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3-D Hydrodynamic Modeling in a Geospatial Framework

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Abstract

3-D hydrodynamic models are used by the Savannah River National Laboratory (SRNL) to simulate the transport of thermal and radionuclide discharges in coastal estuary systems. Development of such models requires accurate bathymetry, coastline, and boundary condition data in conjunction with the ability to rapidly discretize model domains and interpolate the required geospatial data onto the domain. To facilitate rapid and accurate hydrodynamic model development, SRNL has developed a pre- and post-processor application in a geospatial framework to automate the creation of models using existing data. This automated capability allows development of very detailed models to maximize exploitation of available surface water radionuclide sample data and thermal imagery.

INTRODUCTION

The Savannah River National Laboratory (SRNL) is performing research directed at improving its ability to predict the transport and dispersal of radioactive materials in coastal waters. The focus area of the research is the coastal zone of South Carolina and Georgia, where tidal currents, wind stress and buoyancy forces created by salinity and thermal gradients all contribute to the transport of radioisotopes through the complex network of estuaries, tidal creeks, and marshes that link sources of radioactivity such as the Savannah River to the open Atlantic Ocean. Applications of this research include more accurate dosimetry calculations as well as an improved capability to determine the sources of radioisotopes in the environment and the magnitude of the source terms contributing to environmental concentrations.

The analytical tool used by SRNL in this research is a hydrodynamic code (ALGE) designed specifically for surface water transport simulations, the use of which is facilitated by rapid automated geographic information systems (GIS) pre- and post-processing of model input and output. SRNL has applied the ALGE code to a wide variety of surface water transport problems, including cooling lakes, cooling canals, rivers, estuaries and thermal discharges to the open ocean (Garrett and Hayes 1997; Garrett et al. 1999; Garrett 2001).

HYDRODYNAMIC MODEL

ALGE is a 3-D hydrodynamic code that simulates a free water surface and models heat and momentum transfer to and from the atmosphere. Mass (water) sources and sinks can be located at any of the nodes in the computational domain. Water temperature and

radionuclide concentrations also can be specified at those nodes. ALGE solves the set of 3-D partial differential hydrodynamic equations used by most researchers to predict the behavior of bodies of water with free surfaces (Blumberg and Mellor 1983; Oey et al. 1985; Froehlich 1989; Jin and Kranenburg 1993; Johnson et al. 1993). The equations used in ALGE are more fully developed in Garrett and Hayes (1997). The processes modeled include transport, diffusion, deposition of aqueous tracers, and conservation of thermal energy.

ALGE accounts for solar and thermal radiation using a method developed and tested by Garrett (1978, 1980, 1982). In addition, sensible and latent heat fluxes are computed according to the relationships developed by Louis (1979). The net surface longwave radiative flux is computed with a simplified transmission model that treats emission and absorption in combined spectral bands. This model was developed by Kondratyev (1969) and tested by Garrett (1977). ALGE includes a free-surface simulator, first-order chemical reactions, and accounts for radioactive tracer transport/particle transport deposition and resuspension. The advective and diffusive terms in the 3-D hydrodynamic equation set for ALGE are solved by the conservative differencing scheme described by Roach (1972), Jin and Kranenburg (1993), and Johnson et al. (1993).

ALGE GEOSPATIAL FRAMEWORK

As discussed above, the ALGE code has been developed to solve the partial differential equations that account for the physics of surface water and energy transport. The solution of these equations requires the development of a finite difference grid or mesh over which the equations are solved by ALGE. This 3-D mesh is comprised of

spatially equidistant points in the horizontal plane with layers in the vertical direction of uniform thickness. Model parameters such as position, depth, frictional drag, horizontal eddy viscosity and diffusivity, and boundary conditions are specified at each node in this 3-D mesh.

To facilitate rapid development of the ALGE model mesh from geospatial data, an ArcView 3.2 extension was developed to automate the process of generating the finite difference mesh. This ArcView extension includes options to create the 2-D mesh points, attribute the mesh with boundary conditions, assign number of layers in the vertical direction at each point based on depth, and write the ALGE input files. Prior to using the ArcView extension, the required geospatial data must be prepared, consisting of a polygon of the land surface that delineates the shoreline boundary and a bathymetry grid that represents the water depth as a function of location (see Figure 3a).

The first step is to create a rotated rectangle of the model orientation and extent as shown in Figure 1a. Using the ArcView extension, the user specifies the mesh spacing (distance between points) and a point shapefile is automatically created as shown in Figure 1b. The blowup in Figure 1c shows the point density of the mesh.

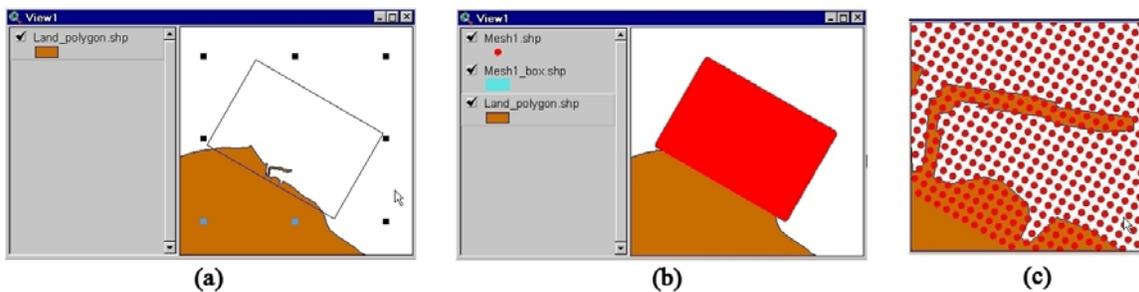


Figure 1. Automated generation of point mesh

The next menu step in the extension automatically assigns water codes for interior and boundary points as shown in Figure 2a. Then the land polygon is intersected with the

mesh points to assign land codes as shown in Figure 2b. The prepared bathymetry grid in Figure 3a is used to interpolate depth values at each point in the mesh. The user specifies layer thickness and the number of layers at each point is computed and assigned as a layer code as shown in Figure 3b. At this point the user can chose an option to write the ALGE input files representing the generated mesh and attributes. Note that the user has the option of manually editing the attributes to represent detail that may be known but not represented in the base data. For example, a dredged channel may not be resolved in the bathymetry grid but could be important in the simulation.

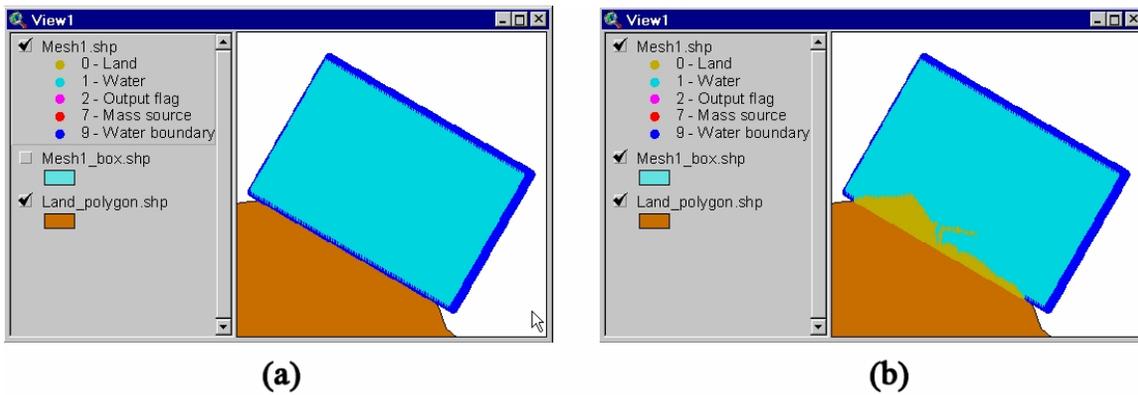


Figure 2. Assignment of codes for (a) water and (b) land

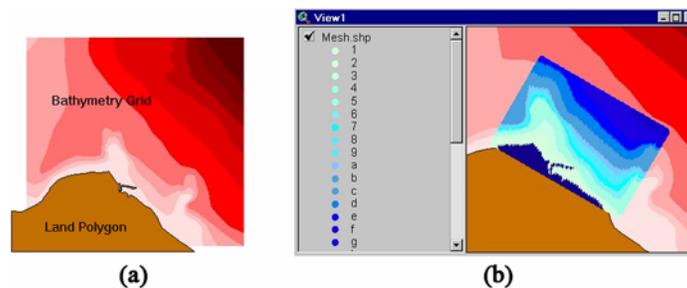


Figure 3. Assignment of layer codes from bathymetry grid data

The ALGE computation using the input files may take from several hours to many weeks to complete depending on the complexity of the problem and is run as a standalone application. After the simulation is complete, the output can be post-processed with ArcView to visualize the results. The primary utility of this post process is to convert the ALGE results from model coordinates back into projected coordinates for overlay with available geospatial reference data.

An ArcView script was written to automatically import the ALGE results into a point shapefile in model coordinates as shown in Figure 4a. The water points in Figure 4a are assigned an attribute with the concentration computed by ALGE. The concentration value at each point is used to create a grid of the concentration as shown in Figure 4b.

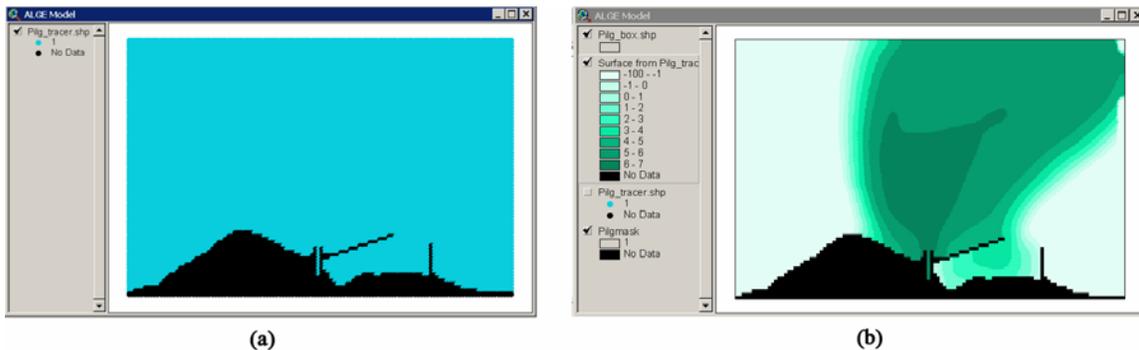


Figure 4. Import of ALGE results in model coordinates

Concentration contours in model coordinates are computed from the concentration grid as shown in Figure 5a. From the pre-processing with ArcView to create the mesh, the conversion between projected coordinates and model coordinates is known. This information is used to transform the contours into projected coordinates for overlay with geospatial reference data as shown in Figure 5b.

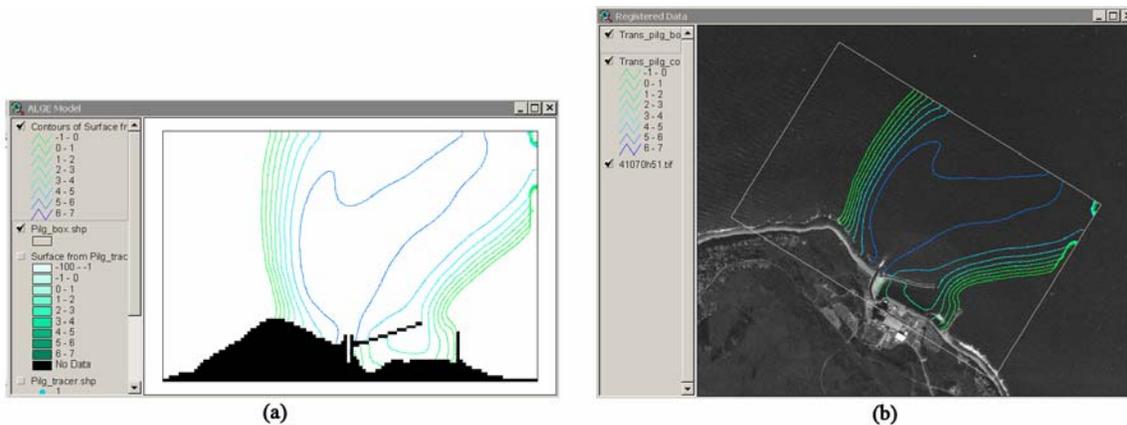


Figure 5. Contours of ALGE results in model coordinates and projected coordinates

The above post process is used to show a final result from the transient ALGE computation, which is often a desirable product. However, it may be useful to visualize the transient computation. The methods described above have been extended with ArcGIS scripts to automate the creation of a grid at each time step in the ALGE computation, to transform each grid to projected coordinates, and to overlay each grid on geospatial reference data in a layout that is then exported as an image file. These image files are then compiled as frames in a movie that shows the transient simulation results.

DESCRIPTION AND RESULTS

Since tritium oxide is a nearly conservative quantity that is passively transported and dispersed in water, it is an ideal tracer for use in research on aqueous transport of pollutants. Residual amounts of tritium that was produced during the Cold War enter the Savannah River from the Savannah River Site (SRS) (see Figure 6), which is located about 150 km from the mouth of the river. Tritium concentrations downstream from SRS

range from about 0.5 pCi/ml to 1.0 pCi/ml. Note that the Environmental Protection Agency (EPA) Drinking Water Standard for tritium is 20 pCi/ml.

The average tritium source term from SRS in the river is 18 +/- 8 Ci/day. Some of this tritium enters the Atlantic Ocean directly from the Savannah River, and some of it enters the marshes and tidal creeks adjacent to the river as a result of tidal pumping. SRNL collected tritium grab samples in tidal creeks, estuaries, and offshore on March 5, 2005. SRNL simulated transport of tritium from SRS down the Savannah River into the Atlantic Ocean with ALGE, and found that a three-month simulation was necessary to reach quasi-equilibrium in tritium concentrations out to approximately 30 km offshore. Comparison of prediction and measurement generally agreed to within about a factor of two (Figure 7).

The simulation that produced the predicted tritium concentration contours in Figure 7 was performed using a coarse 1-km resolution grid in the horizontal plane and 2-m in the vertical plane that was generated using the ArcView pre-processing extension. This coarse resolution allowed only a crude representation of the tidal creeks and marshes that receive some of the SRS tritium from the Savannah River before it reaches the Atlantic Ocean. Both the tritium measurements plotted in Figure 7 and the simulated contours show that a significant part of the tritium enters the marshes on the south (Georgia) side of the river and makes its way to the Atlantic Ocean via a large tidal creek south of Tybee Island.

The simulation used to produce the results shown in Figure 7 treated the marshes as continually covered by water, with the water level varying according to the tidal stage. The water in the marshes at low tide was a fraction of a meter deep, and over two meters

deep at high tide. In reality, the marshes are drained of water at low tide and are no more than about one meter deep at high tide. As a result, the model simulation carried excessive amounts of tritium into the marshes from the Savannah River. This helps to explain the under-prediction of tritium concentration at the mouth of the Savannah River and the over-prediction at the mouth of the tidal creek south of Tybee Island.

SRNL is continuing its research on tritium transport in the coastal waters of South Carolina and Georgia in a three-year collaborative project with the Skidaway Institute of Oceanography (SkIO). This project will make use of data collected by SkIO as well as an extensive database collected after a 5700 Ci release of tritium from SRS in December 1991 (Hamby 1993). SRNL plans to make more realistic simulations of the marshes with higher-resolution computational domains and by adding marsh node drying and rewetting. The use of automation within the geospatial framework is essential to generate the higher-resolution meshes in a timely manner. Also, techniques are being developed to automatically distinguish marsh areas. Initial results of modeling the 1991 tritium release are shown in Figure 8, which contains time series plots of simulated and measured tritium concentrations at Ft. Pulaski, located at the mouth of the Savannah River. Two simulations were performed; one treated the marshes as dry land at all times, and the other treated them as water covered with a variable depth according to the tides. Figure 8 shows that the measured tritium concentrations are bracketed by the two sets of simulated concentrations, which was expected. More accurate simulations will therefore almost certainly require code modifications to incorporate the ability to dry out and rewet nodes representing marshes.

REFERENCES

- Blumberg, A.F. and Mellor, G.L., 1983. Diagnostic and Prognostic Numerical Circulation Studies of the South Atlantic Bight. *J. Geophys. Res.* 88(C8):4579-4592.
- Froehlich, D.C., 1989. Finite Element Surface-Water Modeling System: Two-Dimensional Flow in a Horizontal Plane (Users Manual). *Rep. No. FHWA-RD-88-177*. U.S. Geological Survey, Water Resources Division, Reston, VA.
- Garrett, A.J., 1977. A Comparison of the Observed Longwave Radiation Flux to Calculations based on Kondratyev's and Brunt's Methods. *Arch. Mmet. Geoph. Biokl. Ser. B.* 25(1):127-134.
- Garrett, A.J., 1978. Numerical Simulations of Atmospheric Convection over the Southeaster U.S. in Undisturbed Conditions. *Atmospheric Sciences Group Report No. 7*. University of Texas, Austin, TX.
- Garrett, A.J., 1980. Orographic Cloud over the Eastern Slopes of Mauna Loa Volcano, Hawaii, Related to Insolation and Wind. *Monthly Weather Rev.* 108(7):931-941.
- Garrett, A.J., 1982. A Parameter Study of Interactions between Convective Clouds, the Convective Boundary Layer, and a Forecasted Surface. *Monthly Weather Rev.* 110(8):1041-1059.

Garrett, A. J., and D. W. Hayes, 1997: Cooling Lake Simulations Compared to High Resolution Thermal Imagery and Dye Tracer Data. *J. Hydraulic Engineering*.123: 885-894.

Garrett, A. J., J. M. Irvine, T. K. Evers, J. Smyre, A. D. King, C. Ford, D. Levine, 1999. Application of Multi-spectral Imagery to Assessment of a Hydrodynamic Simulation of An Effluent Stream Entering the Clinch River. *Photogrammetric Engineering and Remote Sensing*. 66(3):329-335.

Garrett, A. J., 2001: Analyses of MTI Imagery of Power Plant Thermal Discharge. *International Symposium on Optical Science and Technology, SPIE 46th Annual Meeting*, San Diego, July 29 – August 3, 2001.

Hamby, D. M. et al., 1993. Environmental Monitoring and Dose Assessment Following the December 1991 K-Reactor Aqueous Tritium Release, *Health Physics*, **65**: 25-32.

Jin, X. and Kranenburg, C., 1993. Quasi-3D Numerical Modeling of Shallow-Water Circulation. *J. Hydr. Engrg.*, 119(4):458-472.

Johnson, B.H., Kim, K.W., Heath, B.B, and Butler, H.L., 1993. Validation of Three-Dimensional Hydrodynamic Model of Chesapeake Bay. *J. Hydr. Engrg.*, 119(4):2-20.

Kondratyev, K.Y., 1969. *Radiation in the Atmosphere*. Academic Press, Inc. New York, NY.

Louis, J.F., 1979. A Parametric Model of Vertical Eddy fluxes in the Atmosphere. *Boundary-Layer Meteorology*. 17(2):187-202.

Oey, L.Y., Mellor, G.L. and Hires, R.I., 1985. A three-dimensional simulation of the Hudson-Raritan Estuary. Part I: Description of the Model and Model Simulations. *J. Phys. Oceanography*. 15(12):1676-1692.

Roache, P.J., 1972. *Computational Fluid Dynamics*. Hermosa Publishers. Albuquerque, NM.

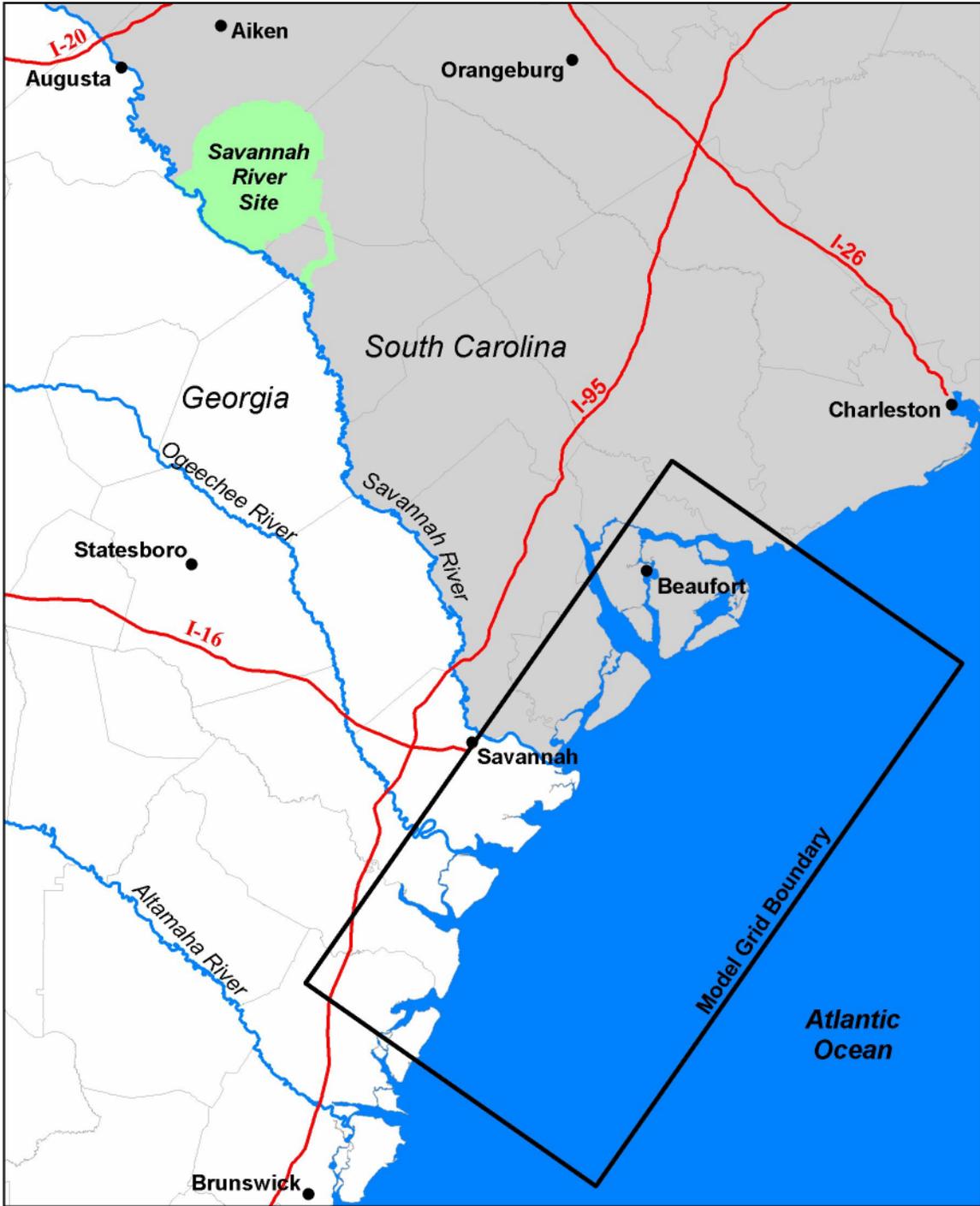


Figure 6: ALGE 1-km Resolution Model Domain along the Georgia-South Carolina Atlantic Coastline

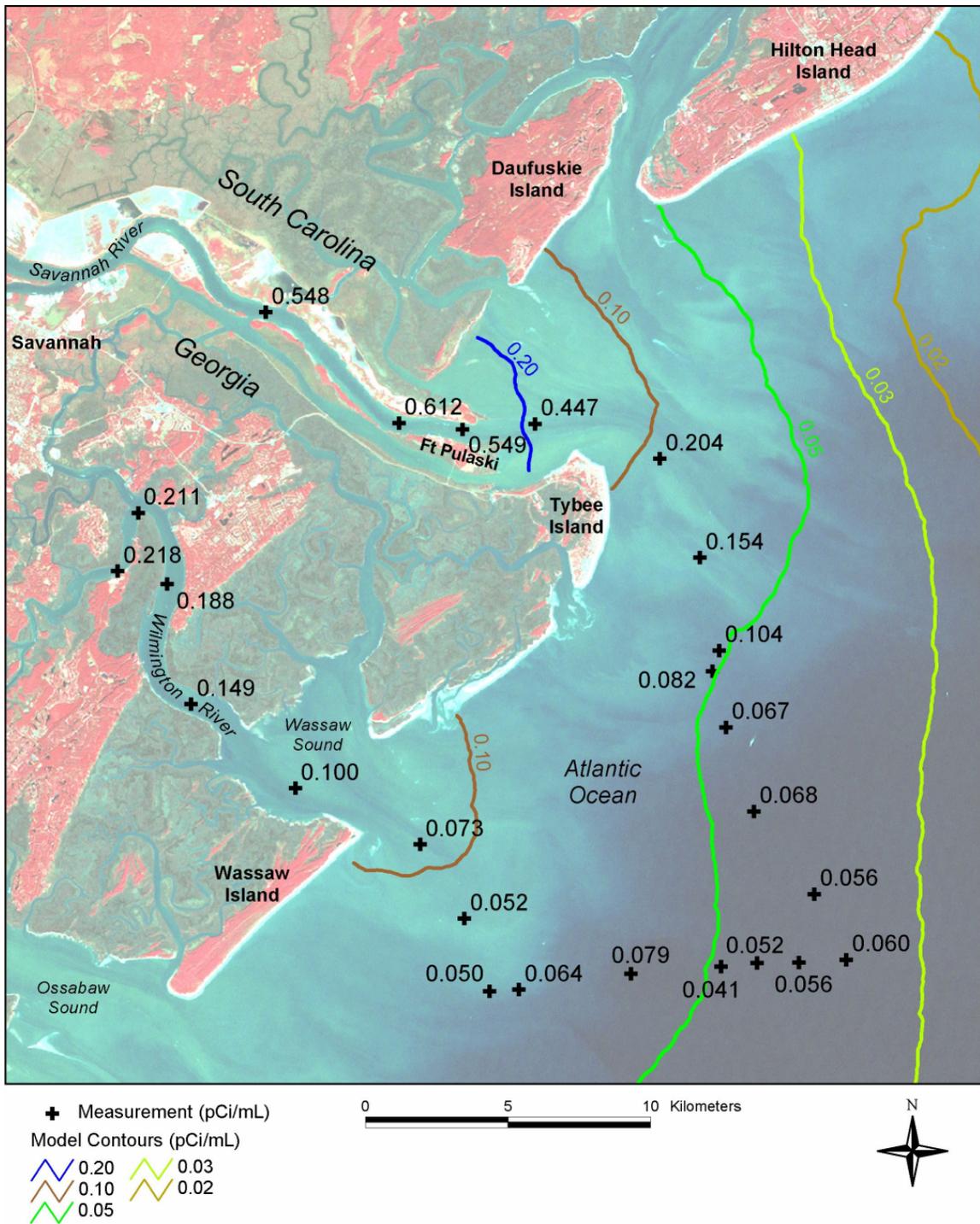


Figure 7: Landsat false-color image with superimposed tritium measurements (plotted) and simulations (contours) for March 5, 2005. Dry land is indicated by red, marshes are green and water is light to dark blue.

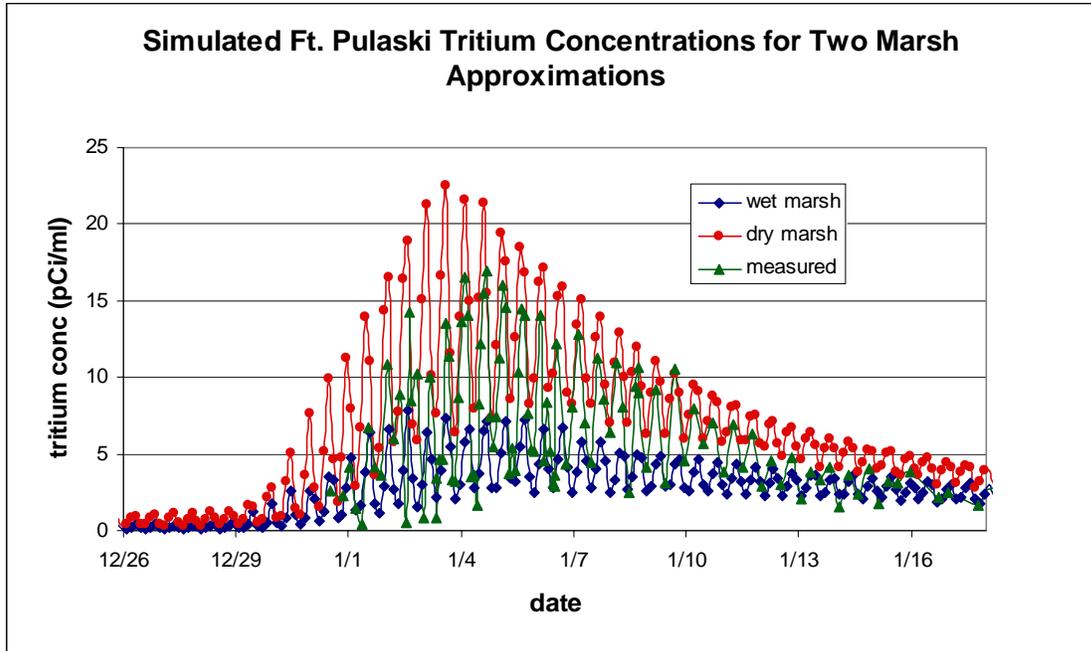


Figure 8: Time series of measured and simulated tritium concentrations at Ft. Pulaski (near mouth of Savannah River) in late December 1991 and January 1992.