Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

Develop SRNL's ALGE3D code for use as national response asset.

ALGE3D is a three-dimensional hydrodynamic code which solves the momentum, mass and energy conservation equations. Its original purpose was to predict movement and dissipation of thermal plumes. To fill a gap in existing emergency response technology this code is being modified to predict the movement and dissipation of tracers as they interact with sediments and move between the dissolved and particulate phase. To increase the usability of the code a pre- and post- processing GUI have been developed to aid the user in developing the inputs for the code and processing the code output into understandable figures for decision makers.

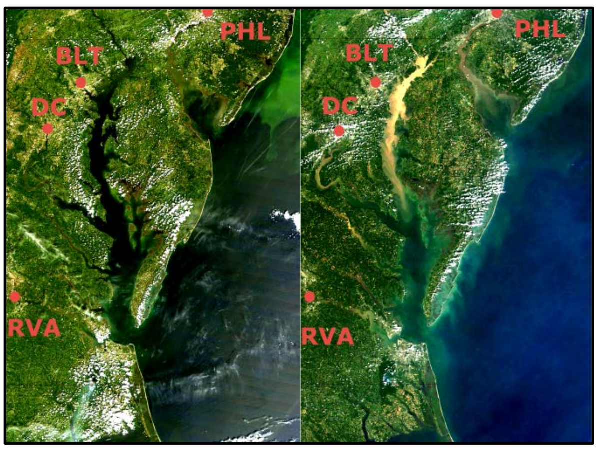

Figure 1. MODIS images of Chesapeake Bay August 23, 2011 and September 12, 2011. Major population centers are labeled.

Awards and Recognition

None.

Intellectual Property Review

This report has been reviewed by SRNL Legal Counsel for intellectual property considerations and is approved to be publically published in its current form.

SRNL Legal Signature

Signature **Date**

Title

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Subcontractor: University of South Carolina

Thrust Area: NS

Project Start Date: October 1, 2017
Project End Date: September 30, 2018

Current national models employed by emergency response agencies have well developed models to simulate the effects of hazardous contaminants in riverine systems primarily driven by one-dimensional flows; however, there is a gap in the support for more complex systems. While many models exist, none are capable of quick deployment in emergency situations that could contain a variety of release situations including mixtures of both particulate and dissolved chemicals in a complex flow area. Adaptations of ALGE3D are planned to update and expand particulate tracer and sedimentation capabilities to allow for a more comprehensive model. Quick-deployment model inputs will also be developed for a few high impact areas to aide in the timeliness of emergency response in key locations. The final product of ALGE3D will allow for coupling of dissolved tracer concentrations, particulate tracer concentrations, and their associated sedimentation effects.

FY2018 Objectives

- Define key locations
- Develop particulate tracer module for ALGE3D
- Develop sedimentation module for ALGE3D
- Verification, testing and publication

Introduction

On average North Americans live within ~3 km of a water body [1]. Of the top 10 most populated US cities from a 2015 US Census Bureau estimate, 7 of the cities are situated near the ocean, a bay, or on one of the Great Lakes [2]. A contamination of the water ways in the United States could be devastating to the economy (through tourism and industries such as fishing), public health (from direct contact, or contaminated drinking water), and in some cases even infrastructure (water treatment plants). For example, Figure 1 shows two visible satellite images for Chesapeake Bay, the first on August 23, 2011 and the second on September 13, 2011. In the second image a large plume of suspended particles in the Bay can clearly be seen. In this case it was a sediment plume caused by a large storm system moving through, and the major impacts included mainly damage to the fishing and oyster industries that year along with beach and recreation area closures [3, 4]. However, a similar plume containing radioactive or chemical material would have resulted in much costlier and wide spread consequences due to the associated human health impacts.

Current US emergency response capabilities for contamination to waterways, either from an accidental release or a planned attack, include the use of a one-dimensional transport model [5, 6]. This works well for most riverine systems which have flow in primarily one (downstream) direction. However, in more complex systems, such as tidal estuaries, bays, or lakes, a more complex model is needed. SRNL will develop ALGE3D to fill this gap in technology for emergency response of multi-dimensional aqueous modeling of scales below the Rossby radius of deformation, where the forces associated with the rotation of the earth are negligible. A three-dimensional model with the capability to handle dissolved and particulate contaminants, model the associated sedimentation effects, and support quick-deployment will provide a unique capability that could support the US emergency response enterprise.

Approach

ALGE3D is a 3-D hydrodynamic code developed by SRNL which solves the momentum, mass, and energy conservation equations to predict the movement and dissipation of thermal or dissolved chemical plumes discharged into cooling lakes, rivers, and estuaries [7]. The first portion of this project included data gathering for Chesapeake Bay and Lake Michigan, two high populated bodies of water with multiple potential sources of accidental release. Data was gathered for each location to provide input files for the model. While data gathering was being accomplished a pre-processor GUI was developed. The highly structured format of the required input files can be limiting and provide an endless source of frustration for users, so to facilitate use in an emergency response situation a program was developed. This program guides the user through the selection of necessary data and generates the necessary input files in the proper format and verifies all required files are present based on the user's selections.

Code modifications were made to include suspended sediment, particulate species, and dissolved species transport. The dissolved species can be adsorbed onto or desorbed off of suspended sediment particles based on the chemical properties specified of the released material. Sedimentation effects, including erosion and deposition were also added into the code and will be verified in the second year of the project. In addition to the transport modules added, modifications were made to the code to reduce the amount of spin up time needed to obtain the physical properties (salinity and temperature) by adding an option to include an initial spatially varying field rather than one set initial value. This modification allows the code to be run in a more operational time frame.

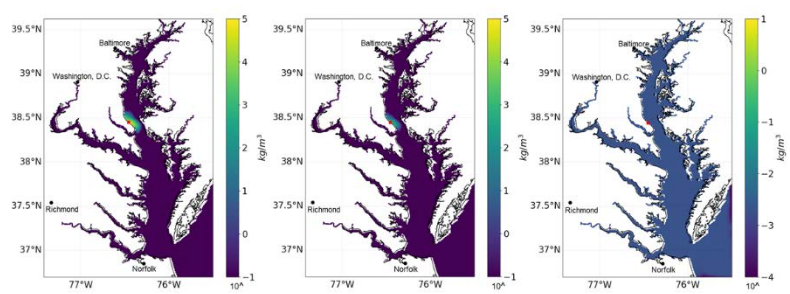

Figure 1. Dissolved species (left), particulate species (middle), and suspended sediment concentrations 24 hours after a theoretical release from Calvert Cliffs Nuclear Power

Results/Discussion

Chesapeake Bay and Lake Michigan bathymetry data was gathered from 30 arcsecond topography horizontal topography with 1 m vertical resolution [8] and interpolated to 500 m and 1 km horizontal resolutions. River coordinates and stream flow data for each domain were gathered from USGS water data [9]. Input files were developed to include bathymetry and grid identifications for each domain and at each scale. The pre-processing GUI allows for user selection of a release location from several different pre-set locations on each main domain, including nearby nuclear power plants. Tidal harmonics were gathered for Chesapeake Bay [10] (Lake Michigan is not tidally forced) and coded into the pre-processor allowing tidal forcing to be calculated based on the user's selection of date. Testing of the predicted tidal forcing was matched against the NOAA tidal forecast.

Code modifications to include suspended sediment, particulate species and dissolved species transport were tested using a stagnant column of water with suspended sediments introduced at the surface and settling through a layer of constantly discharged dissolved species, before settling into a layer with no dissolved or particulate concentration. Scenarios were run with three different classes of sediments with varying diameters, densities, and adsorption/desorption rates (Figure 2). As expected as the suspended sediment settles from the surface layer into the layer with dissolved concentration some of the material adsorbs onto the suspended sediments, moving onto the particulate species form. As the suspended sediments and particulate species settle further into the water column in the area with no concentration some of the material desorbs from the particulate species back into the dissolved species. The suspended sediment material and the particulate species settle into the bottom of the water column and accumulate into the bed, where some adsorption/desorption continues until an equilibrium is reached. This equilibrium is based on the user specific constants provided and are material dependent. Total mass balance was conserved showing there was no mass loss/gain in movement between species.

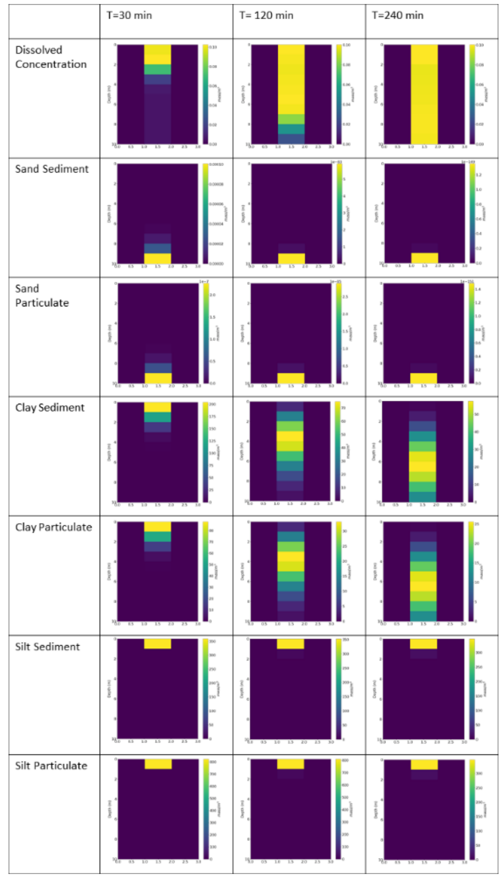

Figure 2. Concentration of dissolved species, suspended sediments, and particulate sediments 30 minutes, 120 minutes and 240 minutes after release.

FY2018 Accomplishments

- Developed bathymetric and identification grid for 2 locations and began development for 3 additional locations.
- Gathered oceanographic and meteorological verification data for 2 developed locations for 1 full year each.
- Identified 1-2 events for validation at each developed location and gathered oceanographic and meteorological data for each event.

- Modified code to include an unlimited number of sediment classes and particulate speciation. This includes sediment bed loading, deposition and resuspension, and adsorption/desorption of dissolved species.
- Verification of particulate and sediment modules was performed using a stagnant water column simulation

Future Directions

- Refine pre- and post- processing GUI
- Configure code to allow GPU processing to significantly reduce model run time
- Validation and verification of simulations.
- Expand library of release locations
- Add library of potential release materials with the appropriate model inputs and critical values for analysis
- Inverse modeling
- Couple with atmospheric dispersion model for inputs of deposition over waterways.

FY 2018 Publications/Presentations

1. Maze, Grace. (2017, December) *ALGE3D: A Three-Dimensional Transport Model*, Presented at the American Geophysical Union Fall Meeting, New Orleans, Louisiana.
2. Maze, Grace. (2018, February) *ALGE3D: A Three-Dimensional Transport Model*, Presented at Ocean Sciences Meeting, Portland, Oregon.
3. Maze, Grace. (2018, March) *ALGE3D: Development as an Aqueous Emergency Response Model*, Presented at the Palmetto Chapter of the American Meteorological Society Mini-Technical Conference, Columbia, South Carolina.
4. Submitted: Maze, Grace (2018, December) *Expanding ALGE3D as an aqueous emergency response model*, Submitted for Presentation at the American Geophysical Union Fall Meeting, Washington, D.C.
5. Submitted: Maze, Grace. (2019, January) *ALGE3D development as an aqueous emergency response model*, Submitted for Presentation at the 99th American Meteorological Society Annual Meeting, Phoenix, Arizona.

References

[1] M. Kummu, H. de Moel, P. J. Ward and O. Varis, "How close do we live to water? A global analysis of population distance to freshwater bodies," *PloS ONE,* vol. 6, no. 6, June 2011.

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[5] R. Bahadur and W. B. Samuels, "Modeling the fate and tansport of a chemical spill in the Elk River, West Virigina," *J. Environ. Eng.,* vol. 141, no. 7, 2005.

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[9] USGS, "Current Water Data for the Nation," [Online]. Available: https://waterdata.usgs.gov/nwis/rt.

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Acronyms

US – United States
USGS- United States Geological Survey
NOAA- National Oceanographic and Atmospheric Administration

Intellectual Property

None to date.

Total Number of Post-Doctoral Researchers

None to date.