variance of biological traits and contamination level at puberty of juvenile common sole from the Gironde estuary. For this purpose, we developed a mechanistic TK model by combining last updated DEB model on *S. Solea* with a basic one-compartment TK model. This allowed to mechanistically model the relative influence of these environmental factors (i.e. water temperature, food quality, food availability) on biological traits, that themselves (combined with food contamination) influence bioaccumulation. The analyses conducted in this paper highlighted that diet composition, through food energy density and food contamination, was the key environmental factor influencing both juvenile sole growth and contamination variabilities. As it is a rather opportunistic feeder species (Cabral, 2000), future Global Change studies should focus on constructing credible scenarios for the future evolution of benthos populations in order to deduce possible changes in the diet of the common sole.

The second aim was to compare the influence of these environmental factors with that of TK parameters uncertainty on the variability of fish contamination levels. Finally, several scenarios of TK parameters were tested with the model to determine which one would give the best fit to the CB153 and L-PFOS contamination data of the Gironde estuary.

Our results also underlined the strong influence of the TK parameters (AE and $\dot{k}_e$) on sole contamination estimations and the importance of using correct values for each chemical, species and environment. A major direct influence of temperature was shown on age at puberty but not on fish contamination.

4.2. Sex difference in juvenile ingestion does not influence sole contamination

First of all, results were obtained for each sex as the DEB model used considers sex-specific parameters (Mounier et al., submitted, this special issue), including one related to food ingestion throughout the entire lifecycle which directly influences dietary contamination. In the present work focusing on the juvenile phase spent in nursery grounds, the influence of these sex differences on fish contamination was found negligible. This result support the assumption that sex-differences in fish contamination observed in adults are rather due to sex-differences in contaminant elimination through gametes emission than to a differential accumulation during their juvenile phase in contaminated areas (Bodiguel et al., 2009; Loizeau and Abarnou, 1994; Peng et al., 2010; Shi et al., 2018). It emphasizes the necessity to use of a DEB model considering sex differences, especially those regarding gametes emission (see Mounier et al., submitted, this special issue), to study fish contamination at the lifecycle scale, and sex-specific impact of reproduction.

4.3. The major role of diet composition

Food quality, based on prey energy density and diet composition, was found to be the main factor influencing life-history traits of age and length at puberty. In our approach, the variability of food quality is only due to the diet composition variability.

The diet variability also appeared to be a major factor influencing food contamination variance for both chemicals. And, food contamination was the only environmental factor significantly influencing fish contamination variance for both chemicals. Fish diet was already put forward, for biomagnified compounds, as a factor that may be responsible for the variability in bioaccumulation between individuals, sites, and seasons, for PCBs (Masset et al., 2019; Stapleton et al., 2002; van der Oost et al., 2003), and between fish species for PFASs (Babut et al., 2017). Diet modifications influence on juvenile

sole growth and contamination is all the more topical that, in the Gironde estuary, as in several other ones, shifts in ecological communities (e.g., Chaalali, 2013; Chaalali et al., 2013a ; Chevillot et al., 2016 for the Gironde) and food web structure and functioning (e.g., Chevillot et al., 2018 for the Gironde; Tecchio et al., 2016 for the Seine) have been highlighted in relation with global changes. And, we can assume that if prey abundances are affected by Global Change, common sole diet is expected to change and adapt as sole is rather an opportunistic feeder species (Pasquaud et al., 2010). This feeding behaviour adaptation of the juvenile sole, as a function of prey abundance, has been demonstrated in the Tagus estuary (Cabral and Costa, 1999).

Results from the variance analysis on food contamination indicated the strong influence of Gammarids and *Nereis* contamination in CB153 and L-PFOS, respectively. *Nereis* is the most consumed prey all year round whereas Gammarids are mainly found in the stomachs of sole in spring (Pasquaud, 2006). As a consequence, seasonal fluctuations in the Gironde estuarine soles' diet could have different effects on the two studied chemicals. These seasonal variations of food contamination due to variations of diet composition may also enhance the influence of birth date on fish contamination, as birth date affects the time of the season when the individual settles in the estuary.

4.4. Substantial direct impact of temperature on the age puberty

Our results highlighted that the direct influence of temperature on growth rates induce substantial changes of the age at puberty that could lead to substantial consequences at the population level. Indeed, the implemented variability of the average annual temperature (i.e. a range of 1.6°C) was responsible for nearly 11% of the variance of age at puberty. As puberty was predicted to vary between 18 and 32 months for females, considering all the environmental variability, an increase of 1.6°C of the average temperature alone could lead to a decrease of several months in the age puberty (e.g. -17 days for +0.16°C, see local sensitivity in supplementary material, Appendix E). Such increase of mean annual temperature is a realistic scenario in the context of climate change as, during the last 3 decades, the water temperature of the Gironde estuary already increased by about 2°C (Chaalali, 2013; Le Treut, 2013). As DEB models can describe the full life cycle of an individual, by combining it with different population models (Charles et al., 2009; Jager and Klok, 2010), this modelling framework allows studying the consequences at the population level of such modifications of female age at puberty.

Our results showed that direct impact of temperature on fish metabolism does not affect fish contamination at puberty. Indeed, considering DEB model properties, although temperature significantly influences growth rate, it does not affect the state variable values at a given point of development (e.g., the length at puberty) because it affects each energy flux in the same way. However, temperature can have indirect impacts on fish by modifying for instance prey distribution and consequently diet composition, which could induce changes in age, length, and contamination at puberty. Thus, the global influence of temperature on fish contamination is difficult to predict simply, due to direct and indirect effects on metabolism and ecological traits.

4.5. TK parameters estimates

Variability of TK parameters

TK parameters variability was shown to be more influent on fish contamination variability than environmental factors, with the exception of food contamination. Moreover, for CB153, they were almost as influent as food contamination. It highlights the importance of the TK parameter values used to study global change influence on fish contamination. Indeed, the amplitude of TK parameters values from the literature reflects both the uncertainty of the estimates from experimental data, and the variability due to the different species studied and the experimental conditions used. Thus, the variability considered on TK parameters estimates may reflect the influence of both environmental

(e.g., temperature and food composition) and biological variabilities (e.g., length and specific metabolic capacities) on the chemical fluxes. Most of these factors are already included in the mechanistic models' equations and parameters. Thus, in the present analysis, the variability on chemical flux predicted considered both environmental variability from the model and the environmental/biological variability implicitly included in TK estimates from literature. Consequently, the apparent strong influence of TK parameters variability mostly indicates that TK estimates must be chosen, and wisely chosen, from the literature for this particular type of model application.

In our results, unlike CB153, L-PFOS food contamination was by far the major factor influencing fish contamination compared to TK parameters. This difference may be due to the much larger range of food contamination levels for L-PFOS than for CB153 (factor 3.5), reducing the influence of TK parameters comparatively to the one of food contamination. Thus, variability in food contamination can have a greater or lesser impact on fish contamination depending on the chemical. The variance analysis showed that for L-PFOS the variance of *Nereis* contamination supported half of the variance of food contamination. However, only 3 measurements of *Nereis* contamination were performed and the large range of contamination was mostly dependent on only one sample with particularly high contamination level (Figure B4). Consequently, further studies on prey contamination may be necessary to exclude that TK parameters uncertainty is not as important as food contamination variability for L-PFOS too.

Uncertainty of TK parameters estimates for S. solea in estuarine environment

Our results highlighted the high variability of TK parameters in the literature and the difficulty to use them in natural environment studies. Indeed, considering the whole range of TK parameters estimates from literature led to an underestimation of fish contamination level and variability in our case study. Results from the sensitivity analyses (i.e. the global one presented in the main document and the "One step at a time" local analysis from the supplementary material, Appendix E) highlighted that an underestimation of fish contamination level could be due to several factors. There were interactions between food contamination, AE and $\dot{k}_e$ values. As food contamination was estimated from prey measurements from the Gironde estuary, we assume that they are reliable. On the contrary, TK parameters were taken from a large review of the literature. Since the values of AE and $\dot{k}_e$ interact on fish contamination, it was not possible to dissociate the effects of each parameter and to estimate them from *in situ* contamination data. To do so, we would have needed contamination-decontamination data from controlled experimental conditions (i.e. $\dot{k}_e$ is the only parameter involved in fish contamination kinetics during the decontamination period).

However, we can assume from our results that the underestimation of fish contamination may be rather due to too high values of elimination rate or to the omission of other uptake routes, as the maximum value of assimilation efficiency parameter (i.e. full assimilation) was included in the range used for simulations. Moreover, results of data comparison to model predictions with the "worst case scenario" (full assimilation and no elimination) showed that the hypothesis of too high values of elimination rate is the most likely one for both compounds.

This conclusion of a smaller error of the model on the assimilation flow (i.e. efficiency from diet assimilation and/or other routes of exposure) compared to elimination flow is also consistent with the knowledge that exchanges with water through gills can be neglected for highly lipophilic compounds (i.e., with an octanol-water partition coefficient (logKow) larger than 6.6; Mackay and Fraser, 2000) like CB153 (logKow = 6.92, Hawker and Connell, 1988). Moreover, this PCB congener does not have any precursor that could be biotransformed into CB153 by the fish metabolism. Finally, the assumption of an overestimation of the elimination flux is also supported by the satisfactory model fits to experimental contamination of *S. solea* in Mounier et al. (submitted, this special issue) and to *in situ* measurements in the present paper, both using TK values with no elimination from Mounier et al. (submitted, this special issue).

PFOS is known to be mainly associated with the particulate phase in estuarine environment, which reduces exposure via respiration (Munoz et al., 2017b). Another likely source of uptake might be considered for PFOS: the biotransformation of precursors, themselves accumulated from the environment (Babut et al., 2017; Martin et al., 2010). Yet, considering PFOS estimates from de Vos et al. (2008) led to higher fish contamination levels without considering these other sources of PFOS. Consequently, an overestimation of $\dot{k}_e$ for PFOS may, more likely, be responsible for fish contamination underestimation. Indeed, de Vos et al. (2008), in a modelling exercise, showed that PFOS elimination was "best described by [mimicking] elimination kinetics of metals" and used an empirical value of $\dot{k}_e$=0.8 10^{-2}.d^{-1}, thus, a 7 fold lower value compared to the minimum threshold of the range used in the present analysis. Using de Vos et al. (2008) values (i.e., AE=0.8 and $\dot{k}_e$= 0.8 10^{-2}.d^{-1}), PFOS contamination would only be overestimated by a factor 2. Moreover, the overestimation with these parameters was likely as the authors also reported that these values led to an overestimation of bioaccumulation factors. This indicates that the elimination rate of PFOS, in our case study, is likely to lie between the one used for metals by de Vos et al. (2008) ($\dot{k}_e$=0.8 10^{-2}.d^{-1}) and the lower bound of the range defined from literature estimates ($\dot{k}_e$=5.2 10^{-2}.d^{-1}, which is close to the one from Goeritz et al., 2013).

Overall, the results reflect that $\dot{k}_e$ values from literature were too high for our species of interest in our case study context. Yet, there was no information about sole in the literature cited. According to Arnot et al., (2008), the inherent variability among species and conditions (life stage and sex) is not well understood while estimates for most chemicals are derived from only one or two tests. It could lead to significantly high estimation uncertainty. Thus, available data in literature probably do not allow for general conclusions about differences in $\dot{k}_e$ values between species, routes of exposure, and environments.

To conclude, the use of non-informative TK parameter values like the common "worst case scenario" showed that, depending on the chemical studied, predictions may greatly overestimate fish contamination, and thus, probably toxic effects in future works. To select the best informative TK estimates from the literature and use it properly in such mechanistic models, it should be necessary to consider the closest species possible as even among fish, between common sole and rainbow trout from Goeritz et al. (2013), results showed that TK parameters seems to differ for L-PFOS. However, the underestimation of sole contamination using Goeritz et al. (2013) estimates for L-PFOS could come from environmental differences rather than from species-specific capacities. Indeed, results showed that elimination rate in sole from the Gironde estuary is lower than the one from rainbow trouts from Goeritz et al. experiment. However, food contamination was greatly higher in the experiment (500 ng.g^{-1} dw) compared to *in situ* contamination (6.2-79.3 ng.g^{-1} dw) and elimination rate is concentration-dependent. Thus, the use of TK parameters estimated from contamination-decontamination experiment should be preceded by an adaptation of the estimates to this mechanistic model. To do so, it should be necessary to have as much information as possible on the experimental design and results used to acquire the estimates (e.g. water temperature, food composition and assimilation by the studied species, food contamination, growth and contamination kinetics).

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- Mounier F.: Conceptualization, Methodology, Software, Formal analysis, Visualization, Writing - Original Draft, Writing - Review
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SUPPLEMENTARY MATERIAL

For:

Dietary bioaccumulation of persistent organic pollutants in the common sole *Solea solea* in the context of global change. Part 2: Sensitivity of juvenile growth and contamination to toxicokinetic parameters uncertainty and environmental conditions variability in estuaries.

Content

Appendix A. Detailed TK equation

A1. General principles

The mechanistic TK model presented below is a one-compartment kinetic model similar to the one presented by Arnot and Gobas (2004), who related bioaccumulation in an aquatic organism to 6 major routes of chemical uptake and elimination: dietary uptake, gill uptake, gill elimination, metabolic transformation, faecal egestion and growth dilution. Applications of this model are usually based on steady-state assumption, which leads to consider that chemical fluxes are constant. This simplification is often accurate for small organisms and short-term experiments in constant environmental conditions (Arnot and Gobas, 2004). However, it should be used with caution when the exchange kinetics are relatively slow (slowly metabolizable chemicals of high hydrophobicity in large, lipid-rich organisms) because steady state takes a long time to achieve (Arnot and Gobas, 2004). The fundamental interest of this DEB-TK model is to consider non-constancy of these different chemical fluxes. We used the DEB theory (Kooijman, 2010) to predict the variation of chemical fluxes due to environmentally induced variations of metabolic activity, ingestion and growth dynamics. In the present model, no retroaction of contamination level on DEB parameters is implemented. Furthermore, as we focus on the juvenile phase, the reproduction and thus the transfer to the gametes are not accounted for.

A2. Uptake

In a first approach, we assumed that trophic contamination was the main route for the two chemicals we considered in this study. Our DEB-TK model, thus only considers food uptake, where food is a mix of different prey. Dietary uptake (Q_{in} in ng of contaminant) was related to food contamination (C_X in ng g_{food}^{-1} dw), dynamic ingestion rate predicted by the DEB model ($\dot{p}_X/\varrho_X$ in g_{food} dw per day, with $\dot{p}_X$ the food ingestion flux in $J.d^{-1}$ and ϱ_X the food energy density in $J.g_{food}^{-1}$) and assimilation efficiency of chemical from food (AE in ng of chemical assimilated per ng of chemical ingested) following this equation:

$$Q_{in} = AE \cdot \frac{\dot{p}_X}{\varrho_X} \cdot C_X \qquad \text{Eq. 1}$$

AE is the TK parameter that describes the proportion of the chemicals ingested with food that is assimilated by the fish. This approach was used in Bodiguel et al. (2009) and Eichinger et al. (2010). In this approach, contaminants in the faeces represent the non-assimilated part of ingested contaminants. Based on ingestion rate dynamics predicted by the DEB model, the uptake flux of contaminants thus depends on environmental conditions as well as their predicted effects on fish growth (i.e., $\dot{p}_X$ depends on growth, temperature, and food availability, see Mounier et al., submitted, this special issue).

A3. Elimination

Previous DEB-TK models (Bodiguel et al., 2009; Eichinger et al., 2010) neglected elimination of their studied compounds as negligible biotransformation and excretion rates are assumed for many PCB congeners (Kim et al., 2016). However, excretion and biotransformation are known to be major processes of decontamination in fish for some PFASs (Hassell et al., 2019) and for some PCB congeners, depending on their chemical structure (Arnot et al., 2008; Kannan et al., 1995; Sijm et al., 1992).

In our DEB-TK, elimination was considered using a second TK parameter, the elimination rate ($\dot{k}_e$, in d^{-1}), that quantifies gill elimination, metabolic transformation, and faecal elimination (i.e., due to the chemical partition between the organism and the digested food in guts). As well as other metabolic

rates, elimination rate is supposed to be affected by temperature (see Kooijman et al., 2009 for general theory, and Borgå et al., 2010 for an application of this principle to the study of climate change impacts on bioaccumulation in a food web). Thus, $\dot{k}_e$ was defined as the daily diminution of the contaminant concentration in fish (c in ng.cm^{-3}) at the reference temperature (T_{ref} =20°C). It was then corrected by the actual temperature (T) following the same Arrhenius temperature correction factor as for all the DEB energetic fluxes (cT, dimensionless, see Mounier et al., submitted, this special issue). We assumed first order elimination kinetics (i.e., no saturation). Consequently, the daily evolution of c due to elimination is equal to:

$$\dot{c}_{out} = \dot{k}_e \cdot cT \cdot c \qquad \text{Eq. 2}$$

A4. Computation of fish contamination

Fish internal concentration is expressed per unit of somatic volume (V_w in cm^3). V_w is the sum of the structural volume (V) and the reserve volume (V_E) computed from the DEB model (with $V_E = E/(\varrho_E \times d_V)$, which assumes that densities of reserve and structure are equal).

The equation describing the evolution of the fish internal concentration (c in ng.cm^{-3}) from ingestion of contaminated food, growth dilution and elimination is:

$$\frac{dc}{dt} = \frac{Q_{in}}{V_w} - \frac{1}{V_w} \cdot \frac{dV_w}{dt} \cdot c - \dot{c}_{out} \qquad \text{Eq. 3}$$

By using Eq. 1 and Eq. 2, Eq. 3 can be written in details as follows:

$$\frac{dc}{dt} = \frac{AE \cdot \frac{\dot{p}_X}{\varrho_X} \cdot C_X}{V_w} - \frac{1}{V_w} \cdot \frac{dV_w}{dt} \cdot c - \dot{k}_e \cdot cT \cdot c \qquad \text{Eq. 4}$$

Chemical body burden (Q in ng) can be thus calculated as the product of c and V_w. Contaminant mass concentrations in fish (C_w in ng g_{fish}^{-1} ww) can be calculated from Q and corresponding total weight predicted by the DEB model (W_w).

Appendix B. Graphic representations associated to the datasets used

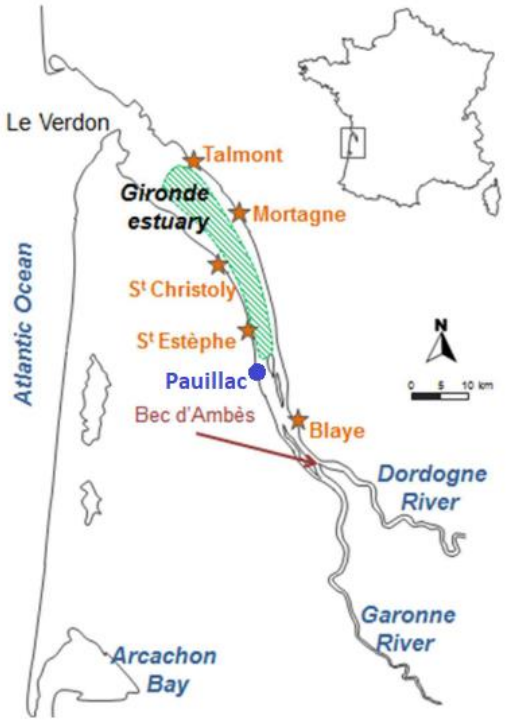

Figure B1 - General setting of the Gironde estuary (SW France) adapted from Munoz et al. (2017). Location of intertidal mudflats sampling sites for benthic invertebrates (orange stars), fish sampling zone (green hatched area) and MAGEST water measurement station (blue dot).

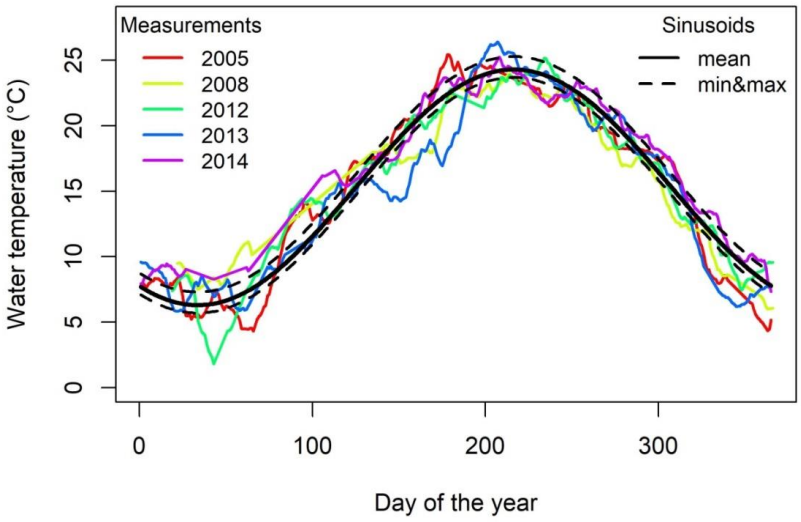

Figure B2 - Daily mean water temperature in Pauillac (central part of the Gironde estuary) from MAGEST monitoring program for the 5 selected years (years with limited missing data from 2005 to 2016) and sinusoids with mean (solid line), minimum and maximum (dotted lines) average annual temperature ($\widehat{T}$) (see section Erreur ! Source du renvoi introuvable. of the main document).

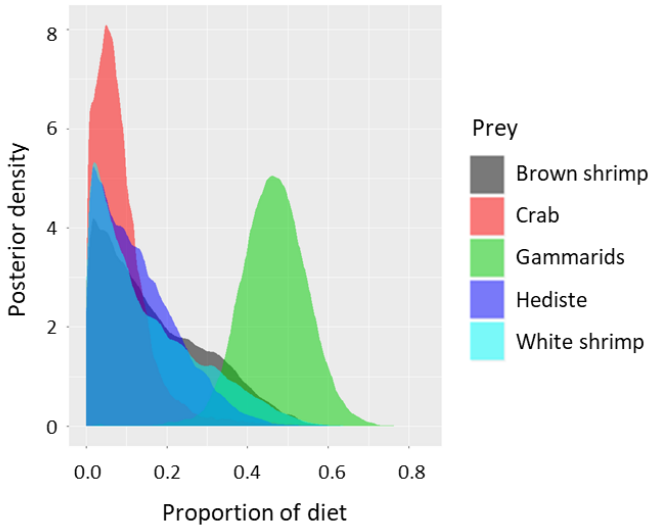

Figure B3- Probability density (in y-axis) of the proportion (in x-axis) of each of the listed preys in the diet composition of the common sole in the Gironde estuary estimated by ESCROC using both N- and C- isotopic ratios and 5 PFAS concentrations. Figure from (Ballutaud et al., 2019)

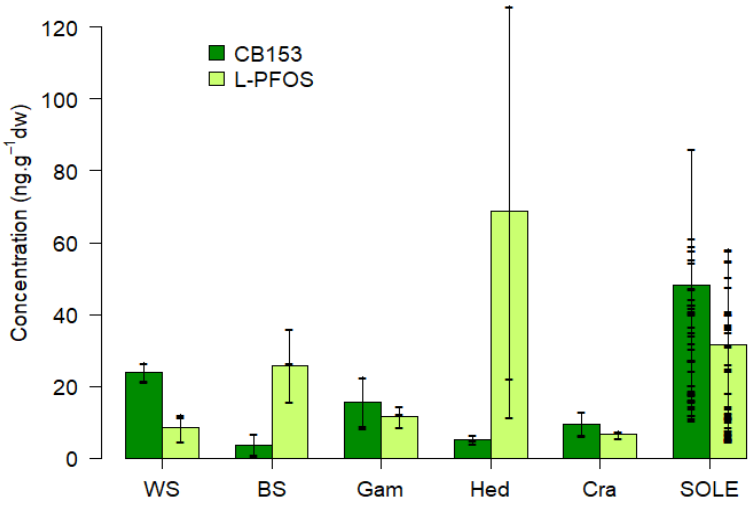

Figure B4 - Preys and fish contamination levels reported for the Gironde estuary for CB153 (from Lauzent 2018) and L-PFOS (Munoz 2015; Munoz et al. 2017). Barplots represent contamination mid-ranges. Vertical bars cover contamination ranges. Ticks represent each sample value. WS: White shrimp, BS: Brown shrimp, Gam: Gammarids, Hed: ragworm, Cra: shore crab.

Appendix C. Temperature sinusoids considering birth date variability

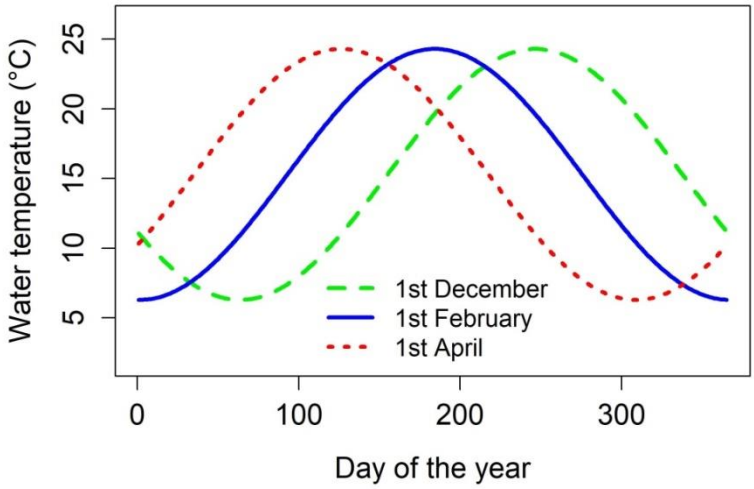

Figure C1 - Temperature sinusoids associated with fish born at the reference birth date (1st February in blue solid line), the earliest (1st December in green dashed line) and the latest (1st April in red dotted line) birth dates from the spawning season.

Appendix D. Detailed results from global sensitivity analysis

Table D1 - Sobol' indices (Si and STi) computed values for each sex, each model output and each model input.

		Female				Male			
		Si		STi		Si		STi	
Output	Input	original	std. err.	original	std. err.	original	std. err.	original	std. err.
Age	birth	0,018	0,012	0,027	0,001	0,015	0,013	0,023	0
	temp	0,093	0,012	0,1	0,002	0,089	0,013	0,095	0,002
	avail	0,195	0,011	0,204	0,003	0,193	0,011	0,203	0,003
	quality	0,676	0,005	0,688	0,01	0,688	0,005	0,697	0,011
Length	birth	0,001	0,012	0	0	0,001	0,013	0	0
	temp	0,001	0,012	0	0	0,001	0,013	0	0
	avail	0,231	0,011	0,232	0,003	0,23	0,011	0,232	0,004
	quality	0,768	0,003	0,769	0,011	0,768	0,004	0,769	0,011
CB153	birth	0,001	0,019	0	0	0,001	0,017	0	0
	temp	0,001	0,019	0	0	0,001	0,017	0	0
	avail	0,001	0,019	0	0	0,001	0,017	0	0
	quality	0,008	0,019	0,012	0	0,008	0,018	0,012	0
	contam	0,381	0,017	0,48	0,013	0,383	0,017	0,481	0,012
	AE	0,226	0,02	0,307	0,008	0,227	0,018	0,308	0,007
	ke	0,258	0,02	0,339	0,008	0,256	0,019	0,337	0,008
L-PFOS	birth	0	0,014	0	0	0	0,015	0	0
	temp	0	0,014	0	0	0	0,015	0	0
	avail	0,001	0,014	0,001	0	0,001	0,015	0,001	0
	quality	0,003	0,015	0,006	0	0,003	0,014	0,006	0
	contam	0,704	0,007	0,76	0,013	0,705	0,006	0,76	0,013
	AE	0,09	0,016	0,119	0,002	0,09	0,016	0,119	0,002
	ke	0,139	0,016	0,177	0,003	0,138	0,015	0,176	0,003

Appendix E. Local sensitivity analysis « One step at a time »

E1. Method

A local sensitivity analysis was carried out to quantitatively measure the influence of each model input on both types of model outputs we selected (related to growth and contamination predictions). It consists in applying to one input parameter at a time a small variation around its nominal value.

First, reference values for selected outputs were estimated by setting all input parameters to their nominal value. Then, sequentially, nominal value of each model input was increased by 25% of its range of variability, while keeping the other ones at their nominal values. The effect of the input variation on model outputs was quantified by the percentage difference of the predicted output to its reference value. For age and length outputs, sensitivity to food contamination and TK parameters inputs weren't studied.

Ranges of variability and nominal values are summarised in Table SI 2. Ranges were defined in the section 2.4 of the main document. Nominal values were set using the same data as presented in the section 2.4 of the main document and defined as follows: $\hat{T}$ to the mean of $\hat{T}$ values for the different years, d_b to the mid-time of the spawning period (the 1st of February), f to the median of f estimated for the 8 males considered, ϱ_X to the median of computed ϱ_X for the different diets, C_X to the median of computed C_X, and AE and $\dot{k}_e$ to their respective mid-range of variation for each contaminant.

Table E1- Summary of inputs nominal values and range of variability used in the sensitivity analysis.

Description	Symbol	Unity	Nominal [Min – Max]
Average annual temperature (temp)	$\hat{T}$	°C	15.3 [14.7 – 16.3]
Day of the year at birth (birth)	d_b	d	32 [335 – 90]
Food availability (avail)	f	-	0.588 [0.547 – 0.627]
Food energy density (quality)	ϱ_X	$J.g^{-1}$ dw	16,412 [14,047 – 18,034]
Food contamination (contam)	C_X	$ng.g^{-1}$ dw	CB153: 12.4 [3.3 – 24.5] L-PFOS: 20.6 [6.2 – 79.3]
Assimilation efficiency of contaminant	AE	-	CB153: 0.63 [0.26 – 1] PFOS: 0.76 [0.53 – 1]
Elimination rate at 20°C	$\dot{k}_e$	$10^{-2}.d^{-1}$	CB153: 1.34 [0.45 – 2.24] PFOS: 8.25 [5.22 – 11.28]

E2. Results

Overall, local sensitivity analysis showed that fish contamination is more sensitive than age and length to small variations of model inputs one at a time (Figure). Indeed, the deviations of the predicted contamination from their reference values were approximately 8 fold higher than those for age and length. Among biological outputs, age deviations to its reference were up to 10 times greater than for length for which all deviations exhibited negligible increases (i.e., less than 1 mm variations, see Table). Also, age at puberty was the only model output for which a difference between female and male was observable in the sensitivity to model inputs variations (i.e., 7 days, c.f. SI section 4).

Compared to the other model inputs, the date of birth within the spawning season (“birth”) had nearly no effect on the model outputs. Mean annual temperature (“temp”) only affected age at puberty, by lowering it by approximately 2% (i.e., ≈2 weeks, c.f. SI section 4).

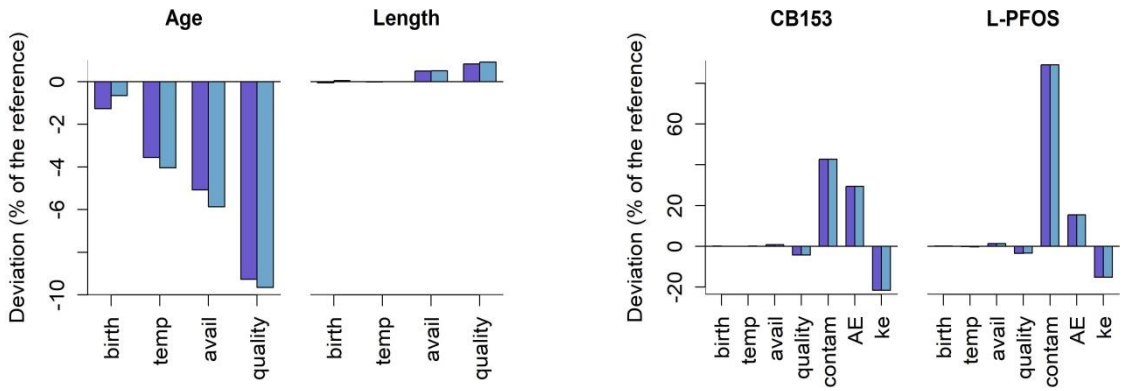

Figure E1 - Percentage of deviation from the reference value (y-axis) for age, length, CB-153 and L-PFOS contamination level predicted at puberty for female (F) and male (M) for a +25% increase of each model input (x-axis). Reference values of model ouputs and deviation values can be found in Table SI 2.

Model inputs related to food had greater impacts on biological traits and fish contamination. An increase in food availability (“avail”) or energy density (“quality”) led to a decrease in age at puberty and an increase in length at puberty. For both of these model outputs, availability had approximately half the effect of quality. For female, “avail” and “quality” respectively induced, at puberty, a decrease of approximately 3 and 5 weeks in age and of 0.4 and 0.8 mm in length.

Fish contamination wasn’t substantially affected by sex and environmental inputs (<2%), with the exception of food contamination (“contam”), whose variation had a greater impact on L-PFOS than CB153 (36 and 17% respectively). Concerning TK parameters, a 10% increase in the assimilation efficiency (“AE”) nominal value induced a 20% increase for both contaminants. The increase in the elimination rate (“ke”) induced a decrease of 3% and 5% for CB153 and L-PFOS contaminations respectively.

Table E2 - Detailed results from local sensitivity analysis. Model outputs deviations to their reference value are given in their unit and their percentage of deviation are given in brackets. Reference values of model outputs are given in their respective units. Model input variations of +25% of their range of variability are given in brackets. Contaminant-specific inputs values are presented as follows: "CB153 / L-PFOS".

	Output	**Age at puberty days**		**Length at puberty cm**		**[CB153] ng.g^{-1} ww**		**[L-PFOS] ng.g^{-1} ww**	
	Sex	F	M	F	M	F	M	F	M
	Reference value	777	757	21.79	20.62	1.85	1.87	0.70	0.71
Environment	birth (+ 30 days)	-10 (-1.3%)	-5 (-0.7%)	-0.01 (-0.05%)	0.01 (0.05%)	0.00 (0.14%)	0.00 (0.04%)	0.00 (0.18%)	0.00 (0.11%)
	temp (+ 0.40 °C)	-28 (-3.6%)	-31 (-4.0%)	-0.00 (-0.02%)	0.00 (0.00%)	-0.00 (-0.06%)	-0.00 (0.07%)	-0.00 (-0.18%)	-0.00 (-0.31%)
	avail (+ 0.02)	-39 (-5.1%)	-44 (-5.9%)	0.1 (0.49%)	0.1 (0.50%)	0.02 (0.82%)	0.02 (0.84%)	0.01 (1.4%)	0.01 (1.3%)
	quality (+ 997 J.g^{-1} dw)	-72 (-9.3%)	-73 (-9.6%)	0.2 (0.8%)	0.2 (0.9%)	-0.08 (-4.3%)	-0.08 (-4.3%)	-0.02 (-3.4%)	0.02 (-3.4%)
	contam (+ 5.3 / 18.3 ng.g^{-1} dw)	0.0	0.0	0.0	0.0	0.79 (42.7%)	0.80 (42.7%)	0.62 (89.0%)	0.63 (89.0%)
TK	AE (+ 0.2 / 0.9)	0.0	0.0	0.0	0.0	0.54 (29.4%)	0.55 (29.4%)	0.11 (15.4%)	0.11 (15.4%)
	ke (+ 0.4 / 1.5 10^{-2}.d^{-1})	0.0	0.0	0.0	0.0	-0.40 (-21.6%)	-0.40 (-21.6%)	-0.11 (-15.2%)	-0.11 (-15.1%)

N.B.: Considering DEB model properties, temperature doesn't affect the state variable values at a given point of development as it affects each energy flux in the same way. So, the slight effect on length and contamination of temperature change included in "birth" and "temp" was due, in our results, to the discretization of model predictions leading to a slightly different state of the system considering the first time step after crossing the maturity threshold.

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