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ScienceDirect

Environmental Modelling & Software 22 (2007) 488–501

Environmental Modelling & Software

www.elsevier.com/locate/envsoft

Simulation of constituent transport using a reduced 3D constituent transport model (CTM) driven by HF Radar: Model application and error analysis

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Received 11 November 2004; received in revised form 5 July 2005; accepted 12 February 2006
Available online 26 May 2006

Abstract

Data-driven constituent transport models (CTM), which take surface current measurements from High Frequency (HF) Radar as input can be applied within the context of real-time environmental monitoring, oceanographic assessment, response to episodic events, as well as search and rescue in surface waters.This paper discusses a numerical method that allows for the evaluation of diffusion coefficients in anisotropic flow fields from surface current measurements using HF Radar. The numerical scheme developed was incorporated into a data-driven CTM and through model error analyses, the effects of using spatially variable transport coefficients on model predictions were examined. The error analyses were performed on the model by varying the cell Reynolds number, $Re = f(\boldsymbol{u},\boldsymbol{K},\Delta\boldsymbol{x})$ between 0.15 and 100, where $\boldsymbol{u}$ is the velocity vector within the flow field, $\boldsymbol{K}$ is a diffusivity tensor and $\Delta\boldsymbol{x}$ is the computational grid cell size.Two instantaneous releases of conservative material were then modeled, the model being initialized at two different locations within the domain. From the two simulation runs, marked differences in the predicted spatial extent of the conservative material resulting from the spatially varying diffusivity values within the study area were observed. Model predictions in terms of variance or size estimates of a diffusing patch were found to be more affected from using inaccurate diffusivity estimates, and less affected from using inaccurate current measurements. The largest errors occurred at $Re > 2$ associated with changing diffusivity values, going up to as much as a 25-fold difference in variance estimates at $Re = 100$. Very little effect on variance estimates due to varying velocity values were observed even at $Re > 2$. This model was applied within the framework of constituent tracking to Corpus Christi Bay in the Texas Gulf of Mexico region.

Keywords: Coastal; Diffusion coefficients; Mixing processes; Modeling; Pollutant transport; Transport processes; USA; Gulf of Mexico; Texas; Corpus Christi Bay

1. Introduction

Mixing processes (turbulence and shear) in surface waters are important as they govern the overall distribution of constituents within the domain of interest, including constituents that may be biogenic or anthropogenic in origin. In conjunction with sampling and measurements, constituent transport modeling (CTM) can be a valuable tool for environmental assessments, forming the bedrock of most water quality and pollutant tracking applications in surface waters. A number of these models have been developed for use in various applications covering a wide range of spatial and temporal scales. An excellent review of models and their applications can be found in Martin and McCutcheon (1998) while Reed et al. (2004) describes an application for simulating dispersant application in a shallow bay. Mechanistic models such as ADIOS developed by the National Oceanic and Atmospheric Administration Hazardous Materials Response Division (Lehr et al., 2002) and SIMAP developed by Applied Science Associates (McCay, 2003) have specific application to oil spills while others such as WQMAP (Spaulding et al., 1999) are more general in their application to water quality. These models are based on the solution of

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doi:10.1016/j.envsoft.2006.02.010

coupled sets of partial differential equations (PDEs) comprising two distinct modules. One module provides hydrodynamic information through direct numerical simulation (DNS) while the other module provides solution from the constituent (mass, heat, solute, etc.) transport equations. The DNS module is a set of PDEs, comprising the well-known Navier–Stokes equations based on momentum conservation while the constituent transport module is a set of advection–diffusion reaction PDEs based on mass conservation laws.

The governing equation of constituent transport will have a diffusive component that is based on Fick's law of diffusion and applicable when the scale of the transport phenomenon is larger than the characteristic scale (time or length) of the diffusion process. This derives from the material balance in turbulent flow within an elemental fluid volume accounting for the combined turbulent fluctuations in the currents field and the constituent of interest. For conservative materials, the resultant temporal gradient (or time rate of change) of solute concentration is the sum of the spatial gradients of the advective and diffusive fluxes. This argument although developed within the context of turbulence can be extended to include other effects that are known to influence diffusive processes such as current shear (Bowden and Howe, 1963; Elliot, 1986). Since the turbulent field in bays exhibits anisotropy, one would expect to find the diffusive process characterized by the diffusivity values exhibiting spatial–temporal variability (Ojo and Bonner, 2002). The spatial variability of diffusivity was investigated as part of this study.

From the foregoing, two sets of coefficients are required in the governing equation of transport: the advection (velocity) coefficients and the diffusion coefficients (turbulence or shear). Advection coefficients are provided either through direct observations or through DNS as outlined above and in this study, these were obtained from direct observations using HF Radar. Diffusion coefficients can be estimated using one of the following methods:

- Method A: From the evaluation of the temporal variation of the magnitude and direction of currents (Paul et al., 1989; Taylor, 1920, 1954).
- Method B: Based on the evaluation of the spatial variation of the velocity field (Csanady, 1980 (reprinted); Elder, 1958; Taylor, 1953).
- Method C: From the evaluation of the first and second moments of concentration distribution of a diffusing cloud (Murthy, 1975; Okubo, 1971).
- Method D: An inverse problem based on the governing equation of advection–diffusion (Ernest et al., 1991; Lam et al., 1983).

The first three of these four methods have been applied in a series of related studies within Corpus Christi Bay (Ojo et al., submitted for publication-a-b, in press) aimed at estimating diffusivity values from direct observations of current in surface waters.

The spatial extent typical of bays and estuaries is such that the incorporation of hydrodynamic information into a CTM defaults to the DNS method, which couples a hydrodynamic numerical scheme to a mass transport scheme within the modeling framework. While the required model parameterization are in many cases based on turbulence–closure schemes that have been developed by a number of researchers (Wijesekera et al., 2003), there are inherent uncertainties in their application especially within shallow wind-driven bodies of water typical of Texas bays. Improved accuracy can be achieved in CTM applications by incorporating direct measurements of velocity (or advective coefficients) in near real-time into constituent transport and water quality models predicated on recent advances in surface current measurements using HF Radar.

As outlined above, the diffusion coefficients can be estimated from the velocity time series, which are then incorporated into the modeling framework. In this study, Method A was applied where the diffusion coefficients were evaluated using the statistical properties of a turbulent flow field, leading to the development of a data-driven CTM. Since HF Radar only provides surface currents (2D velocity profile) within the domain of interest, in order to develop a 3D current field, Acoustic Doppler Current Profiler (ADCP) measurements were used in providing velocity time series along the vertical coordinate axis.

The objectives of this study are the following:

1. To estimate diffusion coefficients based on direct observations of hydrodynamic data on spatial scales ∼30 km and temporal scales covering several tidal cycles.
2. To develop a framework for incorporating direct hydrodynamic observations and derived turbulent diffusivities into a simplified data-driven CTM.
3. To examine through model error analysis:
   a. The effect of inaccuracies associated with current measurements on model predictions.
   b. The results of using spatially averaged values of diffusion coefficients typically obtained from diffusion diagrams or tracer experiments vs. using spatially distributed values obtained through current measurements as outlined above.
4. To apply the resulting simplified data-driven CTM to near real-time constituent tracking in Corpus Christi Bay, Texas.

The integration of numerical modeling (Ernest et al., 1991; Lee et al., 2000; Sterling et al., 2004a,b) with real-time measurements (Ojo et al., 2003) is important for characterizing bays and estuaries as well as within the context of response to episodic events in surface waters. This is part of ongoing research within our laboratory with the overarching objective of developing an operational environmental and oceanographic assessment system for the coastal and nearshore environments.

2. Background theory

The generalized form of the governing equations that form a coupled set for a CTM is given in Eqs. (1) and (2) where u_x, u_y, u_z are the component velocities, N_x, N_y, N_z are eddy