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Integrating Numerical Models with Data Analysis in Site Assessment

Timothy R. Keen (keen@nrlssc.navy.mil) and James D. Dykes
(Naval Research Laboratory, Stennis Space Center, Mississippi)

ABSTRACT: The characterization and assessment of contaminated sites can be made more effective with the interactive use of in situ data, historical records, and results from predictive process-based numerical models. These three components can be difficult to merge because of space and time scales, as well as data formats and availability. We are developing an Application and Programming Interface (API) tool to make this procedure more accessible to a range of interested groups. This tool consists of two components: (1) a GUI-based toolbox of data processing and analysis software and (2) a numerical modeling system for hydrodynamics, sedimentation, and mass transport. The toolkit includes modules to analyze data in four dimensions and merge different data types as well as compute derived variables. The modeling system includes models that calculate waves; circulation due to tides and the wind; entrainment of bottom sediment; and the transport of dissolved and suspended material. The components of the API have been tested on the potential entrainment and transport of contaminants in San Francisco Bay, California, and St. Louis Bay, Mississippi. The models have proven valuable at predicting the movement of dissolved and suspended contaminants both within enclosed bays as well as in estuaries and the inner shelf. The results indicate that integration of the models with available data for planning containment and remediation strategies would reduce the effort required to characterize a contaminated site using field methods alone.

INTRODUCTION

The U.S. Navy has more than 40 coastal and nearshore contaminated sediment sites that are included on the National Priorities List (Superfund sites) (CNO, 2005). Navy remediation policy requires that the source(s) for these sites must be identified and that a monitoring plan must be in place before data collection begins. Both of these tasks can be made easier by the use of mathematical models of the site-specific processes that impact contaminant behavior and public health risks. For example, inactive contaminant sources can be identified from historical records and the current distribution of sediment-bound contaminants, but this straightforward approach cannot predict remobilization by physical mechanisms.

Contaminant transport by water and sediments can be simulated in numerical hydrodynamic, sediment dynamics, and water quality models. These models are capable of simulating post-depositional processes and can help identify sources and evaluate remobilization. The quantitative predictions from numerical models can be used to define zones of potential future contamination and assist in determining an efficient sampling strategy for monitoring. Sediment and contaminant transport modeling is often conducted on a site-specific basis. This approach works especially well for rivers and lakes (Connolly et al., 2000) but accuracy depends on dense sampling because local models cannot include the impacts of external influences. With the recognition of pollution problems in estuaries, the simulation of contaminant dispersal in open bodies of water has become

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more widespread. The accurate prediction of contaminant transport in coastal waters requires comprehensive hydrodynamic descriptions (i.e., river input, tides, wind-driven flow, heat and mass mixing, and surface waves). The U.S. EPA encourages the use of numerical models for pollutant transport (e.g., the Chesapeake Bay Program: www.chesapeakebay.net), which is especially important for long-term effects caused by rare events (e.g., severe storms) and the cumulative effects of weaker processes.

Numerical models are typically used only where there is public interest or a potential health threat (e.g., Aldridge et al., 2003). NAVFAC's *Implementation Guide* recommends that modeling should be considered as a tool to integrate site data (NAVFAC, 2003), but conceptual site models are routinely used at Navy sites instead of numerical models. Nevertheless, the Naval Oceanographic Office (NAVOCEANO) and Naval Research Laboratory (NRL) have developed and successfully validated several models for littoral environments (Harding et al., 1999).

INTEGRATED AQUATIC DATA ANALYSIS AND SIMULATION

Our approach consists of two components: (1) a suite of numerical models and the software required for their use and (2) an analysis toolkit built on Geographic Information System (GIS) libraries. This system is being actively developed and the results presented herein represent an intermediate level of implementation rather than a completed API.

Numerical Models. Numerical models are routinely used for atmospheric and oceanographic forecasting at production centers, forward centers, and even at the fleet level (Flather, 2000; Burnett et al., 2001). The forward deployment of ocean modeling is simplified somewhat from the production centers because of reduced computational resources, but local models are supplied with required boundary conditions from the major centers. This approach has been demonstrated for different physical processes in several regions (Keen and Holland, 2010).

Simulations of mass transport in estuaries and nearshore areas are dependent on water levels and currents calculated by circulation models. Computing chemical behavior is further reliant on salinity and temperature. Local hydrodynamic models are more flexible than global and basin models because they do not incorporate data assimilation schemes. A tailored model can thus be implemented for a specific problem. In addition to flow calculations, it is often necessary to simulate waves and mass transport processes (e.g., sedimentation), requiring either additional numerical models or comprehensive observations. The examination of complex sites where multiple sources are present and remobilization is possible would likely require the simulation of the wind, waves, currents, temperature and salinity, sedimentation, boundary layer processes, and mass transport within a small area, as well as the surrounding estuary or ocean. Remediation experts thus find themselves forced to choose between using a parametric model that is dependent on random sampling, and using numerical models that require expert knowledge for reliable operation.

One solution to this problem is to implement numerical models of physical processes in the littoral ocean in the following manner. First, it is a simple matter to take advantage of operational ocean models run by NAVOCEANO. These fields of water levels, currents and waves can be a first approximation of environmental forcing in many areas. The second step is to utilize local models in a reach-back mode, which is largely implemented to provide environmental support for Navy operations (Malley et al., 2005). Finally, this approach can be implemented as a network-centric system as has been proposed for operational forecasting (Jimenez, 2009).

Analysis Toolkit. NAVOCEANO has implemented an operational support center for antisubmarine warfare (ASW) oceanographic modeling and forecasting. This reach-back cell (RBC) is staffed by subject-matter experts whose analyses are aided by the ASW Reach-Back Cell Oceanography Analysis System (ARCOAS). ARCOAS is a GIS-based toolkit incorporating a customized ArcMAP application tailored for meteorological and oceanographic (METOC) analysis of data and model forecasts. ARCOAS has extensive capabilities, including georeferencing using a standard datum (e.g., NAD83), the statistical analysis of different databases on their original locations or collated for specified times, spatial and temporal averaging, and the inclusion of other data (e.g., USA Prime Imagery server).

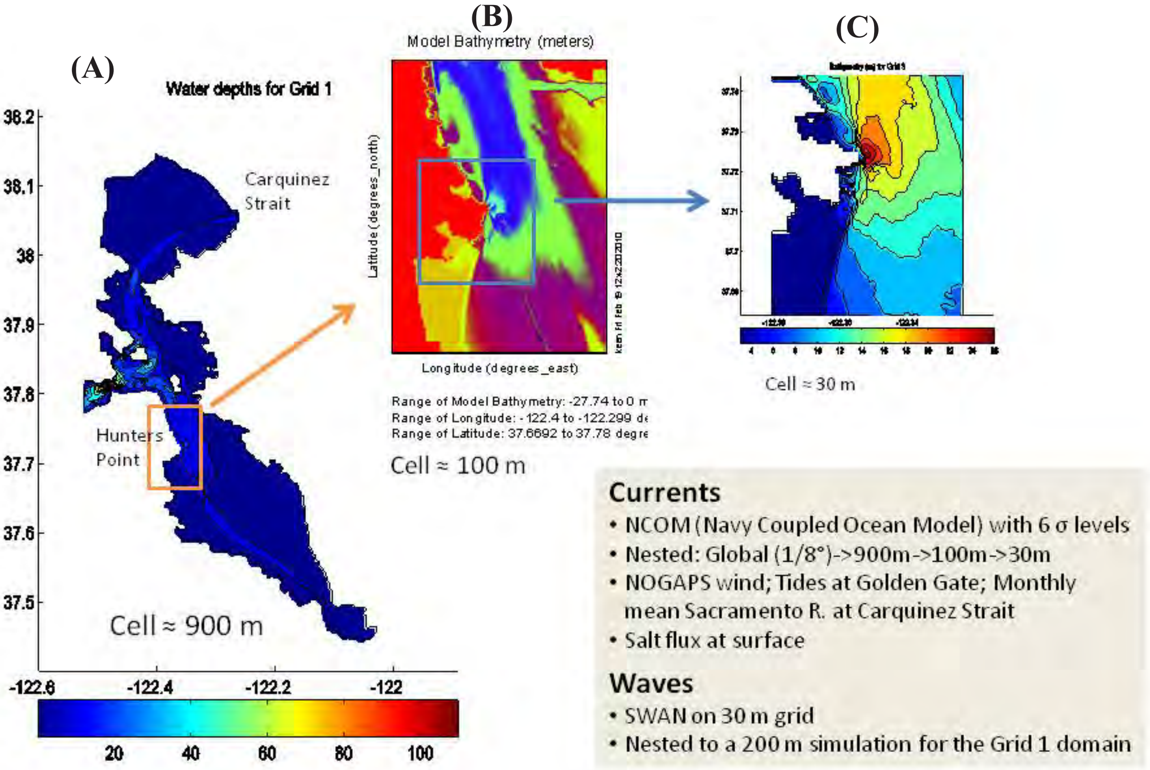
ARCOAS can easily be expanded to include additional METOC and other geophysical tools as the need arises because it is programmed using an inherently flexible and full-featured platform. This advantage permits access and analysis of all data and information in one place. ARCOAS both addresses operational Navy requirements and lends itself to interoperability with other systems using similar protocols and formats. A primary objective is to provide critical environmental characterization of the battlespace within the concept of network-centric operations using a services-oriented architecture (SOA) (Meyer, 2007). In line with this Navy METOC requirement, the RBC concept provides the ability for forward-deployed teams to request in-depth analyses from the RBC, thus freeing them to provide tailored support to their customers. Some ARCOAS tools may also be suited for users outside of the RBC.

EXAMPLE PROBLEM: HUNTERS POINT SHIPYARD

The south basin at Hunters Point Shipyard (SBHP) is a small (< 0.5 km^2) tidal basin in San Francisco Bay (SFB) (Figure 1). Potential remobilization in SBHP depends on whether sediment-bound contaminants can escape into SFB by natural mechanisms. To address this problem, it is necessary to examine the potential release of contaminants from the bottom and to evaluate their potential transport by physical processes. This complex problem has been studied using wind forecasts from the Navy Operational Global Atmospheric Prediction System (NOGAPS), and Pacific Ocean temperature, salinity, and sea surface height (SSH) from the global Navy Coastal Ocean Model (NCOM). These products supply boundary conditions to local grids for NCOM to calculate currents and SSH, and SWAN (Simulating Waves Nearshore), which computes significant wave height (SWH). The predicted currents and waves are used to compute sediment entrainment with the Littoral Sedimentation Model (LSM). The currents are also used to calculate dissolved tracer concentrations and particle transport.

Modeled Hydrodynamics at Hunters Point. This example focuses on the contaminant remobilization during periods of southeasterly winds and tides. The largest waves in SBHP occur when the wind is from the SE due to the increased fetch (Zimmerman et al., 2008; Keen and Holland, 2010). The NOGAPS wind is southeasterly (max = 13 m/s) between 6 and 10 January 2004. The predicted SWH from SWAN in SBHP exceeds 35 cm on 8 January. The ebb-tide model currents (short-dash line in Figure 2) reach

6 cm/s toward the SE along the eastern shoreline of SBHP despite the southeasterly wind. This flow extends from the NE corner of the inner basin to the outer basin. The tidal flow is into SBHP during the flood tide. This inflow/outflow cycle is repeated daily. There is also a strong ebb tide flow (> 20 cm/s) from Yosemite Creek (long-dash line in Figure 2) in the NW end of SBHP. The model currents during high water show a counterclockwise transport within SBHP that is in agreement with the observations and residual sediment fluxes (Zimmerman et al., 2008). This transport regime includes a SE flow driven by the ebb-tide that the observations from 2001 did not capture. The model also reveals a widespread flow into the outer basin and transport along the eastern shore.



Currents

- NCOM (Navy Coupled Ocean Model) with 6 σ levels
- Nested: Global (1/8°)->900m->100m->30m
- NOGAPS wind; Tides at Golden Gate; Monthly mean Sacramento R. at Carquinez Strait
- Salt flux at surface

Waves

- SWAN on 30 m grid
- Nested to a 200 m simulation for the Grid 1 domain

FIGURE 1. Grids used for numerical simulations in this study: (A) the SFB grid; (B) the Hunters Point (HP) grid; and (C) the SBHP grid. The box in A indicates the domain of B, and the box in B is the SBHP grid.

Resuspension of Bottom Sediment. The predicted max shear stress τ_m is 8.7 Pa. The depth of erosion can thus be qualitatively compared to the results from laboratory experiments on sediments from Hunters Point (Zimmerman et al., 2008). The Sedflume device was used to measure the erosion rates for homogenized sediments after 1 hr and 16 d of consolidation. The erosion rate for sediments at 1 and 13 cm in a core (16 d settling) at a shear stress of 6.4 Pa was 0.01 and 0.008 cm/s, respectively. The same core had a constant erosion rate of approximately 0.03 cm/s at a shear stress of 8 Pa. This result suggests that the surface sediments would have been instantly removed.

FIGURE 2. Summary of currents and tracer predictions for SE wind event during a tidal cycle on 8-9 January. The maximum tidal outflow is 20 cm/s (long dashed line) and tidal inflow/outflow is 6 cm/s (short dashed line). The wind speed is labeled and the direction is indicated by the arrow. The tracer concentration is contoured after 24 h of release from the locations indicated by stars (dimensionless). The measured concentration of PCBs (µg/kg) is indicated by the solid circles (Battelle et al., 2002).

The LSM calculates total suspended solids (TSS) as well as an active layer depth, which is the thickness of disturbed sediment, and the equivalent bed depth of sediment particles in suspension. The predicted TSS (Figure 3) reaches peaks of 450 and 360 mg/L during consecutive low tides; the resulting active layer exceeds 14 cm and the resuspension depth is 0.54 mm. The similarity of the measured (400 to 600 mg/L in 2001) and predicted TSS suggests an erosion depth of about 10 cm, below which the sediment would have been too consolidated to erode.

The depth of erosion can be used to evaluate the release of contaminants from the bottom sediment. For example, the measured concentrations of metals from grab samples (Table B3 in Battelle et al., 2002) suggest elevated levels within the predicted erosion depth. These metals could thus be introduced to the water column during SE wind events. The mechanism for their exchange between the sediment and water would need to be represented by a water quality model that is not part of our system. The available profile data for SBHP are not easily analyzed because typical sample intervals were 2 feet (60 cm) except for Pb^{210} data, which were collected at ~10 cm intervals.

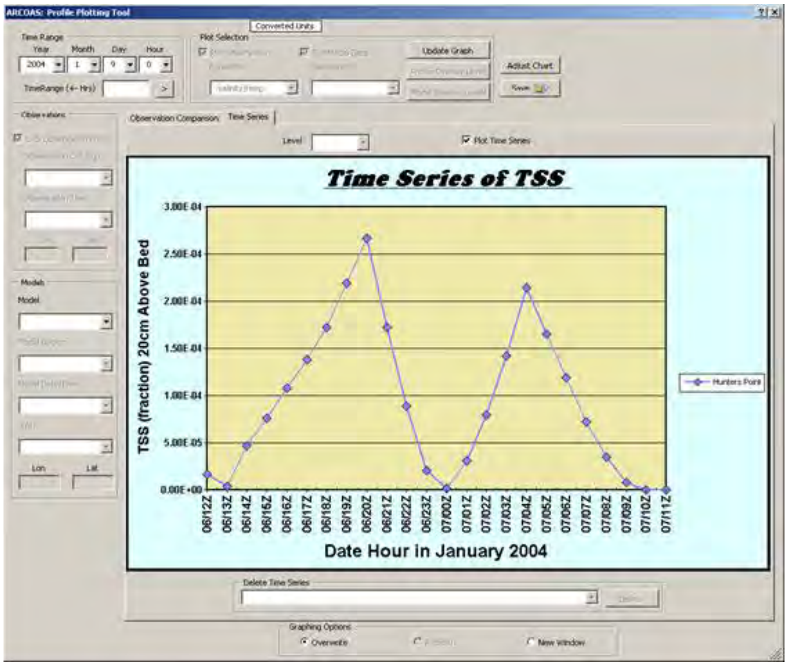

Year 2004
Month 1
Day 9
Hour 0

FIGURE 3. Hourly TSS 20 cm above the bed computed by LSM in SBHP (water depth = 1.82 m).

Contaminant Transport. Contaminants within the seafloor can be released when the bottom sediment is disturbed. The timing of the potential releases in this study is directly related to the wave energy predicted by SWAN through the bottom shear stress. The most likely times for contaminants to be released into the tidal basin are when TSS is high (Figure 3). This potential release is simulated in the model using a concentration of 5 (units are arbitrary) at the locations indicated in Figure 2.

The initial tracer release coincides with the first resuspension event, which occurs at low tide. During the ensuing flood-tide, the tracer released within the inner basin is transported westward and collects along the western shore. The CCW circulation within the south basin causes accumulation of the tracer along the western side of the inlet as well. The flood tide works with the SE wind to transport the surface water back to the NW and into the inner basin. The following ebb tide transports the tracer along the eastern shore into the outer basin (Figure 2).

A second approach to evaluating the paths of contaminants released from sediments at SBHP is to use particles as Lagrangian tracers. This method is useful for complex flows where the kinematics of particle behavior are not well constrained. The particle model uses the currents calculated by NCOM on the SBHP grid for January 2004 (Figure 4). After 31 days of transport, the heavier particles, which are representative of silt, are primarily distributed around Hunters Point (yellow points in Figure 4) and become trapped within the southern basin. The lighter particles (aqua circles) have been transported into SFB. The interesting result from this simulation is that particles with finite settling velocities have reached the main bay. This transport occurs over several days under a range of flow conditions. The implication is that, even if toxins adsorbed to clay particles require several days' exposure to sea water to become dissolved, it is likely that some contaminant would be dissolved into the waters of the main bay.

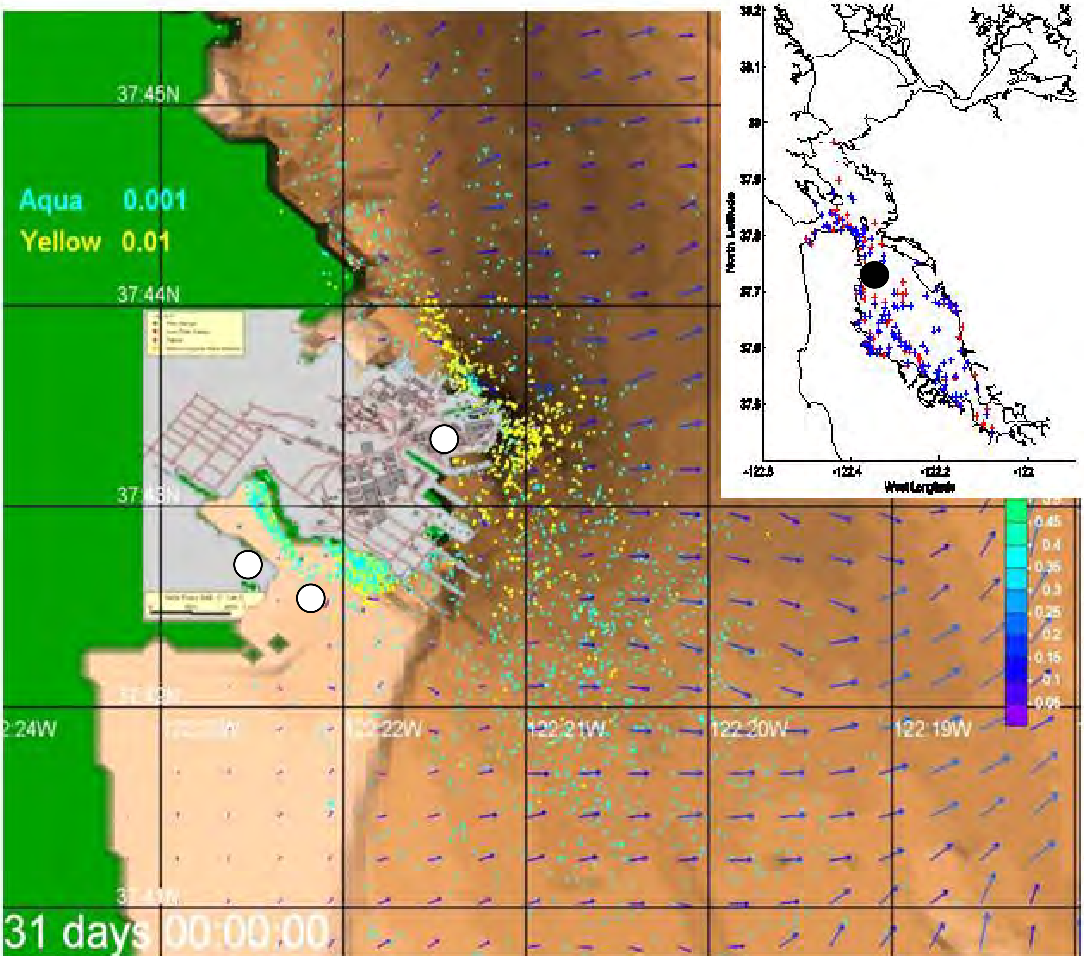


FIGURE 4. Particle distributions near Hunters Point computed by a particle tracking algorithm for January 2004. Particles were released at the locations indicated by the circles. The aqua particles have a settling speed of 10^{-3} mm/s, which is representative of clay flocs. The yellow particles have a settling speed of 10^{-2} mm/s, which is more typical for large flocs and silt. The bathymetry is represented by shading. The vectors are the surface currents calculated by NCOM on the 30-m grid. Current speed (m/s) is indicated by shading as shown on the colorbar. The inset map shows the particles after 15 days (red pluses) and 28 days (blue pluses) for February 2004. The currents are from the NCOM SFB grid. One particle was released every 24 hours.

SUMMARY

The paper has two objectives: (1) shed light on the question of whether and how sediment-bound toxins in a small tidal basin can escape into San Francisco Bay and (2) briefly demonstrate the potential integration of numerical modeling methods with data collected from the field in studying this problem. Part (1) is a straightforward application of multiple models to the problem but it is complicated by the importance of environmental factors that operate at a range of scales. This problem demonstrates the importance of tides and atmospheric events like the southeasterly winds in SFB. These environmental factors, which are external to the study area, are critical in understanding the hydrodynamics and potential release of sediment-bound contaminants. The internal factors like local wind and still-water depth were not as critical in this example but they play important roles for the long-term stability of the bottom sediment. There is no easy way to include both internal and external environmental factors in a numerical study but this example shows one approach that does not require the development of new models. It does, however, rely on access to operational or archived environmental forcing. This is where the reach-back cell concept becomes important, as has been the case for ASW.

This study has demonstrated some of the problems associated with multi-scale, multi-physics simulations. As with most estuary models, the water depth is critical. The shallow water in the south basin is a determining factor in sediment resuspension. A small uncertainty in depth can decrease the wave-current bottom stress below the critical threshold for entrainment and completely change the results. Thus, it is important to simulate the tidal amplitude and phase accurately so that the water depth is correct. The wind direction was critical in this example because of the generation of larger waves from the SE. The range of potential environmental factors that can impact the hydrodynamics and sediment dynamics in an estuary is a strong motivation for implementing the RBC concept using network-centric software like ARCOAS. This approach can bring the computational and data resources of the entire defense establishment into the hands of remediation managers at forward deployments.

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