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RESEARCH ARTICLE

ESCROpath, a Bayesian mixing model to quantify diets and trophic flows in aquatic food webs

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Abstract

1. Food-web modelling is a key tool to provide a global and comprehensive knowledge on community structure, biodiversity and ecosystem processes and functioning. In particular, it allows computing integrative and holistic indices describing food web characteristics, topology and functioning. However, one of the main sources of uncertainty in most food-web models is the estimation of diet matrices.
2. In the present work, we propose an innovative approach that combines (a) a Bayesian mixing model using both isotopes and contaminants as chemical tracers with (b) classical mass-balance equations. This dual approach allows the simultaneous estimation of diet composition, isotopic enrichment, contaminant biomagnification, and contaminants and biomass flows in the whole food web. This original model named ESCROpath also provides food-web indices derived from ecological network analysis (ENA). As a case study, the approach was implemented in the Gironde estuarine food web (SW France) for which isotopes, contaminants and trophic data exist. Two sets of priors were constructed accounting for more or less uncertainty in trophic parameter estimates. Outputs were compared with previous published Ecopath results.
3. A constrained calibration led to very similar outputs as Ecopath (which shows that the method is able to find the initial set of parameters if it is forced to do so), whereas a free calibration led to slight differences in trophic parameters and ENA indice estimations (which shows that the Ecopath solution was not fully optimal). Quite different diet matrices and estimations of flows distribution within the food web can thus be obtained.
4. ESCROpath is an original flexible food-web modelling tool that, for the first time, makes it possible to go from a model mainly built on an 'estimate' of the parameters based on expert knowledge (which constitutes the main criticism formulated against Ecopath) to a statistical Bayesian framework for the estimation of the trophic parameters. It thus provides a very integrated framework for

food-web modelling by estimating simultaneously trophic parameters, diet compositions and trophic enrichment/magnification factors. By doing this, it notably provides reliable and robust uncertainty estimations for output parameters.

KEYWORDS
Bayesian mixing model, contaminants, food-web modelling, isotopes, uncertainty

1 | INTRODUCTION

Food-web ecology is a key tool to provide a global and comprehensive knowledge on ecosystems combining insights on both community structure and biodiversity in one side and ecosystem processes and functioning on the other side (Livingston, 2002; Thompson et al., 2012). Indeed, trophic interactions are among the main drivers of ecosystem functions (Ings et al., 2009) and have been shown to be modified by ecosystem fragmentation (Terborgh et al., 2001), climate change (Chevillot et al., 2017) or alien species (Cloern, 1996). Moreover, trophic flows are a major pathway for the spread of pollutants in food webs (Kelly et al., 2007).

By providing qualitative features of species interactions and/or quantitative outputs on biomass and energy flows or interaction strength, food-web modelling allows computing integrative and holistic indices describing food web characteristics, topology and functioning (e.g. Christian et al., 2005; Fath et al., 2019). Such network analyses are now proposed as components of aquatic ecosystem assessments. Some indices, mainly derived from the ecological network analysis (ENA; Fath et al., 2007; Kones et al., 2009; Saint-Béat et al., 2015; Ulanowicz, 2004), are being considered to be implemented into environmental directives (Le Guen et al., 2019; Safi et al., 2019) or ecosystem-based management strategies (Mulder et al., 2017; Raoux et al., 2018, 2019). Furthermore, food-web modelling is an important tool to describe and quantify trophic transfer of contaminants (De Laender et al., 2009). This is particularly crucial for many marine and freshwater ecosystems as anthropogenic pollution has been identified as one of the main factors affecting their ecological quality (Matthiessen & Law, 2002; Verhoeven et al., 2006).

One of the main source of uncertainty in most food-web model is the estimation of diet matrices, which define the proportion each prey type in the diet of each predator (e.g. Ainsworth et al., 2010; Bentley et al., 2019; Masi et al., 2014; Morzaria-Luna et al., 2018). There are different strategies to address the construction of diet matrices in food-web models. For instance, in Ecopath with Ecosim (Christensen & Pauly, 1992; Polovina, 1984), one of the most widely used modelling approaches for marine food webs, observation data, literature review and expert knowledge are compiled to achieve one single predator–prey interaction matrix, to which a certain level of uncertainty can be associated. In the last decade, various methods have been implemented to account for this uncertainty (as well as for other trophic parameters; e.g. Guesnet et al., 2015 or Steenbeek et al., 2018) such as Monte Carlo exploration of a range of possible values for each predator–prey interactions. However, the range of possible values still remains mainly compiled from literature concerning other systems or time-scales.

A relevant way to calibrate a diet matrix using in situ observations is to use isotopic data from in situ measurements (Boecklen et al., 2011). In particular, combining knowledge of trophic interactions with outputs from isotopes mixing models such as MixSIR (Moore & Semmens, 2008), SIAR and MixSIAR (Parnell et al., 2008, 2013; Stock et al., 2016, 2018) provides estimate distributions of prey contributions to the predator's diet. Such outputs can be integrated in food-web models such as food-web linear inverse modelling (LIM; Pacella et al., 2013). The EcoDiet tool (Hernvann et al., 2020; Thero et al., 2020) integrated such a Bayesian mixing model approach where gut contents and knowledge from the literature define the topology and the prior distributions of the diet matrix parameters.

Recently, Ballutaud et al. (2019) proposed an original Bayesian method, the ESCROC model. ESCROC, as with classic isotope mixing models like MixSIAR, assumes that the chemical signature of a predator is a weighted mixture of the signatures of its predated preys, plus a potential trophic enrichment (or discriminant) factor (TEF). Chemical signatures are based on any chemical elements that can be used as tracers of trophic interactions through the food web so long as the tracers mix conservatively or with an additive (e.g. isotopes, fatty acids) or multiplicative (such a situation is linear in a log scale, e.g. contaminants) enrichment. This approach simultaneously estimates diet contributions across an entire network of consumers (plus estimating the enrichment factors) using both isotopic composition and contamination data, leading to more robust food-web descriptions. Furthermore, this model provides a reliable and rigorous assessment of both contaminant trophic magnification and accurate estimations of isotope TEF and their associated uncertainties in food webs.

In the present work, we combine biomagnification, diet estimation and food-web modelling into a single, innovative model. This model combines (a) a Bayesian mixing model using both isotopes and persistent organic pollutants (POPs) as chemical tracers with (b) classical mass-balance equations. This dual approach enables the simultaneous estimation of diet composition, isotopic enrichment (TEF), contaminant biomagnification (trophic magnification factor, TMF) and contaminants and biomass flows in the whole food web. This original model derived from ESCROC and named ESCROpath also provides food-web indices derived from ENA.

As a case study, the ESCROpath approach was implemented in the Gironde estuarine food web on which the ESCROC model had been developed (Ballutaud et al., 2019) and for which an Ecopath model already exists (Chevillot et al., 2019). This Ecopath model was reshaped and the calibration adjusted in order to be directly compared with ESCROpath outputs, thereby allowing the discussion of advantages and limitations of both modelling approaches.

2 | MATERIALS AND METHODS

2.1 | The ESCROpath model

2.1.1 | Equations and parameters

The model is derived from the ESCROC model to which has been added a module to describe biomass flows based on Ecopath mass-balanced equations. Since ESCROC is detailed in Ballutaud et al. (2019), we only focus here on the most important aspects of this model and on the modifications brought to build ESCROpath.

Basically, ESCROC relies on the same assumptions as classical isotope mixing models like MixSIAR for describing both isotope signature and contaminant concentration (both referred to as the signature of tracer *t*) of a predator species *e* that consumes prey*p*. The main equation can be written as follows for all chemical tracers:

$$Y_{e,t} = \sum_{p \in prey(e)} \left(\rho_{e,p} \cdot Y_{p,t}\right) + \Delta_t + E_{e,t} \text{ with } E_{e,t} \sim \mathcal{N}\left(0s_t^2\right), \qquad (1)$$

where $Y_{e,t}$ is the average signature for a tracer *t* for species *e*; $\rho_{e,p}$ is the diet contribution of prey *p* for consumer *e*; $Y_{p,t}$ is the measured mean signature of tracer *t* value for prey *p*; Δ_t is the food-web average enrichment factor for tracer *t*; $E_{e,t}$ is the species random effect for species *e* and tracer *t* with s_t^2 the associated variance.

The measured signature $Y_{i,e,t}$ of an individual *i*, from species *e*, for tracer *t* is assumed to follow a normal distribution:

$$Y_{i,e,t} \sim \mathcal{N}\left(Y_{e,t}V_{e,t}\right) \qquad (2)$$

with $V_{e,t}$ the variance of tracer *t* within the species *e* defined as a function of the variances of its prey:

$$V_{e,t} = \sum_{p \in prey(e)} \left(\rho_{e,p}^2 \cdot V_{p,t}\right) + \gamma_t, \qquad (3)$$

where γ_t is an error variable added to account for potential noise.

The main innovation of ESCROC was to acknowledge that contaminants may be used as additional tracers of trophic relationships in a similar way as isotopic ratios. Thus, the previous equations are also valid for a contaminant, except that Δ_t is an indicator of biomagnification (TMF) instead of an enrichment factor (TEF). Thus, it allows estimating these parameters (TEF, TMF, hereafter called TEF) and diet composition simultaneously at the whole food web scale.

Since diets are key input parameters of most food-web models, we combine here ESCROC with trophic mass-balance equations in order to use biomass as an additional tracer of trophic relationships. In order to make our model understandable and accessible to the greatest number of users, it is based on the Ecopath model (Christensen & Pauly, 1992; Polovina, 1984), widely used in aquatic ecology. However, the equations remain generic. Thus, in ESCROpath, the biomass of a living prey *p* (B_p) given biomasses of its predators *e*is computed as follows:

$$B_p \cdot EE_p \cdot (P/B)_p = H_p + \sum_{e \in pred(p)} \rho_{e,p} \cdot (Q/B)_e \cdot B_e. \qquad (4)$$

Equation (4) expresses the part of the production (standing biomass B_p times productivity potential$(P/B)_p$) of *p* consumed in the system (times ecotrophic efficiency EE_p) as the sum of harvesting (H_p, if any, e.g. catches by fisheries) and the total biomass of *p* consumed by all its predators *e*. The latter is equal to the sum, over all *e*'s predators, of the biomass of *p* they consume (biomass of *e* times their consumption rate $(Q/B)_e$) times the contribution of *p* to their diet ($\rho_{e,p}$). Ecotrophic efficiency (*EE*) is a particular parameter that measures the proportion of production utilized in the food web through direct predation or fishing (Heymans et al., 2016).

Note that, in Equation (4), we assumed for simplicity that there is neither biomass accumulation nor export of living biomass to adjacent systems (e.g. migration, except for detritus), but that can be accounted for if required.

All parameters are assigned a prior distribution (see the following section), except harvesting (H_p) that is considered known without error.

Using ESCROC, it was not possible to estimate the signature of 'source species', that is species that do not feed on other species (typically primary producers or detritus). Similarly, it is not possible here to compute the biomass of top predators since no species consumes them. Therefore, we impose a large uniform prior for the biomass of top predators.

Once biomass is known for species *p*, it is possible to compute several flows associated with *p*:

$$\text{Consumption:} \quad Q_p = B_p \cdot (Q/B)_p, \qquad (5)$$

$$\text{Production:} \quad P_p = B_p \cdot (P/B)_p, \qquad (6)$$

$$\text{Unassimilated food:} \quad U_p = Q_p \cdot (U/Q)_p, \qquad (7)$$

$$\text{Respiration:} \quad R_p = Q_p - P_p - U_p, \qquad (8)$$

$$\text{Predation mortality:} \quad BC_p = \begin{cases} 0, \text{ if } p \in \text{top predator} \\ \sum_e \rho_{e,p} \cdot (Q/B)_e \cdot B_e, \text{ else} \end{cases}, \qquad (9)$$

$$\text{Other natural mortality:} M_p = P_p \cdot \left(1 - EE_p\right). \qquad (10)$$

It is beyond the scope of the present paper to explain how each parameter can be estimated using ecological data and/or empirical relationships. However, we can refer the interested reader to the Ecopath literature and especially the user guide (Christensen et al., 2005) for examples concerning aquatic ecosystems.

Detritus *Det* and Primary Production *PP* are particular groups as they do not consume anything. We thus deal with them in a different way that is described in SI (SI1).

Biomasses are estimated using observations (noted *obs*) coming from various sources (e.g. scientific surveys) that can be used to fit the model:

$$Bobs_e \sim \mathcal{N}\left(B_e \sigma^2_{Bobs_e}\right)$$

with $\sigma^2_{Bobs_e}$ the variance of the observation data.

2.1.2 | Model priors

As ESCROpath can be seen as a combination of ESCROC and Ecopath mass-balance equations, two types of priors must be provided regarding each part of the model.

The ESCROC model priors are as follows: diet matrix compiling all diet contributions of each prey to each predators ($\rho_{e,p}$), TEFs for each tracer (isotopes and contaminants—Δ_t) and signatures of source species ($Y_{e,i,t}$). For more details on how these priors are elicitated, see Ballutaud et al. (2019).

In addition, ESCROpath requires priors on the biomasses *B* of top predators, the import of detritus ($Import_{Det}$) and the mass-balance parameters: *EE*, *P/B*, *Q/B* and *U/Q*. Indeed, for instance and contrary to Ecopath, ESCROpath does not compute *EE* as a combination of other mass-balance parameters but provides sets of parameters combinations (including *EE*) that fulfil the mass-balance constraint. For all these parameters but $Import_{Det}$ and *EE*, we use uniform priors between minimum and maximum bounds, based on literature for instance. However, as respiration (R_e) has to be positive, the following condition needs to be verified:

$$(Q/B)_e \cdot \left(1 - (U/Q)_e\right) > (P/B)_e. \tag{11}$$

Thus, while the user provides a prior on *P/B*, we did not use it in the model and instead introduced a new parameter to mimic it, A_e, for which an associated prior based on $(P/B)_e$, $(Q/B)_e$ and $(U/Q)_e$ values is computed.

$$A_e = \frac{(P/B)_e}{(Q/B)_e \cdot \left(1 - (U/Q)_e\right)} < 1. \tag{12}$$

Then, before running the model, 1,000 values of *A* are sampled by drawing uniform production rate (*P* / *B*), consumption rate (*Q* / *B*) and rate of unassimilated consumption (*U/Q*) in their respective uniform priors. The few values greater than 1 are removed and a beta distribution on the resulting sample is fitted for A_e. The parameters of this beta distribution are then used as a prior for A_e.

For *EE*, since this parameter value ranges from 0 to 1 by definition, a beta distribution can be used. A beta distribution Beta(α, β) is defined by two parameters α and β, with mean equals to $\alpha/(\alpha+\beta)$ and concentration equals to $\alpha+\beta$ (which tunes the importance of the prior, a large concentration leading to more informative priors).

For the import of detritus, we propose to use a normal distribution:

$$Import_{Det} \sim \mathcal{N}\left(\mathrm{ImportDetobs}\sigma^2_{\mathrm{importDet}}\right) \tag{13}$$

2.2 | Illustrative example and comparison perspectives

2.2.1 | Comparison perspectives

In order to explore possible uses of ESCROpath and to compare with a standard Ecopath approach, two sets of priors were used regarding trophic parameters. The first one is called $\text{ESCROpath}_{\text{free}}$ and mimics a typical use of ESCROpath, that is a situation in which the modeller has vague idea of the parameters based on the literature and wants to account for the uncertainty in the estimates. A second set of priors, $\text{ESCROpath}_{\text{cons}}$, aimed at mimicking the traditional Ecopath approach in which the user provides a single value for parameters (i.e. not accounting for the uncertainty) except for the *EE* which is traditionally estimated by solving the sets of production and consumption equations in Ecopath. $\text{ESCROpath}_{\text{free}}$ and $\text{ESCROpath}_{\text{cons}}$ are here proposed as ‘standard’ implementations that can easily be used as basis depending—for instance, on available data.

The two sets of priors can be built (summarized in Table 1) from mean plausible parameter values as computed in a standard Ecopath approach and then uncertainty around them can be included: a large uncertainty (uninformative priors) for $\text{ESCROpath}_{\text{free}}$ and a very low uncertainty (very informative priors) for $\text{ESCROpath}_{\text{cons}}$. In more details, we used uniform priors for *P/B*, *U/Q* and *Q/B* ranging from 0.8 to 1.2 times the mean plausible parameter values in $\text{ESCROpath}_{\text{free}}$ while they were constrained in mean plausible values ±0.005 in $\text{ESCROpath}_{\text{cons}}$. We used normal priors for the biomasses, with means equal to mean plausible values and coefficients of variation of 20% for $\text{ESCROpath}_{\text{free}}$ and 1% in $\text{ESCROpath}_{\text{cons}}$. We used beta priors for *EE* with values comprised between 0 and 1. For $\text{ESCROpath}_{\text{cons}}$, we used Beta(1,1) priors, equivalent to uniform distributions from 0 to 1. For $\text{ESCROpath}_{\text{free}}$, a plausible mean *EE* value based on information about the food web from literature has to be estimated and then a ‘concentration’ based on expert knowledge about the level of confidence has to be assigned (see below for an estimation method from the Gironde example).

Regarding $Import_{Det}$, a normal distribution can be used with mean equals to mean plausible value, and $\sigma^2_{\text{importDet}}$ corresponding to a coefficient of variation of 30% for $\text{ESCROpath}_{\text{free}}$ and 0.5% for $\text{ESCROpath}_{\text{cons}}$.

Finally, diet compositions for both ESCROpath sets of priors can be based on a standard diet matrix. For $\text{ESCROpath}_{\text{free}}$, similar to

TABLE 1 Examples of priors proposed for the trophic parameters in the **ESCROpath$_{\mathbf{free}}$** and **ESCROpath$_{\mathbf{cons}}$** approaches. $\overline{P}$ designates the mean plausible value of each parameter. See text for details and Ballutaud et al. (2019) for ESCROC priors. α, β and $\overline{P}$ has to be calibrated. See Table 2 for examples of priors for *EE*

Parameter	Prior distributions	ESCROpath$_{\text{free}}$	ESCROpath$_{\text{cons}}$
P/B, *U/Q* and *Q/B*	Uniform	$\mathcal{U}\left(\left[0.8 \cdot \overline{P} 1.2 \cdot \overline{P}\right]\right)$	$\mathcal{U}\left(\left[\overline{P} - 0.005, \overline{P} + 0.005\right]\right)$
B	Normal	$\mathcal{N}\left(\overline{P}\left(0.2 \cdot \overline{P}\right)^2\right)$	$\mathcal{N}\left(\overline{P}\left(0.01 \cdot \overline{P}\right)^2\right)$
EE	Beta	Beta(α, β)	Beta(1,1)
$Import_{Det}$	Normal	$\mathcal{N}\left(\overline{P}\left(0.3 \cdot \overline{P}\right)^2\right)$	$\mathcal{N}\left(\overline{P}\left(0.005 \cdot \overline{P}\right)^2\right)$
$\left\{\rho_{e,1} \cdots \rho_{e,n}\right\}$	Dirichlet	*Dirichlet* $\left(\left\{\lambda_{e,1} \cdots \lambda_{e,n}\right\}\right)$ where $\lambda_{e,p} = 1$ if *e* feeds on *p* and $\lambda_{e,p} = 0$ otherwise	*Dirichlet* $\left(\left\{100 \cdot \overline{P}\right\}\right)$

the implementation of ESCROC, uninformative priors can be built using a Dirichlet distribution which parameter values are 1 if the species *e* feeds on the prey *p* and 0 otherwise. In ESCROpath$_{\text{cons}}$, to ensure having a diet matrix similar to the one used in Ecopath, we used Dirichlet priors for each species *e*: *Dirichlet* $\left(\left\{100 \cdot \rho_{e,p}\right\}\right)$, with $\rho_{e,p}$ the mean plausible diet values as used in Ecopath.

2.2.2 | The Gironde estuary case study

As an illustrative example, ESCROpath was implemented on data from the Gironde estuarine food web.

For comparison purpose, the previously published Ecopath model (see SI for details) was reshaped to match the same structure (same 16 species) as the ESCROC application from Ballutaud et al. (2019). The tracers used for ESCROpath application were those already combined in ESCROC by Ballutaud et al. (2019) to compute a diet matrix of the Gironde estuary food web. More specifically, it includes a dataset on perfluoroalkyl substance (5 PFAS) contamination in the Gironde estuarine food web (Munoz, 2015; Munoz et al., 2017) and stable isotope signatures of carbon and nitrogen. Details on the data and the priors used for implementing ESCROC can be found in Ballutaud et al. (2019).

Mean plausible values for mass-balance parameters could have been compiled in the same way as they were in Chevillot et al. (2019) for Ecopath modelling. However, again for comparison purpose and simplicity, we directly used Ecopath values, which can be considered as the median of mean plausible values, except for *EE*. Plausible mean *EE* values and associated 'concentration' were estimated based on information about the food web from literature and on our expert knowledge about the level of confidence (Table 2).

2.3 | Implementation and comparisons between Ecopath and ESCROpath outputs

2.3.1 | Implementation

ESCROpath was implemented in the R (R Core Team, 2018) and the integrated development environment (IDE) R-studio. The model being run using CODA (Plummer et al., 2006) and RUNJAGS packages. JAGS (Plummer, 2003) was used to carry out the MCMC sampling, with the R library RUNJAGS (Denwood, 2016) to provide the interface between R and runjags. Convergence can be checked both graphically and with Gelman and Rubin tests (Gelman & Rubin, 1992).

The R package based on the ESCROCR package (Drouineau & Lobry, 2020; Drouineau et al., 2018) implementing the method is available on GitHub (https://github.com/Irstea/escroc). One single package for both methods is provided. Functions were adapted to switch easily between ESCROC and ESCROpath. Thus, if users provide mass-balance data, they will switch automatically to ESCROpath, otherwise they will switch to ESCROC.

Here, ESCROpath was implemented using the dataset and priors defined above. Three parallel chains were run for 150,000 iterations (one-third iterations were kept for analysis) after an adaptation stage of 100,000 iterations and a burnin of 1,000,000 iterations. Convergence was checked both graphically and with Gelman and Rubin tests.

2.3.2 | Outputs

Main outputs of ESCROpath consist in posterior distributions of the estimated ESCROC parameters and above listed ESCROpath trophic parameters.

Furthermore, a set of ecological indices derived from the ENA framework can be computed from ESCROpath outputs. Eight ENA indices are implemented in the present R Package version using the same formulas as in ENAtool (see Chevillot et al., 2019; Guesnet et al., 2015 for details). These indices are as follows: internal Ascendency (Ai—flowbits), relative internal ascendency (Ai/Ci noted Ai_Ci—no unit), Average Path Length (APL), Comprehensive cycling index (CCI—no unit), internal Capacity (Ci—flowbits), Finn Cycling Index (FCI—no unit), Mean Trophic Level (of the catches, MTL—no unit) and Total System Throughput (TST—kgC km^{-2} year^{-1}).

The definitions and interpretations of those indices were detailed by Kones et al. (2009), Saint-Béat et al. (2015) and Ulanowicz (2004).

TABLE 2 Priors for Ecotrophic efficiency (*EE*) in ESCROpath$_{\text{free}}$. The concentration ($\alpha + \beta$) of the beta distribution for *EE* is based on the level of confidence in mean *EE* (expert knowledge). The parameter α was computed from the concentration ($\alpha + \beta$) of the beta distribution and the plausible mean for *EE* ($\alpha/(\alpha + \beta)$)

Group	Comments	Plausible mean *EE* values	References	$\alpha + \beta$	α
1	Potentially abundant prey with potential predators and catch by the CNPE	0.50	Pasquaud et al. (2008, 2012) and Pierre and Lobry (2020)	10	5
2	No predator, no catch	0.10		15	1.5
3	No predator, no catch	0.10		15	1.5
4	No predator, some catches	0.25		10	2.5
5	Abundant prey with potential predators and catch by the CNPE	0.50		10	5
6	No predator, no catch	0.10		15	1.5
7	No predator, no catch	0.10		15	1.5
8	No predator, some catches	0.25		10	2.5
9	Potentially abundant prey with potential predators and catch by the CNPE	0.50		10	5
10	Potentially abundant prey with potential predators and high catches by fisheries and the CNPE	0.75	Béguer (2009), Béguer et al. (2011, 2012), Pasquaud et al. (2008, 2012) and Pierre and Lobry (2020)	10	7.5
11	Potentially abundant prey with potential predators and high catches by fisheries and the CNPE	0.75		10	7.5
12	Abundant prey with potentially high predation rates (fish)	0.25	Chaalali et al. (2013), Chevillot et al. (2016, 2017), David et al. (2005, 2006) and Pasquaud et al. (2010)	5	1.25
13	Abundant prey with potentially high predation rates (fish)	0.25		5	1.25
14	Abundant prey with high predation rates (fish and mysids)	0.50		5	2.5
15	Potentially abundant prey with potentially high predation rates (fish)	0.25	Bachelet and Leconte (2015) and Selleslagh et al. (2016)	5	1.25
16	Lots of uncertainties on biomass and trophic parameters incl. Preys and predators	0.90		1.5	1.35
17	Estuarine food web poorly based on PP	0.25	Savoye et al. (2012)	1.5	0.375

2.3.3 | Comparisons between Ecopath and ESCROpath outputs

First, in order to address uncertainty in reshaped Ecopath parameter values from Chevillot et al. (2019), the ENAtool routine (Guesnet et al., 2015) was implemented. In a first approach and to be consistent with the ESCROpath$_{\text{free}}$ calibration (see above), uncertainty was set to 20% around each parameter (diet contributions and Ecopath parameters) in the resampling procedure and a set of 50,000 balanced models was retained. Uncertainty was assessed analysing the ENA indices the model computes.

Posterior distributions for diet contributions, Ecopath parameters and the eight ENA indices from the two calibrations with ESCROpath were compared with each other and with corresponding ENAtool samples from the reshaped Ecopath model from Chevillot et al. (2019).

3 | RESULTS

ESCOpath$_{\text{free}}$ was run in 1 h 10 min on three 3.5GHz cores. The values of Gelman indices confirmed the model convergence for most parameters. R statistics were lesser than 1.05 for 442/448 parameters with ESCROpath$_{\text{free}}$ (uncomplete convergence for 7 $\rho_{e,p}$ and 1 $E_{e,t}$) and for 418/448 parameters with ESCROpath$_{\text{cons}}$ (uncomplete convergence for 23 $\rho_{e,p}$ and 7 EE_e).

The general diets, compared based on median diet contributions of prey, can be different between methods (Figure 1). For example, ESCROpath$_{\text{free}}$ concludes to a plausible importance of detritus in the Anchovy diet (approx. 30%), whereas ENAtool and ESCROpath$_{\text{cons}}$ conclude to a negligible contribution (<0.05%). Another key difference is the large shift in the importance from detritus to copepod in the diet of sprat from constrained (approx. 35%) to free (near 85%) runs. Differences can also be highlighted in terms of diet diversity

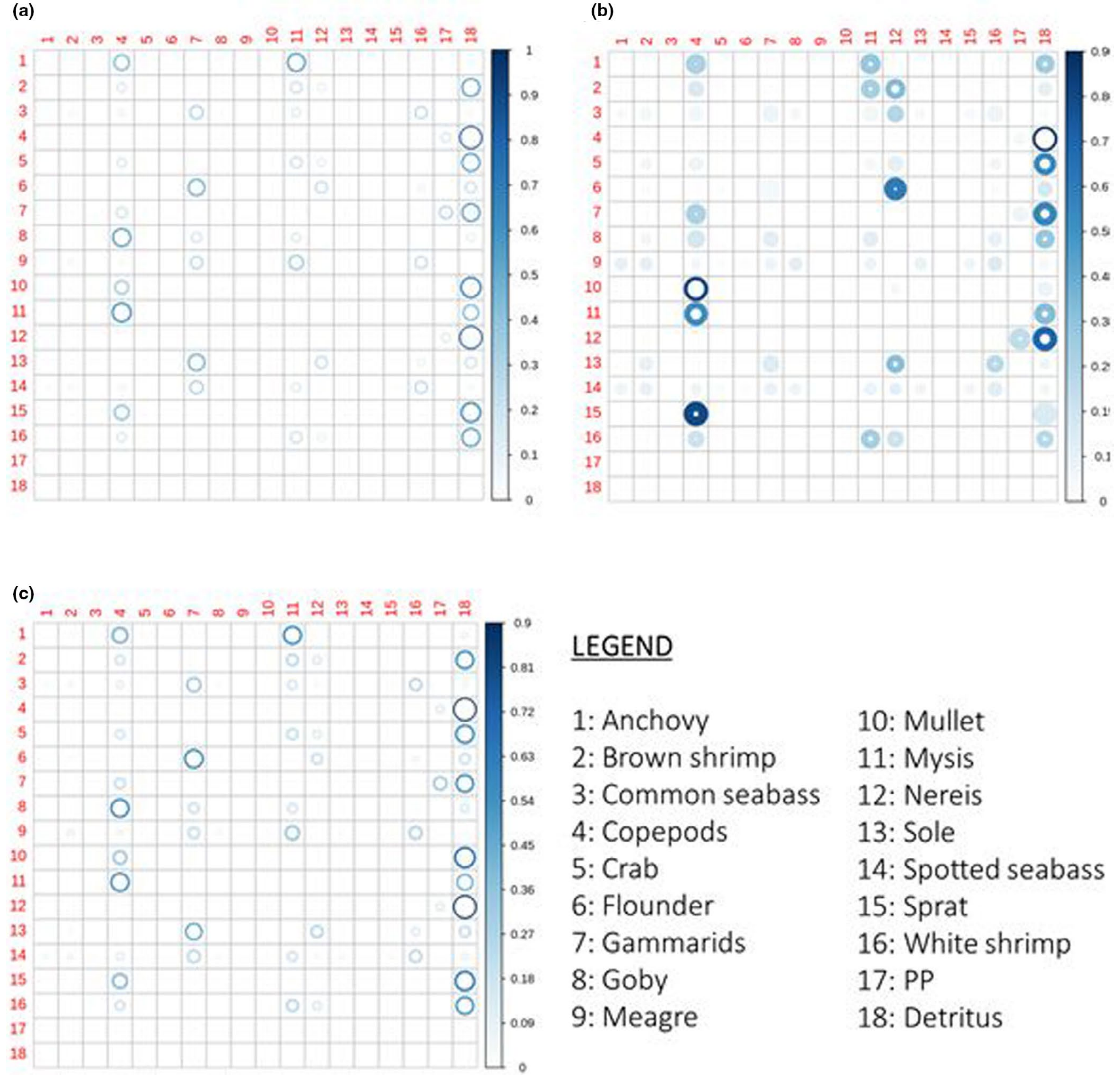

FIGURE 1 Posterior diet matrix values estimated by ESCROpath (b: 'free', c: 'cons' bottom left) and distributions of diet matrices in ENAtools samples (a). Predators are in rows and prey in columns. The size of the circles and the blue colour intensity corresponds to the median of the posterior distribution of the proportion of the prey in the diet of the predator. The thickness of the circle corresponds to the spread of the distribution: the radius internal white circle corresponds to the quantile 2.5% and the radius of the external white circle corresponds to the quantile 97.5% of the posterior distribution. For ENAtool, diagrams stand for the distribution of samples, not posterior distributions. Trophic groups are numbered from 1 to 18 (see legend)

(see SI) and uncertainty. For the latter, ENAtool and ESCROpath$_{\text{cons}}$ provide similar results, with low uncertainty around diet contributions, while diets posterior distributions are wider for ESCROpath$_{\text{free}}$ (Figure 1).

The ranges of TEF/TMF estimates produced by ESCROpath are not significantly different from those produced by ESCROC (see SI for details on values). In addition, although median values can be contrasted between methods, TEF values for δ^{15}N and δ^{13}C estimated by ESCROC, ESCROpath$_{\text{free}}$ and ESCROpath$_{\text{cons}}$ (2.76, 2.61, 2.30 and 1.60, 1.74, 2.32 respectively) are all in line with literature range values (resp. 1.5–5 and 0–3).

By construction, the ranges in trophic parameter output values from ENAtool are directly comparable to the posterior distributions from ESCROpath for each species (Figure 2). Since ESCROpath$_{\text{cons}}$ priors were very narrow, posteriors distributions were thinner and more centred around Ecopath values than ENAtool and ESCROpath$_{\text{free}}$ outputs (except for *EE* which were the only 'free' parameters). Interestingly, despite very limited uncertainties around

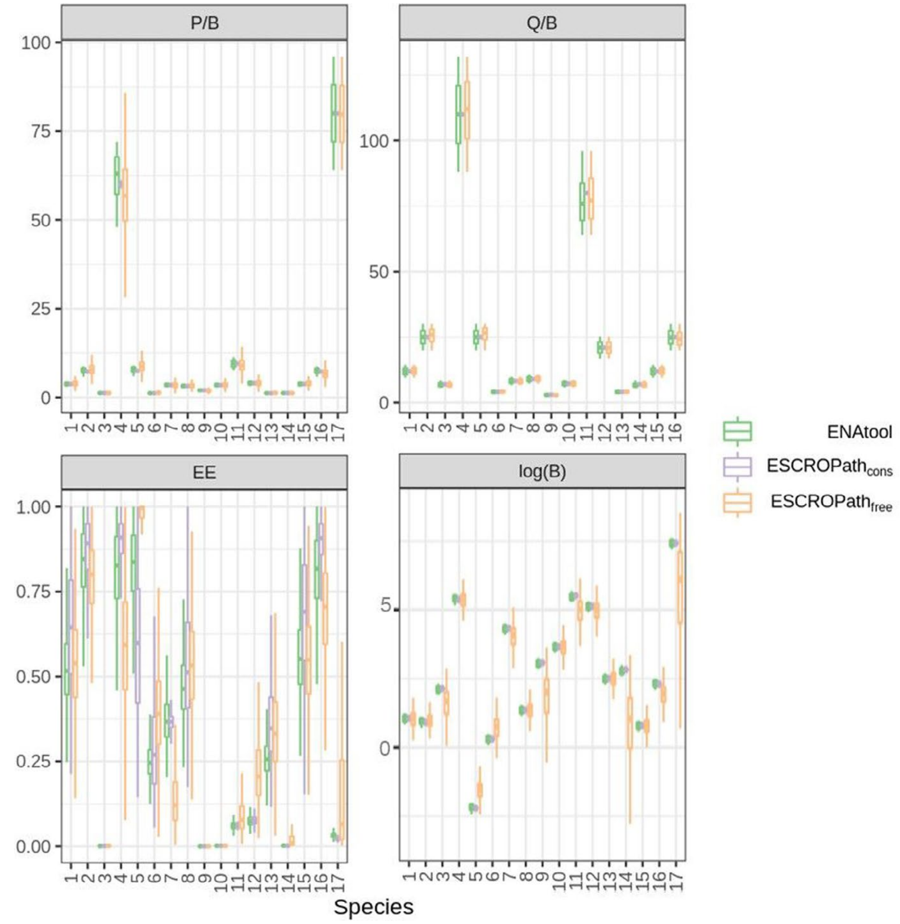

FIGURE 2 Boxplots of (1) Ecopath parameters values and their associated uncertainty computed with ENAtool (in green) and (2) posterior distributions of ESCROpath parameters (in purple and orange) for each species or living group numbered from 1 to 17. P/B (production-biomass ratio, in year^{-1}), Q/B (consumption-biomass ratio, in year^{-1}), EE (ecotrophic efficiency, no unit) and B (biomass, in kgC/km^2). Uncertainties are predicted for the ESCROpath model (but influenced by informative priors; but not for EE) and are an input (less unbalanced possibilities) for the ENAtool. Biomasses are represented in a log scale. See Figure 1 for the legend of the group numbers

most parameters in ESCROpath$_{cons}$, the posterior distributions of *EE* values were very large.

Most computed values are very similar between ENAtool and ESCROpath$_{free}$ for each parameter, including *EE* (Figure 2). *P/B* and *Q/B* values are strictly similar, whereas larger differences concern Biomass of Primary Producers (and to a lesser extent of Sprat and Copepods) and *EE* of Goby, Mysids and Primary Producers (and to a lesser extent of Meagre and Crab).

ENA indice distribution values computed from Ecopath and ESCROpath outputs were graphically compared. Figure 3 shows that values are in similar order of magnitude. Outputs from ENAtool and ESCROpath$_{cons}$ are particularly close. However, except for APL, large differences exist between ESCROpath$_{free}$ values obtained compared with the other method. In particular, the TST values computed with ESCROpath$_{free}$ are approximately 40% lower than those obtained using ENAtool. Consequently, differences are also larger for most indice values derived from TST, namely Ai, FCI, CCI and Ci.

4 | DISCUSSION

4.1 | Highlights

ESCROpath is an original and flexible food-web modelling tool that, for the first time, makes it possible to move from a model mainly built on an 'estimate (and, in some cases, a guesstimate)' of the parameters based on expert knowledge (which constitutes the main criticism formulated against Ecopath) to a statistical Bayesian estimate of all settings directly based on the integration of trophic data. Thus, ESCROpath represents a major methodological leap in food-web modelling. Such an advance is made possible because the model directly integrates isotopes and contaminant data and addresses uncertainty in both trophic parameters and diet matrix simultaneously.

4.2 | Similarities and differences between Ecopath and ESCROpath

By design, ESCROpath is similar in implementation and output to Ecopath. Results show that ESCROpath successfully reproduces Ecopath in a Bayesian implementation. We implemented and compared two parameterizations of ESCROpath to the Gironde estuarine food web. The first, ESCROpath$_{cons}$, mimicked a typical use and resulted in similar outputs of an Ecopath model. This shows that the method is valid, that is able to find the initial set of parameters if it is forced to do so. On the other hand, the free calibration leads to slight differences in trophic parameters and ENA indice estimations, implying that the Ecopath solution was probably over-restrictive and not always consistent with trophic data and that others can be found.

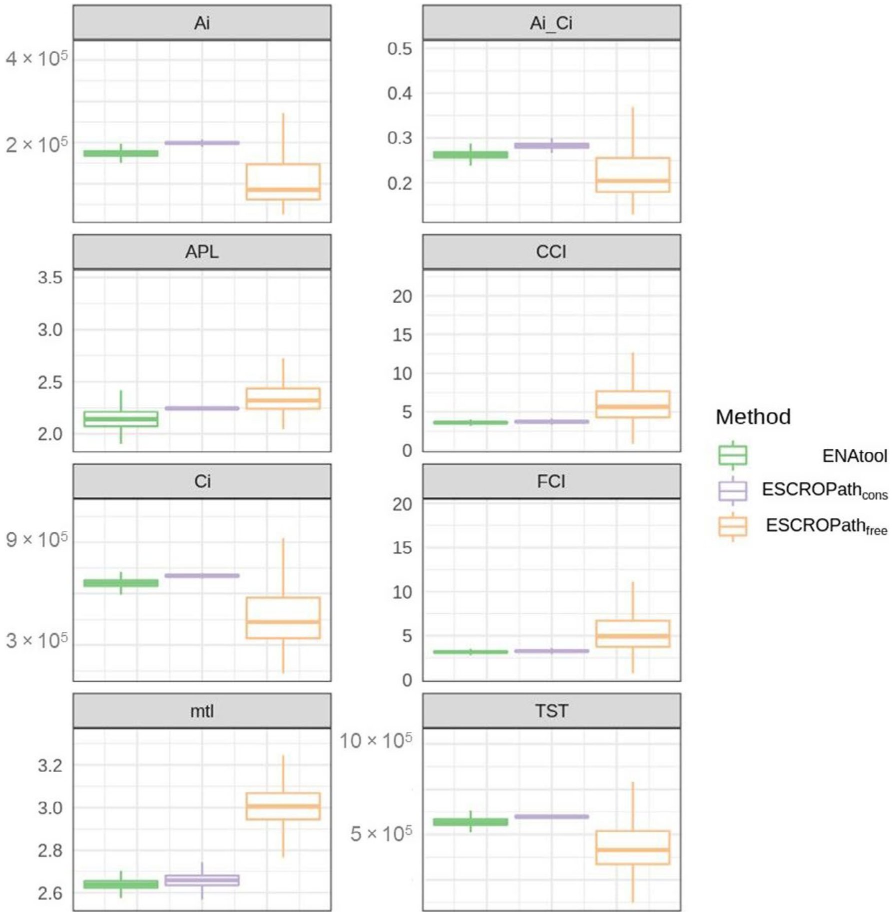

FIGURE 3 Boxplots of ENA indice distribution values computed using ENAtool and ESCROpath. See text for details on the names and units. Ai (internal Ascendency, in flowbits), Ai_Ci (relative internal ascendency Ai/Ci—no unit), APL (Average Path Length), CCI (Comprehensive cycling index, no unit), Ci (internal Capacity, flowbits), FCI (Finn Cycling Index, no unit), MTL (Mean Trophic Level of the catches, no unit) and TST (Total System Throughput, in kgC km^{-2} year^{-1})

First, by essence, the diet matrices are computed differently. In most Ecopath models, they are based on a compilation of in situ observations (mainly contributions inferred from previous stable isotopes studies and stomach contents), expert judgements and literature data (potentially ex situ). This was the case in the Gironde application used here (Chevillot et al., 2019). The same kind of data can be used in the ESCROpath approach (literature and expert knowledge through priors on the diet matrix, isotopes signatures through signature observations), but ESCROpath also incorporates chemical tracers (isotopes, contaminants or other tracers) and species biomasses to compute inference and estimate all parameters. Thus, it allows calibrating a whole food-web model directly on trophic data. This can lead to different diet matrices hence to different estimations of flow distribution within the food web. In the Gironde case study, inferred diet matrices were more uncertain with ESCROpath$_{\text{free}}$ than the space explored by ENAtool (theoretically 20% around Ecopath value, though the exploration might be restricted to achieve mass-balance). However, this is more representative of the real uncertainty surrounding this matrix since it integrates all sources of uncertainty. Since diets and, consequently, flow matrices differ, the mass-balance for each trophic group can thus be impacted and provide different outputs for trophic parameters (i.e. notably for *B* and *EE*). For instance, in the Gironde food web, both brown and white shrimps have very similar trophic parameters in the Ecopath calibration (based on literature), whereas ESCROpath$_{\text{free}}$ led to different estimates of *EE*. Conversely, shifts on Anchovy and Sprat diets between constrained and free runs can be explained by a wider exploration of the range of parameter values. For instance, *EE* values of Copepods are less constrained in ESCROpath$_{\text{free}}$ allowing greater predation flows to Sprat, facilitating greater inclusion of Copepods into the diet that better reflects their known trophic ecology as zooplanktivores (Pasquaud et al., 2010). This, once again, highlights the fact that Ecopath constrained and rigid sets of calibration parameters can lead to forced and not necessarily realistic solutions, whereas ESCROpath, by rigorously exploring uncertainty, enables access to more plausible outputs. Moreover, there was poorer convergence for the constrained than for the free implementation. Strongly constraining the model with priors that are not necessarily compatible or consistent leads to restricted combinations of parameter values. Thus convergence could be more difficult to reach, especially for *EE*. However, by being pragmatic, one can assume that uncompleted convergence is not necessarily problematic as posterior distributions for the parameters concerned are very large. Better-informed priors could probably improve convergence.

Another notable difference in the present application lies in the difference of biomass outputs between ENAtool and ESCROpath$_{\text{free}}$. In the latter, there were no priors implemented for the diets of primary consumer groups feeding on Detritus and PP (Copepods and Nereis) while such input values are obligatorily set in Ecopath DC matrices. In addition, there were no chemical signatures for PP. This likely explains the difference, ESCROpath$_{free}$ yielding a food web with a lower biomass but more efficient PP (i.e. a lower primary production with a larger part of consumed production and thus a higher *EE*). Note that, while such priors were not used in ESCROpath$_{free}$, ESCROpath allows the use of informative priors on the diets of any species (this was done for example in ESCROpath$_{cons}$ to 'mimic' the Ecopath diet matrix) and the use of chemical signatures for PP if such data are available. Such priors for diet can for instance be constructed by using the Ecodiet framework proposed by Thero et al. (2020) and Hernvann et al. (under review).

The difference in primary production between the two models leads to difference in the flow matrix, and consequently on ENA indices. More specifically, the higher *EE* value combined with a lower biomass in ESCROpath$_{free}$ leads to a limited flow of PP to Detritus compared to ENAtool. Mechanistically, this difference explains the difference in TST and all TST-derived ENA indices.

Interestingly, *EE* posterior distributions were large given the limited uncertainty on other parameters. This could be related to a poorer convergence of the Markov chains during simulations. However, this also suggests that the n-dimensional space defined by all parameter values in the initial Ecopath calibration (by Chevillot et al., 2019) is difficult to appropriately explore and sample, probably because of strong correlations among parameters. More specifically, *EEs* in Ecopath are very sensitive to other parameter values. Ecopath is a purely top-down model. By extension, and as we used the same mass-balance equations with the same *EE* buffer parameter, ESCROpath is a top-down model as well. However, the Bayesian estimation framework leads to a much more bottom-up propagation of the constraints. Indeed, (a) predator diets are estimated based on prey signatures and (b) all parameters are estimated together (including relative values between P/B and Q/B for both preys and predators). These two points counterbalance the top-down nature of the mass-balance equations and lead to a well-balanced approach of the food web.

4.3 | Originality

ESCROpath provides a statistical framework for the estimation of all food-web parameters. This directly relies on an innovative mixing model for the estimation of the whole diet matrix (Ballutaud et al., 2019). Indeed, classical mixing models have certain technical and methodological limitations. First, in MixSIAR approaches, predators are considered one by one independently, which imposes to multiply MixSIAR estimation procedures when the considered food web include numerous predators. Second, mixing model estimates are highly sensitive to the uncertainty in TEF values (Bond & Diamond, 2011; Caut et al., 2009) which are generally fixed (and then discussed) before the estimation procedure. Similar to Isoweb (Kadoya et al., 2012), ESCROC addresses these limitations by proposing a novel isotope mixing model that (a) estimates the diet composition of all consumers in a food web simultaneously and (b) addresses uncertainty in TEF. Furthermore, ESCROC also uses contaminants as trophic tracers that allows computing diet matrices using both isotopic composition and contamination data, leading to more robust food-web descriptions. This kind of approach has already been used with fatty acids for instance (Neubauer & Jensen, 2015) and is potentially useful across a range of food-web studies (Majdi et al., 2018).

Most importantly, the main strength of ESCROpath is that it provides a reliable and robust way of quantifying the uncertainty in input parameters of food-web models and propagate it to the calculation of various indicators. By directly integrating biotracers in the model, ESCROpath allows a direct and realistic assessment of this uncertainty that is related to the diet matrix, which, to our knowledge, has never be done due to the difficulties of coupling tools such as LIM and SIAR (Pacella et al., 2013).

These two above specificities differentiate ESCROpath from some other modelling frameworks that have attempted to integrate uncertainty as part of the model calibration. For instance, even if the base equations are not exactly the same, it shares some principles with the Chance and Necessity (CaN) modelling approach (Planque & Mullon, 2020) as it is based on priors that translate a combination of constraints and uncertainty. However, compared to CaN food-web modelling, LIM or the Ecosampler plug-in of Ecopath (Steenbeek et al., 2018), ESCROpath is clearly one of the first models to be able to combine both food-web flow representation (i.e. biomass, productivity and consumption rates are included) and diet estimation; and that it is a great opportunity for studying the uncertainty in food-web model outputs coming from diet information. In particular, compared to Ecosampler, ESCROpath is a way of propagating realistic uncertainties, not guesstimates of uncertainty around parameter guesstimates.

4.4 | Flexibility

The Bayesian framework in which is implemented the model provides flexibility, for example when data are scarce, highly variable or uncertain. Such variability and uncertainty can then be rigorously incorporated in uncertainty estimates. Formally, the data needed for calibrating ESCROpath are the same as most food-web models. Practically, implementing ESCROpath requires at least biotracer data and biomass observations/estimations while values and distributions of other trophic parameters can be more easily found in literature.

As with the recently published Rpath tool (Lucey et al., 2020), the ESCROpath model is implemented in the R language. Providing a food-web model available on the R platform is a way to better adapt food-web models to specific cases, combining the simplicity of the well-known and widely used Ecopath equations and the flexibility of the R language, rather than a restrictive user interface. This also permits to combine it with various food-web indice estimation tools, namely the R packages NetIndices (Soetaert, 2009) and enaR (Borrett & Lau, 2014; Lau et al., 2015). Thus, this allows computing the eight ENA indices recommended for instance by Safi et al. (2019) for ecosystem assessment in the context of European Directives.

ESCROpath might thus be a useful tool in order to implement the ENA framework for ecological assessments, in particular when ecosystems are contaminated and pollutants are monitored. ESCROpath can be used with any chemical tracer, provided this chemical tracer can be considered as an indicator of trophic interactions (e.g. POPs, trace metals, mercury, fatty acids…).

4.5 | Limitations and perspectives

The main limitation lies in the availability of isotopes/chemical data at the relevant spatio-temporal scale. Indeed, ESCROC and ESCROpath have theoretically the same constraints and assumptions as isotopic food-web studies: spatio-temporal congruence, relevance of measurements and sources, accounting for turnover time (Carter et al., 2019) etc. While deviations from assumptions are possible, this requires consistent hypotheses and a reliable consideration of uncertainty and possible biases. Furthermore, in a first approach, the TEF is element specific in ESCROC and ESCROpath. However, the species-specific random effect taken into account in the TEF estimates (Equation (1) partially accounts for the variability between species. Actually, there is neither mathematical nor computational obstacle to consider and estimate a TEF value at the consumer or consumer/prey level. Implementing this possibility in the code might be a future development.

Moreover, short-term, ESCROpath flexibility has to be tested in data-poor situations and implemented with other tracers. The accessibility of the package will favour the test application of the model to many types of other tracers. Accounting for these limits, ESCROpath offers interesting perspectives in food-web comparisons when, for instance, various habitats and associated food webs are sampled. Eight ENA indices are computed in the current version of ESCROpath but other food-web indices or isotopic-like functional indices can be computed to investigate food web functioning. Furthermore, ENA-like contamination indices (such as a POP cycling index) could be developed and implemented in a next version of the package.

To conclude, rigorous statistical adjustments and therefore observations are required to build robust ecosystem approaches. So far, we are limited to empirical estimates, based on stomach contents (that are not always easy to interpret) and few isotope signatures (that do not easily allow solving a whole food web mixing model with many groups). ESCROpath opens a new way, showing that all it takes is data from chemical tracers to build the robust statistical approach required. These data are becoming more readily available, as they are required by more rigorous monitoring regimes and are now more cost-effective. Our approach allows reconciling ecosystem modelling and trophic ecology, making the former more realistic and reliable.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHORS' CONTRIBUTIONS

J.L. and H.D. conceived the ideas, designed the methodology and analysed the data; H.D. wrote the code; P.L. and H.B. collected and provided the chemical data; X.C. provided the trophic data; F.M., M.B. and D.G. contributed to the data analysis and tested the code; J.L. and H.D. led the writing of the manuscript. All authors contributed critically to the drafts and gave final approval for publication.

PEER REVIEW

The peer review history for this article is available at https://publons.com/publon/10.1111/2041-210X.13808.

DATA AVAILABILITY STATEMENT

The R package of the ESCROpath model, based on the ESCROCR package (Drouineau et al., 2018; Drouineau & Lobry, 2020) implementing the method, is available on GitHub (https://github.com/Irstea/escroc; https://doi.org/10.5281/zenodo.5226371). The dataset used for the implementation on the Gironde case study is described in Munoz (2015) and Munoz et al. (2017). Details on the data and the priors used for implementing ESCROC can be found in Ballutaud et al. (2019). All these data are included and available on the R package stored in a zenodo repository (Lobry et al., 2021).

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