Ecological Modelling 221 (2010) 1080–1088

Contents lists available at ScienceDirect

Ecological Modelling

journal homepage: www.elsevier.com/locate/ecolmodel

Simulating property exchange in estuarine ecosystem models at ecologically appropriate scales☆

James N. Kremer[a,*], Jamie M.P. Vaudrey[a], Dave S. Ullman[b], Deanna L. Bergondo[c], Nicole LaSota[b], Chris Kincaid[b], Dan L. Codiga[b], Mark J. Brush[d]

[a] UCONN, United States
[b] URI, United States
[c] US CGA, United States
[d] VIMS, United States

ARTICLE INFO

Article history:
Available online 21 January 2010

Keywords:
Estuarine
Ecology
Modeling
Hydrodynamic modeling
ROMS
Box model

ABSTRACT

A computational scheme has been developed and tested to simulate property exchange by advection and dispersion in estuaries at time and space scales that are well suited to ecological and management simulations, but are coarse relative to the demands of physical hydrodynamic models. An implementation of the Regional Ocean Model System (ROMS) for the Providence River and Narragansett Bay (RI, USA) was used to determine property exchanges between the spatial elements of an ecological box model. The basis for the method is the statistical tabulation of numerical dye experiments done with the full ROMS physical model. The ROMS model domain was subdivided into fifteen coarse boxes, each with two vertical layers, defining 30 elements that were used for the box model simulations. Dye concentrations were set to arbitrary initial concentrations for all ROMS grids in the large elements, and the ROMS model was run for 24 h. The final distribution of the dye among the elements was used as a tracer for property exchange over that day and was used to develop an exchange matrix. Box model predictions of salinity over 77 days in each element compared favorably with ROMS simulated salinity averaged over the same spatial elements, although the disparity was greater in areas where large river inflows caused strong gradients in ROMS within elements assumed to be homogeneous in the box model. The 77-day simulation included periods of high and low river flow. Despite the large size of the spatial elements, dispersion artifacts were small, much less than the modeled daily exchanges. While others have taken a similar approach, we found a number of theoretical and practical considerations deserved careful attention for this approach to perform satisfactorily. Whereas the full ROMS model takes 9 days on a powerful computing cluster to compute the physics simulation for 77 days, the box model simulates physics and biology for the same interval in 5 s on a personal computer, and a full year in under 1 min. The exchange matrix mixing model is a fast, cost effective, and convenient way to simulate daily variation of complex estuarine physics in ecological modeling at appropriate scales of space and time.

1. Introduction

Numerical hydrodynamic models are commonly being used to simulate ocean dynamics on very fine scales of space and time (*MIT general circulation model*: Marshall et al., 1997a,b; *Finite-Volume Coastal Ocean Circulation Model* (FVCOM): Chen et al., 2003, 2004; *Princeton Ocean Model* (POM): Oey et al., 1985; Galperin and Mellor, 1990; *Regional Ocean Model System* (ROMS): Haidvogel et al., 2000; Warner et al., 2005a). Time steps of less than a minute and spatial scales of 100 m or less are common for full-estuary models employing state of the art computational power. This resolution is necessary to resolve important aspects of the physics. Indeed, even with modern powerful computers and clusters, physical modelers still must make tough decisions to use coarser time and space scales than would be preferred for resolving physical processes because of practical reasons of limited computing power. Even so, execution times are quite long, especially for full year or multiyear runs, and implementation on personal computer platforms is impractical.

These scales are vastly finer than most marine ecologists feel are appropriate for our understanding of ecological processes, at

☆ This is contribution number 105 of the National Oceanic and Atmospheric Administration's Coastal Hypoxia Research Program. This is contribution number 3062 of the Virginia Institute of Marine Science.

* Corresponding author at: Univ. of Connecticut, Marine Sciences, UCONN, Avery Point, Groton, CT 06340, United States. Tel.: +1 860 405 9027; fax: +1 860 405 9153.
E-mail address: James.Kremer@uconn.edu (J.N. Kremer).

0304-3800/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.ecolmodel.2009.12.014

least as they are formulated in estuarine ecosystem models. Yet it is common to implement the ecology on the same scale, "since we are running the physics anyway." Some widely used ecosystem simulations take this approach. ROMS and FVCOM include an ecological package. The models implemented for research and management in the Chesapeake Bay (Cerco and Cole, 1994; HydroQual, 1999), Long Island Sound (HydroQual, 1991, 1996; LISS STAC, 2003) and Boston harbor outfall (HydroQual, 2000) used this approach.

Others have suggested that ecological models do not require the fine scales used for hydrodynamics (Bird and Hall, 1988). Whether such fine scales are even appropriate for ecological analyses is a question not often addressed. Of course, all processes actually function continuously in real time and space. When modeling is undertaken to investigate the implications of diel or shorter time scales, simulation of small scales is feasible and useful. However, when models are designed for purposes outside the heuristic goal, and especially when the results are destined to inform management and policy decisions, the small scales may be inappropriate. Firstly, in many cases, the coefficients and assumptions implemented in the ecological formulations represent at best a daily approximation of ecological processes. Secondly, rate formulations are often chosen in hopes of simulating average conditions representative of ecological regions and seasons. Thirdly, ecological data available for comparison (or model initialization) are never available at such scales. In fine-scale models, model performance must be averaged over many spatial compartments and compared with observations sparse in space and time.

Next, fine scales complicate and probably weaken the process of evaluating the adequacy of model performance, since poor fit can always be potentially attributed to a mismatch of the model prediction in space and time from the observations. Finally, the computational burden of running ecology in the full physical domain of the hydrodynamics is great, even when stored advection and diffusion rates are used for the ecological simulations rather than running the hydrodynamics concurrently.

In this study, we evaluated the extent to which a coarse box model can reproduce the physical exchanges of a detailed hydrodynamics model. We suggest that many modeling studies use computational scales that cannot be validated, are not necessary for the patterns in space and time that are of interest, and thus are at best unnecessary and perhaps inappropriate. While others have used a similar approach to that tested here (see below), the methodology is rarely explained in detail and direct evaluation of its adequacy is not given.

In our ongoing study of hypoxia in upper Narragansett Bay (funded by NOAA's Coastal Hypoxia Research Program, project NA05NOS4781201), the modeling is directed toward two goals. The first is to simulate and test our understanding of vertical mixing at short scales of space and time with the Regional Ocean Model System (ROMS). The second is to explore various causal interactions for intermittent hypoxia observed in the upper bay (Bergondo et al., 2005). For the first goal, running ROMS at fine scales is necessary. But for the second, we believe that this computationally intensive physical model is actually counterproductive. The need to run the ecological simulations many times to explore large uncertainty in ecological formulations and parameters is inhibited by the required use of large and expensive computer clusters and long run-times. Further, the space and time scales of our conceptual model of ecological processes, and the field data available to build and test the model, are much coarser than imposed by the full physical model. To avoid this constraint, we sought a way to capture the physics of the fine-scale ROMS simulations in a fast-running, conceptually simple mixing model for use with the ecological modeling.

For our ecological questions, we feel that constraints implicit in the formulations limit the appropriate spatial scale to large boxes with limited vertical resolution. Horizontal boxes of O(1–5 km) with two or three vertical layers are adequate and perhaps ideal. Each of these crude computational "elements" comprises hundreds of gridpoints within a typical high-resolution ROMS grid. Temporally, while ROMS runs with $\Delta t = O(10\,\mathrm{s})$ for the physics, for ecological considerations time scales of 6–24 h are appropriate.

Historically, box models such as we use here have often been used for ecological simulations. The approach of defining the dynamics of the box's physics from a fine-scale hydrodynamic model is often not well documented, though it has been done for some time. Kremer and Nixon (1978, see p. 27–36) used a 2D finite difference model (Hess and White, 1974) to calibrate a coarse box model of the ecology of Narragansett Bay, much as we are proposing again here. Williams (1978) similarly used particle tracking in a 2D physical model to define a transfer matrix of exchanges for a box model of Port Phillip Bay, Australia. This approach was later used in a model of the same estuary by Walker (1997, 1999). Williams (2006) and Raillard and Ménesguen (1994) cite other studies where fine-scale model results were averaged over time and space to drive box models (Chen and Smith, 1979; Radford and Joint, 1980; Lindeboom et al., 1988; Bacher, 1989). Some have compared box models of differing resolution versus the full-scale parent (Ménesguen et al., 2007). Some recent management models have used a similar approach (Nobre et al., 2005; Ferreira et al., 2008). Thus this approach has some acceptance especially for applied problems. However, the details of the translation process are rarely reported. Typically, the process is explained as "the fluxes were integrated" or "hydrodynamic outputs were averaged over time and space." In this study, we sought to evaluate in detail how well this box model conversion worked to reproduce the parent fine-scale hydrodynamic model. We found the process to be fraught with subtlety requiring careful attention.

Our approach is conceptually straightforward. The concentration of an arbitrary material "dye" is initialized to a certain value at all ROMS grid cells within a given source element (and zero elsewhere) and then the ROMS model simulates the movement of this dye throughout the model domain. The dye is assumed to track the movement of hydrographic and other biological variables of interest. After a specified time interval, the distribution of dye is the result of physical processes, and the mass of dye within each box model element is determined. Knowing the initial mass of dye in the source element, the fraction of dye in each element is then computed. We have chosen to call this fraction the *gross exchange* between the source element and any destination element, because exchanges in the reverse direction are also computed and tabulated separately by tracking unique dyes for each element. That is, the net transfer of material between elements i and j over a time interval is the result of exchanges from i to j and from j to i. We call the numerical summary of these transfers a *Gross Exchange Matrix* (GEM).

Tabulating gross exchanges among large-scale elements can be done over any specified time interval. For use in the ecological model, we defined the time scale of interest to be 1.0 day, therefore the ROMS dye-exchange runs were carried out over 1-day periods. Although the ecological model does not resolve tidal variations, the presence of tidal processes in the hydrodynamic model makes it important to carry out the dye runs over the same time period as the box model time step. This is because element volumes change over the tidal cycle and this process is captured by the gross dye exchanges.

Finally, even with the crude representation of the estuary by a few two- or three-layered boxes, a large number of exchanges need to be defined. We use ROMS to simulate all exchanges among each of the large-scale elements over 24.0 h simultaneously with different dyes. In addition, we use additional numerical dyes to track the input and movement of river inflows and the exchange at the open ocean boundary.