Ecotracer: analyzing concentration of contaminants and radioisotopes in an aquatic spatial-dynamic food web model

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A B S T R A C T

Ecotracer is a tool in the Ecopath with Ecosim (EwE) software package used to simulate and analyze the transport of contaminants such as methylmercury or radiocesium through aquatic food webs. Ecotracer solves the contaminant dynamic equations simultaneously with the biomass dynamic equations in Ecosim/Ecospace. In this paper, we give a detailed description of the Ecotracer module and analyze the performance on two problems of differing complexity. Ecotracer was modified from previous versions to more accurately model contaminant excretion, and new numerical integration algorithms were implemented to increase accuracy and robustness. To test the mathematical robustness of the computational algorithm, Ecotracer was tested on a simple problem for which we know an analytical solution. These results demonstrated the effectiveness of the program numerics. A much more complex model, the release of the cesium radionuclide $^{137}$Cs from the Fukushima Dai-ichi nuclear accident, was also modeled and analyzed. A comparison of the Ecotracer results to sampled $^{137}$Cs measurements in the coastal ocean area around Fukushima show the promise of the tool but also highlight some important limitations.

1. Introduction

Prediction of the levels of radioisotopes or contaminants in aquatic environments is important for several reasons. Certain contaminants such as methylmercury, PCPs, lead, or $^{137}$Cs (from, e.g., the Fukushima-Daiichi nuclear accident) bioaccumulate in marine organisms to reach levels that are toxic or carcinogenic to the fish themselves or the humans that eat them. Other contaminants, such as $^{14}$C from the nuclear fuel cycle, may be examined to give insight into the trophic interactions of an ecosystem (Muir et al., 2017; Tierney et al., 2017).

There has been significant research into modeling the bioaccumulation and biomagnification of different contaminants. In general, the goal of such simulations is to calculate $C_i/B_i$, or, the amount of contaminant (in Bq for radioisotopes, or $\mu$g, etc. for other contaminants) per unit biomass of each species $i$ in a system. Note that here we define $C_i$ as the total amount of contaminant (e.g., Bq), not the amount per biomass (Bq/kg). However, we define the environmental contaminant amount $C_0$ as a concentration (e.g., Bq/m$^3$). Throughout the paper, the words contaminant, activity, or tracer may be used interchangeably - the methodology applies the same to radioisotopes as well as other contaminants such as methylmercury. To avoid confusion, we will refer to the amount of contaminant in units of Bq, though other units can easily be used (e.g., $\mu$g).

The simplest models utilize concentration ratios (Vanderploeg et al., 1975; Brown et al., 2008; Howard et al., 2013), as defined below:

$$CR_i = \frac{\text{Activity concentration in biota whole-body (Bq/kg)}}{\text{Activity concentration in (filtered) water (Bq/m}^3)} = \frac{C_i}{B_0}$$

(1)

Where, $CR_i$ is the concentration ratio for a given species $i$. This single number takes into account all environmental uptake rates, excretion rates, and trophic interactions. This method is very simple to apply once the CR’s have been obtained simply multiply the CR by the water activity concentration to obtain the activity concentration in the biota. However, there are significant limitations to the CR approach. CR values in the literature have very large uncertainties possibly due to the conditions of different measurement environments, such as feeding habits, habitat, etc (Howard et al., 2013). These values may also change over time, with differences in water temperature, pH, etc. More importantly, the CR method assumes an equilibrium state between the environment and the biota, which may be a poor assumption if the environmental concentration is changing rapidly (e.g., a leak of radio-nuclides from a nuclear accident). Certain species/contaminants may take days to years to reach equilibrium (Coughtrey and Thorne, 1983;
Brown et al., 2004). Concentration ratios are set conservatively, and are very useful as a risk-assessment tool for long-term contamination. However, the method lacks the ability to take into account changing ecosystems (e.g., predation variation due to changes in relative abundances) or transient effects (Vives i Batlle et al., 2008).

A more sophisticated approach is to set up and solve a differential equation for the contaminant concentration, which may be referred to as a dynamic transfer model (Thommann, 1981; Landrum et al., 1992; Rowan and Rasmussen, 1995; Trudel and Rasmussen, 1997, 2006; Luoma and Rainbow, 2005; Vives i Batlle et al., 2008). This generally has the form:

$$\frac{dC_i(t)}{dt} = \alpha - \beta C_i(t)$$  \hspace{1cm} (2)

Where, the input coefficient $\alpha$, and loss coefficient $\beta$ may be dependent on other variables such as environmental concentration, food concentration, relative biomasses; and on parameters such as environmental uptake rate, metabolism rate, etc. This can be related back to the concentration ratio approach by looking at the equilibrium value:

$$\frac{dC_i(t)}{dt} = 0 \rightarrow C_{eq} = \alpha/\beta = CR_CB_i$$  \hspace{1cm} (3)

This allows the method to give identical steady state results by constraining the parameters influencing $\alpha$ and $\beta$ such that this equality is maintained. Additionally, it can give results that are not at steady state, as well as allowing change in model parameter values and inputs.

We describe here a method that uses the dynamic approach of Eq. (2) while at the same time solving the spatial and temporal biomass dynamics using the Ecopath with Ecosim software. This method, Ecotracer, is integrated in the Ecopath with Ecosim (EwE) software (Christensen and Walters, 2004). The basic Ecotracer accounting code has been available in EwE since the early 2000s, and has been applied in a wide variety of cases involving contaminant (e.g., mercury) and radionuclide concentrations (e.g., Booth and Zeller (2005); Sandberg et al. (2007); Razinkovas (2007); Niiranen et al. (2008); Sanderson et al. (2010); Larsen et al. (2016); Booth et al. (2016)). These examples mainly involved prediction of equilibrium concentration differences among trophic groups (bomagnification factors), and showed that Ecotracer gives reasonable predictions of these concentrations when compared to data. But not until the Sandberg et al. (2007) paper were the basic equations of Ecotracer even documented in published literature, and there were no careful checks on the original computer code developed by C. Walters (UBC, pers. comm.) for logical consistency and accuracy of numerical integration methods for time dynamic predictions. In this work we develop Ecotracer further, provide a more detailed description of the approach, and test it more thoroughly to on simplified and spatial-dependent situations.

2. Ecopath with ecosim (EwE)

Ecopath with Ecosim (Christensen and Walters, 2004) is an open source ecological/ecosystem modeling software suite. EwE has three main components: Ecopath a static, mass-balanced snapshot of the system; Ecosim a time dynamic simulation module for policy exploration; and Ecospace a spatial and temporal dynamic module initially designed for exploring impact and placement of protected areas. The EwE software package can be used to:

- Address ecological questions
- Evaluate ecosystem effects of fishing
- Explore management policy options
- Analyze impact and placement of marine protected areas
- Model effect of environmental changes
- Facilitate end-to-end model construction
- Predict movement and accumulation of contaminants and tracers (Ectracer)

This paper will focus on the description, further development, and analysis of the Ectracer component of EwE, but we will first describe the main components of EwE that are central to Ecotracer.

Ecoptah uses a simple mass balance approach for the production of each functional group (e.g., species, or group of similar species) in a system using the following:

$$P_i = B_i + Y_i - E_i + \sum_j Q_{ij}$$ \hspace{1cm} (4)

where, $P_i$ is the biomass production rate, and $E_i$ is the ecotrophic efficiency rate ($E_i$), predation rate ($Q_{ij}$), immigration rate ($I_i$), immigration rate ($I_j$), predation rate of group $i$ from group $j$ ($Q_{ij}$)).

Ecosim (Walters et al., 1997, 2000; Christensen and Walters, 2004) is a time-dynamic simulation tool based on a differential equation derived from Eq. (4) (assuming that $P_i = g_i Q_{ij}$).

$$\frac{dB_i}{dt} = g_i \sum_{j \text{ prey}} Q_{ij} - \sum_{j \text{ predators}} Q_{ij} + Y_i - E_i - M_i B_i$$ \hspace{1cm} (5)

Where, $g_i$ is the net growth efficiency (i.e., production/consumption ratio $P_i/Q_i$), and $M_O$ is the non-predation (‘other’) natural mortality rate, corresponding to $P(1 - EE)$.

At each time-step, Ecosim calculates the following values for each species (or species-age for species with multi-stanza (i.e., age class) representations (Walters et al., 2010)).

1. Biomass $B_i$ [tons]
2. Consumption rate of species $i$ by species $j$: $Q_{ij}$ [tons/yr]
3. Fishing catch rate: $Y_i$ [tons/yr]
4. Fishing mortality rate: $F_i = Y_i/B_i$ [1/yr]
5. Natural/other mortality rate $M_O$ [1/yr]

Ecospace (Walters et al., 1999) calculates these as a function of space $(x,y)$, and also calculates the biomass flow rates between cells.

1. $a_{in}(x,y)$ is the gross flow rate [1/yr] out of the north boundary of cell $(x,y)$
2. $a_{in}(x,y)$ is the gross flow rate [1/yr] out of the south boundary of cell $(x,y)$
3. $a_{out}(x,y)$ is the gross flow rate [1/yr] out of the west boundary of cell $(x,y)$
4. $a_{out}(x,y)$ is the gross flow rate [1/yr] out of the east boundary of cell $(x,y)$

The outflow rates of one cell are the inflow rates to another cell, so the biomass inflow to cell $(x,y)$ can be represented as:

$$I(x,y) = a_{in}(x,y) B(x,y) - a_{out}(x,y) B(x,y) + a_{inw}(x,y) B(x,y) + a_{inw}(x,y) B(x,y) + a_{inw}(x,y) B(x,y)$$ \hspace{1cm} (6)

A diagram of this inflow is shown in Fig. 1. The $a_i$ coefficients are calculated based on diffusion/advection model, with habitat preferences and migration parameters.

3. Ectracer equations

The Ectracer module of EwE models the flow and accumulation of contaminants or tracers in ecosystems while the biomass dynamics of Ecosim/Ecospace are being solved in parallel. The contaminant molecules or isotopes are assumed to be either in the environment (i.e., the water for aquatic applications), or in the biota. The environment and each species (or each stanza of a multi-stanza
representation of species) are considered as “compartments” with their own concentration of tracer. The contaminant may flow or transfer between all of these compartments, as well as into and out of the system, through processes such as environmental input, predation, mortality, direct uptake, excretion, or radioactive decay. This general type of compartment model has been around for a while (Thomann, 1981), but the ability to calculate all these compartment transfers using a spatial-dynamic ecosystem model is new.

In Ecotracer, the contaminant concentration in each “compartment” is modeled using a mass balance equation.

\[
\frac{dC_i}{dt} = \text{intake} - \text{loss} \tag{7}
\]

One thing to note is that the variable \( C_i \) [Bq] is the total contaminant amount in compartment \( i \), not the per-biomass amount as is modeled in other work, e.g., Thomann (1981). This allows for a slightly simpler solution to the problem, since growth dilution does not have to be included in the formulae. The biomass is calculated separately in the Ecospace and Ecosim routines.

### 3.1. Contaminant intake

The contaminant intake [Bq/yr] into a compartment is divided into two factors: direct uptake from the environment, uptake from food sources, and migration. Direct uptake from the environment can be expressed as follows:

\[
\text{Direct uptake} = u_i B_i C_0 \tag{8}
\]

where, \( C_0 \) [Bq/m³] is the environmental concentration of the contaminant, \( B_i \) [tons, t] is the biomass of compartment \( i \), and \( u_i \) [m³/t·yr⁻¹] is the environmental uptake rate for compartment \( i \) (mass of contaminant intake/biomass/environmental concentration/year).

Uptake from food is given by:

\[
\text{Food uptake} = f_i \sum_{j=\text{predators}} Q_i C_j B_j \tag{9}
\]

where, \( C_j / B_j \) [Bq/ton] is concentration/biomass in the food, \( Q_i \) [t/yr] is the rate of consumption of species \( j \) by species \( i \), and \( f_i \) is the assimilation efficiency (i.e., how much of the eaten contaminant that is assimilated into the body tissue).

Uptake from immigration is expressed as:

\[
\text{Immigration} = c_i I \tag{10}
\]

where, \( c_i \) [Bq/ton] is the concentration/biomass in the immigrating population, and \( I \) is the immigration rate (t/yr). This term is only used in Ecosim. In Ecospace, the movement of species is handled explicitly. For each biomass pool, the outflow rates are calculated for each cell. The immigration rate to each cell is calculated as the sum of the outflow rates of the surrounding 4 cells.

\[
\text{Immigration} = a_{i \leq 0} (x + 1, y) B_i (x + 1, y) + a_{i,w} (x + 1, y) C_i (x + 1, y) + a_{i,N} (x, y - 1) C_i (x, y - 1) + a_{i,s} (x, y) C_i (x, y + 1) \tag{11}
\]

where, \( a_{i,w} (x, y) \) is the outflow rate (1/yr) of biomass in pool \( i \) to the west, in spatial cell \((x, y)\). The coefficients \( a_{i,E}, a_{i,N}, a_{i,W} \) are the outflow rates on the east, north, and south borders, respectively. These coefficients are the same flow rates as are calculated for biomass movement in Ecospace.

Finally, there is an additional inflow of contaminants to the current compartment if the compartments are being considered as different ages of the same species (i.e., a multi-stanza representation).

\[
\text{Age inflow} = \frac{1}{\Delta t} \frac{B_{k-1}}{B_{k-1}} C_{i-1} \tag{12}
\]

where, \( B_{k-1} \) is the biomass that is from functional group i aging up from age class \( k - 1 \) to age class \( k \) at the current Ecosim/Ecospace timestep \( t \), and \( \Delta t \) is the Ecosim/Ecospace timestep. At present, the tracer concentration per biomass is assumed to be constant across ages within a given stanza age group. This is a possible source of error, as likely the older fish will have higher tracer concentrations. It should however, only be a problem if the stanza represents a large age span and also is not the oldest age stanza.

### 3.2. Contaminant loss

The loss of contaminant [Bq/yr] from a compartment comes from several sources: mortality, emigration, metabolism, decay, and graduation to a different age-class.

Mortality is considered from three separate sources: predation, fishing, and other mortality.

\[
\text{Mortality loss} = \left( \sum_{j=\text{predators}} \left( Q_i / B_j \right) + F_i + M_i \right) C_i \tag{13}
\]

where, \( Q_i \) [tons/yr] is the rate of consumption of biomass in compartment \( i \) eaten by compartment \( j \), \( F_i \) [1/yr] is the fishing rate, and \( M_i \) [1/yr] is the other mortality rate. These terms differ in that the natural/other mortality is added to the detritus inflow, the predation mortality is an inflow to compartment \( i \), and the fishing mortality is removed from the system.

Emigration is handled in the same fashion as immigration. In Ecosim, emigration is defined simply:

\[
\text{Emigration} = E_i C_i \tag{14}
\]

where, \( E_i \) is the Ecosim emigration rate [1/yr]. In Ecospace, we have:

\[
\text{Emigration} = (a_{i,E} (x, y) + a_{i,W} (x, y) + a_{i,N} (x, y) + a_{i,s} (x, y)) C_i (x, y) \tag{15}
\]

where, the \( a's \) are defined the same as for the uptake terms.

Contaminant losses due to excretion/metabolism are calculated as:

\[
\text{Excretion} = m_i C_i \tag{16}
\]

The excretion/metabolism rate \( m_i \) [1/yr] is the rate at which the contaminant is released from tissue back out to the environment (\( C_i \)). It is noted that there is only a single excretion rate per compartment. There is currently no ability to have different excretion rates from different tissue types (e.g., soft tissue and bone), as has been noted in some studies (Boisson et al., 1998). Some other tracer models have taken this into account explicitly (Vives i Batlle et al., 2008). This can be handled in Ecotracer by running two separate Ecotracer models, one for the slow excretion rate and one with the high excretion rate, using a different assimilation efficiency for each (i.e., the fraction that goes to soft tissue and the fraction that goes to bone). This assumes that there is no transfer between the slow and fast compartments.
Losses due to decay can be radioactive decay or biological breakdown of the contaminant molecule. Decay losses are removed from the system entirely.

\[
\frac{dC_i}{dt} = \alpha_i - \beta C_i(t)
\]  
(22)

where, \(\alpha\) is the sum of the inflow terms, and \(\beta\) is the sum of the outflow terms. Note that the inflow is dependent on the Ecosim/Ecospace parameters (e.g., \(B_i\)'s, \(Q_{ij}\)'s, etc), as well as the tracer amounts in other compartments \((C_0\) and \(C_j\)’s), but not on the compartment concentration \(C_i\). In general, the Ecosim/Ecospace parameters are changing slowly with respect to the main timestep \(\Delta t\). Because of this, and for simplicity, these parameters are assumed to be constant during the timestep when computing the Ecotracer solution. This means that \(\beta\) is constant during a timestep, but a will change if the tracer concentrations are not close to equilibrium.

In order to solve Eq. (22), an Adams-Bashforth multi-step integration scheme is used.

\[
C_i(t + \Delta t) = C_i(t) + \frac{3}{2} \frac{dC_i(t)}{dt} \Delta t - \frac{1}{2} \frac{dC_i(t - \Delta t)}{dt} \Delta t
\]  
(23)

The differential equation is stiff, meaning that a very small timestep may be required for a stable solution using an explicit integration method. Since this timestep may be much smaller than the Ecosim/Ecospace timestep, (which is typically a month) several sub-timesteps are used for with Ecotracer for every Ecosim/Ecospace timestep. The Ecotracer timestep should be no larger than the smallest characteristic time for the balance equation (\(\beta^{-1}\)). Therefore, the number of Ecotracer timesteps per Ecosim/Ecospace timestep is calculated as:

\[
nt = \text{ceiling} \left( \frac{\Delta t}{\min_{ij} \beta_{ij}} \right)
\]  
(24)

This implies that the Ecotracer timestep is equal to:

\[
\Delta t' = \frac{\Delta t}{nt}
\]  
(25)

At each sub-timestep, the \(\alpha_i\) values are re-calculated based on the \(C_j\) values of other compartments \(j\) from the previous sub-timestep, and a step is taken in Eq. (23). After all the sub-timesteps are completed, a standard Ecosim/Ecospace timestep is taken, and the new Ecosim/Ecospace parameters are used for the next set up sub-timesteps. This timestep/sub-timestep scheme is shown in Fig. 3 for the case of two Ecotracer sub-timesteps per Ecosim/Ecospace timestep (i.e., \(nt = 2\)).
4. Mathematical analysis of a simple case

From the equations discussed in the previous section, it is interesting to look at what these equations predict under certain simplified or idealized situations. One such case is to look at predictions of the equilibrium tracer concentration. To do this, we consider a closed system with constant $C_0$, constant biomass, no migration, fishing, decay, or age effect, and set $dC/dt = 0$.

$$\frac{dC}{dt} = 0 = u_i B_i C_0 + \sum_{j=pred} f_j Q_{eq}/B_j - \left(\sum_{j=pred} Q_{eq}/B_j + MO_i + m_i\right) C_{eq}$$

If we solve for the equilibrium concentration $C_{eq}$, we get:

$$C_{eq} = \frac{u_i B_i C_0 + \sum_{j=pred} f_j Q_{eq}/B_j}{\sum_{j=pred} Q_{eq}/B_j + MO_i + m_i}$$

(26)

where, the numerator represents input terms (environmental uptake and prey consumption) and the denominator represents the loss terms (mortality from predation, other mortality, and excretion). A further simplification can be made if we write that the total mortality rate is $Z_i$ (i.e., $P/B_i$). If we further consider that there is only a single prey species $j$, then if we solve for the concentration per biomass $C_{eq}/B_i$, we get:

$$C_{eq}/B_i = \frac{u_i C_0 + f_j Q_{eq}/B_j}{Z_i + m_i}$$

(27)

This equilibrium tracer per biomass can be related back to the concentration ratio method discussed earlier.

$$CR_i = \frac{C_{eq}/B_i}{C_0} = \frac{u_i + f_j Q_{eq}/B_j}{Z_i + m_i}$$

(29)

or,

$$CR_i = \frac{u_i + f_j Q_{eq}/B_j}{Z_i + m_i}$$

(30)

For a primary producer (i.e., $Q_j = 0$), then the equation simplifies to

$$CR_i = \frac{u_i}{Z_i + m_i}$$

(31)

Thus, it is fairly straightforward to select values of $u_i$ and $m_i$ such that under the conditions in which the $CR_i$ values were calculated (i.e., the same $B$, $Q$, $Z$), etc., the same equilibrium values are obtained with this biokinetic method as with the CR method. With the $u_i$ and $m_i$ values set, one could then easily explore the effect of changing abundances, trophic interactions, etc.

If the direct environmental uptake is considered small, then neglected, the amount of biomagnification (i.e., the ratio of the concentration to biomass from predator to prey) can be calculated as:

$$\frac{C_{eq}/B_i}{C_{eq}/B_j} = \frac{f_j Q_{eq}/B_j}{Z_i + m_i}$$

(32)

In a steady state system, the total mortality rate $Z_i$ [yr$^{-1}$] is equal to the production/biomass rate $P/B_i$. The growth efficiency is the amount of total biomass growth per ingested biomass:

$$c_{eq} = (P/B_i)/(Q_{eq}/B_i)$$

(33)

This allows us to cast the biomagnification factor in a slightly different form:

$$\frac{C_i/B_i}{C_j/B_j} = \frac{f_j}{c_{eq} + m_i/(Q_{eq}/B_i)}$$

(34)

By definition, $c_{eq} < 1$, so biomagnification will occur unless the excretion rate $m_i$ is large relative to $Q/B$, or the absorption factor $f_j$ is small. Further, concentration is expected to decrease with increasing growth efficiency, as predicted by similar models (Rowan et al., 1998).

5. Simplified model analytical solution compared to ecotracer solution

The first step in testing the mathematical model is to devise a system so simple that it can be solved analytically, then compare the results of Ecotracer to the analytical solution.

The simplest interesting model used to test this has two hypothetical species: a primary producer (algae), and a single consumer (zooplankton). Migration and fishing will be ignored in this model for simplicity. The main model parameters are given in Table 1.

The algae only obtain tracer through direct uptake, and the zooplankton is the total consumption rate. The environmental uptake parameter is chosen such that:

$$u_i B_i T \ll 1$$

(35)

where, $T$ is the total simulation time. This implies no effect of the
organism contamination of the level of contamination in the medium, a classical and justified hypothesis when the biomass of organisms is low compared to volume of the medium. The environmental concentration \( C_0 \) changes very little due to uptake, and will be treated as a constant.

\[
C_0(t) = C_0(0) = 1.0
\]  

(36)

The differential equation governing the algae tracer concentration \( C_1 \) is given by:

\[
\frac{dC_1}{dt} = u_t B_1 C_0 - MO_1 C_1 - Q_{12} C_1 / B_1
\]  

(37)

In this problem, the predation mortality is very small \((Q_{12}/B_1 = (Q_{12}/B_2)B_2/B_1 \ll MO_1)\), so can be ignored here. The equilibrium concentration of the algae can be calculated by setting \(dC_1/dt = 0\):

\[
C_{1,eq} = \frac{u_t B_1 C_0}{MO_1}
\]  

(38)

The time-dependent solution of Eq. (36) can be solved (assuming a constant \( C_0 \)):

\[
C_1(t) = \frac{u_t B_1 C_0}{MO_1} \left( 1 - e^{-MO_1 t} \right) = C_{1,eq} \left( 1 - e^{-MO_1 t} \right)
\]  

(39)

The zooplankton \( (C_2) \) is assumed to have zero environmental uptake, with the differential equation:

\[
\frac{dC_2}{dt} = f_z Q_{12} C_1 / B_1 - MO_2 C_2
\]  

(40)

This has the equilibrium solution:

\[
C_{2,eq} = \frac{f_z Q_{12} C_{1,eq}}{MO_1 B_1}
\]  

(41)

The time-dependent solution is given as:

\[
C_2(t) = C_{2,eq} 1 + \left( \frac{MO_2}{MO_1 - MO_2} e^{-MO_1 t} - \frac{MO_1}{MO_1 - MO_2} e^{-MO_2 t} \right)
\]  

(42)

The results for the Ecotracer numerical solution and the analytic solutions (Eqs. (39) and (42)) of this system are shown in Fig. 4. The equilibrium values for the tracer concentrations are given by the dashed horizontal lines. The algae concentration approaches equilibrium much faster due to their higher turnover rate. The Ecotracer and analytic solutions are almost identical, and differ by less than 0.25% across all timesteps. This is a good indication that the numerical integration scheme in Ecotracer is working properly.

6. Food web dynamics of radionuclides following the Fukushima disaster

A wide variety of models have been developed since the Fukushima disaster in 2011 to explain patterns of biological accumulation and loss of radioisotopes from marine biota in the coastal area near Fukushima (Tateda et al., 2013; Shigenobu et al., 2014; Belharet et al., 2016; Okamura et al., 2016; Vives i Batlle et al., 2016). In hindsight these models have been highly informative about food web and physical transport mechanisms, particularly for \(^{137}\text{Cs}\). But an interesting question is, how soon after the disaster could food web models have been developed to provide broad guidance about likely space-time concentration dynamics, to aid in development of biological monitoring programs?

Within a month of the disaster, physical monitoring programs (water column and sediment sampling) had demonstrated that \(^{137}\text{Cs}\) had declined dramatically in the coastal water column due to advection-diffusion processes, but that there had been substantial accumulation of it in ocean sediments, apparently due to adsorption of it onto sinking clay particles. This sediment contamination was extensive mainly over a distance of roughly 100 km southward from Fukushima (in the direction of prevailing coastal currents; see review in Buesseler (2014)). Thus within a month of the disaster it would have been possible to focus ecological monitoring and modeling on the benthic portion of the coastal aquatic food web.

One of the main reasons why the Ecopath with Ecosim (EwE) software is so widely used (Villasante et al., 2016) is that it allows rapid development of food web models for biomass flow dynamics, using only limited information on abundances, feeding, production, and mortality rate components (unexplained, predation, fishing) of a wide variety of organisms. So armed only with experience in such model development and rough parameter estimates that are widely available (including from Fishbase (Froese and Pauly, 2016), www.fishbase.org, and Ecobase (Collét et al., 2015), www.ecopath.org) for the kinds of creatures that are of concern along the Fukushima coast, we were able to develop a food web model (Fig. 5) similar to that used by Tateda et al. (2013), before we had discovered that reference, with about 2 h of work time. Likely a much more detailed model with more precise parameter estimates could have been developed in a collaborative workshop process with local scientists, in less than one week of work time for a team of 5–10 scientists.

Coastal fisheries were closed after the disaster, and our first step was to use Ecopis to predict possible biomass changes because of this closure (Fig. 6). Since we had assumed high fishing mortality rates \((F = 0.5 \text{ /yr})\) for coastal fish in Ecopis, we predicted moderately large increases in biomass of harvested fishes, and a relatively large dip in benthic invertebrates due to predation from the increased fish population. The benthic fish population first rises due to lowered fishing mortality, then drops due to the rise of benthic piscivores.

We then used the Ecotracer module in Ecosim to predict non-spatial changes in \(^{137}\text{Cs}\) for various scenarios about possible changes in environmental concentrations over time near the power plant (within 20 km), using Ecotracer uptake and loss parameter values given in (Table 2). The initial \(^{137}\text{Cs}\) environmental concentration and phytoplankton uptake rates were scaled such that the Ecotracer \(C/B\) values approximately matched the data 100 days few months after the disaster. The values are clearly not finely tuned, and additional research could provide more accurate parameters. Metabolism-excretion (de- 

parution) loss rates for the biomass pools were estimated by assuming that metabolic rates scale as the 0.8 power of body weight (Zeuthen, 1953; Clarke and Johnston, 1999). For the first or worst case scenario, we assumed no loss of \(^{137}\text{Cs}\) from the coastal area due to physical dispersion (advection/diffusion) processes, and this led to predictions of persistently high \(^{137}\text{Cs}\) concentrations in all biomass pools. For the second scenario, we assumed loss rates of order 0.3/month of environmental concentration due to export processes, based on decline
patterns presented in Tateda et al. (2013, 2017); estimates from various sources indicate environmental export rates from the region as low as 0.1/month (Buesseler, 2014) to as much as 8.0/month in the first few months after the disaster (Tateda et al., 2017). For the third scenario, we included import-export rates (0.3/month) for Ecosim biomasses of phytoplankton and zooplankton, to simulate high movement rates of these planktonic organisms into and out of the area due to oceanographic transport processes, while assuming zero 137Cs concentrations in the imported biomass, (this is obviously a crude approximation; see more realistic scenarios in Belharet et al. (2016). Biomass 137Cs are given in Fig. 7.

As indicated by comparisons to data in Fig. 7, the simple model was able to predict trends in observed 137Cs concentrations fairly well, but only when supplied with reasonable estimates of physical transport (import/export) rates (as in the red and black curves). But even with these rates, it substantially over-predicted persistence of 137Cs in benthic plankton (likely due to underestimation of advective transport of uncontaminated biomass from areas north of Fukushima by prevailing southward coastal currents), and it over-predicted 137Cs concentrations later seen in benthic piscivores by almost an order of magnitude. There are three possible reasons for the incorrect piscivore predictions: (1) we may have underestimated metabolic-excretion loss rate; we used a rate near 0.002/day, while Tateda et al. (2017), Table S1, summarizes literature reporting rates averaging 0.0078/day; (2) we likely underestimated the proportion of piscivore diet coming from less contaminated plankton feeding fish and from plankton-feeding juveniles of benthic fish that feed mainly on invertebrates when they are older; and (3) there may be substantial import-export of uncontaminated biomass due to spatial dispersal and migration of piscivores. High import-export rates appear doubtful considering the really high differential concentrations reported by Tateda et al. (2017) in benthic fish very near the power plant compared to just a few kilometers away, even three years after the disaster. But as Shigenobu et al. (2014) note, the high measured variance in concentrations among individual fish, with some uncontaminated fish sampled even very near the power plant, indicates that there must be at least some spatial movement at scales of at least a few kilometers.

One thing that is clear from both the data and Ecotracer modeling, is that a concentration ratio approach would have yielded quite misleading results. If the 137Cs values were in equilibrium with the environment, then all species would have the same slope in drop-off of 137Cs concentration. However, there are vastly different slopes between the high-metabolism, short-lived species (plankton) and the low metabolism, long-lived species (benthic piscivores). Even long after the environmental concentration has dropped off, benthic piscivore concentration remains relatively high.

To obtain initial predictions of the impact of spatial dilution processes (dispersal, advection and diffusion), we then developed a simple Ecospace model for the coastal area extending 50 km north and south from the power plant, and 20 km offshore, with 5 × 5km grid cells (Fig. 8). For this model, we assumed very slow dispersal rates (0.2 km/month) for benthic invertebrates, low dispersal rates (1 km/month) for pelagic fish, medium dispersal rates (5 km/month) for benthic fish and zooplankton, and fast dispersal rates (0.2 km/month) for phytoplankton and algae. In order to capture the high variability in 137Cs concentration in fish, we assumed import-export rates ranging from 0 to 10 km/month, and we assumed a range of 100 to 2000 km/month for dispersal rates.

Table 2

<table>
<thead>
<tr>
<th>Biomass Pool</th>
<th>Initial C (Bq m⁻³)</th>
<th>Direct abs. export/import</th>
<th>Decay rate (mo⁻¹)</th>
<th>Excretion (mo⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Environment</td>
<td>Benthic piscivores</td>
<td>0, 0.3, 0.1</td>
<td>0.00192</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>Pelagic fish</td>
<td>0, 0.125</td>
<td>0.00192</td>
<td>0.625</td>
</tr>
<tr>
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<td>Benthic fish</td>
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<td>0.00192</td>
<td>0.0875</td>
</tr>
<tr>
<td></td>
<td>Benthic invertebrates</td>
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<td>0.00192</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>Zooplankton</td>
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<td>0.00192</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>Phytoplankton</td>
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<td>0.00192</td>
<td>7.5</td>
</tr>
<tr>
<td></td>
<td>Detritus</td>
<td>0, 0.1</td>
<td>0.00192</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>Varied among scenarios 1, 2, 3.</td>
<td></td>
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Fig. 5. Ecopath parameters and trophic flow pattern for a simple model of the nearshore marine ecosystem near Fukushima. Units are shown only for benthic piscivores (top). The numbers associated with the arrows indicate the fractional diet composition of the consuming species.

Fig. 6. Ecosim predictions of nearshore marine biomass changes due to fishery closures near Fukushima.

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* Varied among scenarios 1, 2, 3.
benthic fish, and much higher diffusion (30 km/month) and southward advection (5 km/day) for environmental concentrations, detritus and plankton organisms. It should be noted that one of our initial concerns in developing the Ecospace model was to estimate the possible extent of biotransport of $^{137}$Cs through dispersal and migration of larger, mobile marine organisms like benthic piscivores; we expected movement rates considerably higher than apparent in the Tateda et al. (2017) fish data.

The temporal predictions from this simple Ecospace model look much like the predictions from Ecosim (Fig. 9), but the predictions of spatial distribution patterns in the biota are less convincing (Fig. 8). The temporal predictions were only more reasonable when we adjusted diffusion rates upward (to 90 km/month) so as to predict the relatively high physical export rate (0.3/month) estimated for the Ecosim model from time series measurements of environmental concentrations. With these high rates, Ecospace predicts a flatter north-south distribution of concentrations in all biomass pools than was actually observed. The basic problem here is that the Ecospace equations for environmental concentration are far too simplistic, failing to properly account for exchange of environmental concentrations between the water column and sediments. This leads to high and persistent sediment concentrations to which benthic organisms near the plant have been exposed.

Probably the best way to use Ecospace in cases like Fukushima would be to not use the simplistic Ecospace environmental (and perhaps phytoplankton-zooplankton) concentration predictions at all, but rather to first run a far more realistic physical model to predict space-
time environmental concentrations (e.g. Belharet et al. (2016); Erichsen et al. (2013)), and then either force the environmental concentrations in Ecospace with the results from that model or directly couple the physical model and Ecospace. There have been numerous applications demonstrating the utility of such linking or coupling. Examples of linking (i.e. forcing Ecospace with results from a physical model) include evaluation of effects of hypoxia on fish and fisheries in the northern Gulf of Mexico (de Mutsert et al., 2016), while coupling (with GOTM-ERSEM) was demonstrated by Beecham et al. (2015). Such linking or coupling with a physical model would allow focus on realistic predictions of spatial mixing dynamics associated with complex spatial behaviors (dispersal, migration) of larger organisms, without having to worry about confounding of predictions about these behaviors with predictions due only to poor representation of physical transport-dilution processes.

7. Discussion

The analysis presented above revealed two fairly serious flaws in the original EwE implementation, which would not affect most predictions in the literature of equilibrium concentrations but could lead to large errors in time predictions for cases like Fukushima where time dynamics are a key issue. First, we discovered an accounting error or inconsistency, where contaminant loss rate to respiration and excretion was modeled with a single decay parameter for which the loss rates were removed from the system rather than being returned to the environmental concentration pool. This could seriously affect model predictions for cases where a high proportion of the total contaminant or radionuclide is stored at any moment in biological pools rather than in physical form (this can happen with C-14 for example), since the model eliminated all respiration-excretion losses from the modeled total system contaminant mass. Second, the time integration procedure was inadequate to deal with stiff situations involving rapid accumulation and equilibration of concentrations in lower trophic level biomass pools (e.g. phytoplankton). The numerical integration procedure led to substantial errors in mass-balance over the first few time steps (typically months), with up to half of the initial total contaminant mass being incorrectly lost over these steps.

As noted above for the Fukushima case, Ecotracer’s representation of environmental (inorganic form) contaminant concentration by a single variable is not adequate for representation of systems for which there are spatially distinct (and perhaps chemically distinct) inorganic contaminant pools, particularly water column and sediment components that move into distinct parts of the aquatic food web (benthic vs planktonic). We could pretend to correct this problem by allowing Ecotracer users to define multiple environmental concentrations or compartments, and to specify exchange rates between these compartments. But for Ecospace applications, we warn that a far better and safer strategy is to utilize well-tested physical transport models like ROMS (Shchepetkin and McWilliams, 2005) or GETM (Stips et al., 2004) to predict physical concentration fields, then drive the Ecotracer environmental concentration(s) with these fields.

A key area for future development of the Ecotracer software will be to provide capability for predicting the extremely high variance in contaminant concentrations among individual organisms that has been observed in cases like Fukushima. This variation is due to a combination of temporal variation in exposure as organisms disperse and migrate through variable spatial concentrations, and to recruitment of young individuals with low contaminant concentrations (for example fish that feed on relatively uncontaminated plankton organisms as juveniles then later move onto the bottom where they are exposed to higher concentrations from sediments). Probably the best way to add this capability will be to use individual-based models (IBM) that move individuals over the landscape while accounting for space-time varying concentrations in their food and environment. Ecospace now has an IBM mode for creating packets of individuals and simulating their movement patterns, but Ecotracer contaminant dynamics for these packets have not yet been implemented in the code.

8. Conclusion

The Ecotracer module of EwE was described in detail, with a focus on the mathematical formulation. Several improvements were made to the code including a better treatment of contaminant excretion and improved numerical algorithms. The numerical algorithms were tested on a simple problem with an analytical solution. The Ecotracer results were almost identical to the analytical solution, differing by less than 0.25% for all contaminants at all timesteps. Next, a much more detailed model of the coast off of the Fukushima-Daiichi was modeled for the prediction of $^{137}\text{Cs}$ concentrations. Comparisons were made with the Ecospace and Ecosim versions of Ecotracer, as well as with measured concentration data. Overall, Ecotracer does a good job of predicting post-Fukushima $^{137}\text{Cs}$ concentration data given the simplicity of the model, but some limitations are noted. In particular, Ecotracer/ Ecospace is unable to do any complex modeling of the environmental concentration, e.g., hydrodynamic modeling, and exchanges between dissolved contaminant and sediment. Rather than incorporating these complex physical transport models into Ecotracer, it is recommended to
use an existing code to force the Ecotracer model.

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