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

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ABSTRACT

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 μg, 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., μg).

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

$$\mathrm{CR}_i = \frac{\text{Activity concentration in biota whole}-\text{body } (Bq/kg)}{\text{Activity concentration in (filtered) water } (Bq/m^3)} = \frac{C_i/B_i}{C_0} \quad (1)$$

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, etcHoward 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 radionuclides from a nuclear accident). Certain species/contaminants may take days to years to reach equilibrium (Coughtrey and Thorne, 1983;

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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 (Thomann, 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:

$$\frac{dC_i(t)}{dt} = \alpha_i - \beta_i C_i(t) \tag{2}$$

Where, the input coefficient α_i and loss coefficient β_i 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:

$$\frac{dC_i(t)}{dt} = 0 \rightarrow C_{i,eq} = \alpha_i/\beta_i = \mathrm{CR}_i C_0 B_i \tag{3}$$

This allows the method to give identical steady state results by constraining the parameters influencing α and β 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 (biomagnification 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 (Ecotracer)

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

Ecopath 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:

$$P_i EE_i = BA_i + Y_i + I_i - E_i + \sum_j Q_{ij} \tag{4}$$

where, P $[tons/yr, t/yr]$ is the biomass production rate, and EE is the ecotrophic efficiency (which represents the fraction of production that is used inside the system). This "production" side of the equation for group i is balanced with the biomass accumulation (BA_i $[t/yr]$), fisheries mortality (Y_i $[t/yr]$), immigration rate (I_i $[t/yr]$), emigration rate (E_i $[t/yr]$), predation of group i from group j (Q_{ij} $[t/yr]$).

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 $P_i = g_i Q_i$).

$$dB_i/dt = g_i \sum_{j=prey} Q_{ji} - \sum_{j=predators} Q_{ij} + I_i - E_i - Y_i - MO_i B_i \tag{5}$$

Where, g_i is the net growth efficiency (i.e., production/consumption ratio P/Q), and MO_i $[t/yr]$ is the non-predation ('other') natural mortality rate, corresponding to $P_i(1 - EE_i)$.

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 MO_i [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. $a_{i,N}(x, y)$ is the gross flow rate [1/yr] out of the north boundary of cell (x,y)
2. $a_{i,S}(x, y)$ is the gross flow rate [1/yr] out of the south boundary of cell (x,y)
3. $a_{i,W}(x, y)$ is the gross flow rate [1/yr] out of the west boundary of cell (x,y)
4. $a_{i,E}(x, y)$ 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:

$$\begin{aligned} I_i(x, y) &= a_{i,N}(x, y-1)B_i(x, y-1) \\ &+ a_{i,S}(x, y+1)B_i(x, y+1) \\ &+ a_{i,E}(x-1, y)B_i(x-1, y) \\ &+ a_{i,W}(x+1, y)B_i(x+1, y) \end{aligned} \tag{6}$$

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. Ecotracer equations

The Ecotracer module of EwE models the flow and accumulation of contaminants or tracers in ecosystems while the biomass dynamics equations 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