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Sensitivity Analysis of Sediment Coagulations in The Chesapeake Bay

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Abstract

Hydrodynamic models are utilized for fast response to environmental hazards. However, limitations within the models may inhibit their accuracy. A three-dimensional aqueous transport model, ALGE, was developed at the Savannah River National Laboratory (SRNL) as a tool for pollutant dispersion. Recently at SRNL, the capability to account for coagulation and break-up of particles to better account for the fate and transport of materials. A sensitivity analysis was performed to determine a threshold for specified particle parameters that still yield accurate results. Dictating these thresholds advances the development of ALGE to become a product for efficient emergency response.

I. INTRODUCTION

Hydrological models are essential for responding to emergency events and evaluate environmental risks. However, limitations, such as simulation time and computational sources within the models may inhibit their complexity. ALGE is a three-dimensional aqueous transport model developed at SRNL in the 1980s originally to observe thermal plumes in cooling ponds near nuclear reactors on site. ALGE was further developed to be utilized for emergency response to situations with respect to aqueous environments. In past years, ALGE was used for an accidental release of tritium at SRNL and a train derailment in Graniteville. ALGE computes the conservation equations for mass, momentum, thermal energy, turbulent kinetic energy, particle mass, sediment mass, and dissolved and absorbed tracer mass. The model is comprised of a GUI, an executable, and a post-processer. The GUI reads in all the input values for specified parameters defined by the user. The executable is responsible for computing the conservational equations and the post-processer plots the results from the executable. ALGE can simulate releases at a series of predefined locations across the continental United States. The predefined locations consist of coastal bays and estuaries, rivers, and lakes. The focal area for this project is the Chesapeake Bay as it is the largest estuary in the United States, holding fresh and salt water with influence of tides .

II. BACKGROUND

The Chesapeake Bay is a coastal plain estuary located in Maryland and Virginia. The Chesapeake Bay is 200 mi (300km) long having widths ranging between 2.8 mi (4.5 km) to 30 mi (50 km) wide. The average depth is 21 ft (7 m) with the greatest depth reaching 175 ft (53 m). The Chesapeake Bay is the largest estuary in North America while also holding the largest watershed in the United States at 64,000 mi^2 (166,000 km^2) [2]. With an intense amount of riverine and oceanic inputs, nearly 5.2 million tons of sediment enter the Chesapeake Bay on average in a year [1].The sources of these sediments come from both watershed sources (eroding land and stream banks) and tidal sources (eroding shorelines and coasts). The Sediment in the Chesapeake Bay is made up of sand, silt, and clay; with clay covering the largest area of 75 km^2 on the bay floor [5]. Clay is the smallest particle with respect to sediment grain size, typically having a diameter of <1/256 mm [4].

Suspended clay particles can greatly affect the water quality of aqueous environments, especially when contaminants are introduced [1]. Due to particle size and density, clay can stay suspended within the water column rather than sink to the bottom. These non-settling particles are able to stick together via coagulation, and form larger and heavier masses of clay called flocs. These flocs can then fall out of the water column onto the bed. Recent modification of code has incorporated the capability to account for coagulation and break-up of clay within ALGE. This improves the accuracy of fate and transport of materials. In this work, various clay parameters are evaluated to determine a threshold to see how far off a user of ALGE can be from an actual measurement and still get accurate modeling of the contaminant leakage/where the contaminant will travel.

III. METHODS

For this study we used ALGE to simulate a contaminant spill within the Chesapeake Bay from a nuclear power plant in Calvert Cliffs, MD. Inputs used for simulation were based on pervious experimental studies and existing weather and buoy data. A time series was produced to compare the concentrations of sediment and particulate materials at 11 locations within the bay, as they travel from the source of release (power plant) to the mouth (Figure 1).

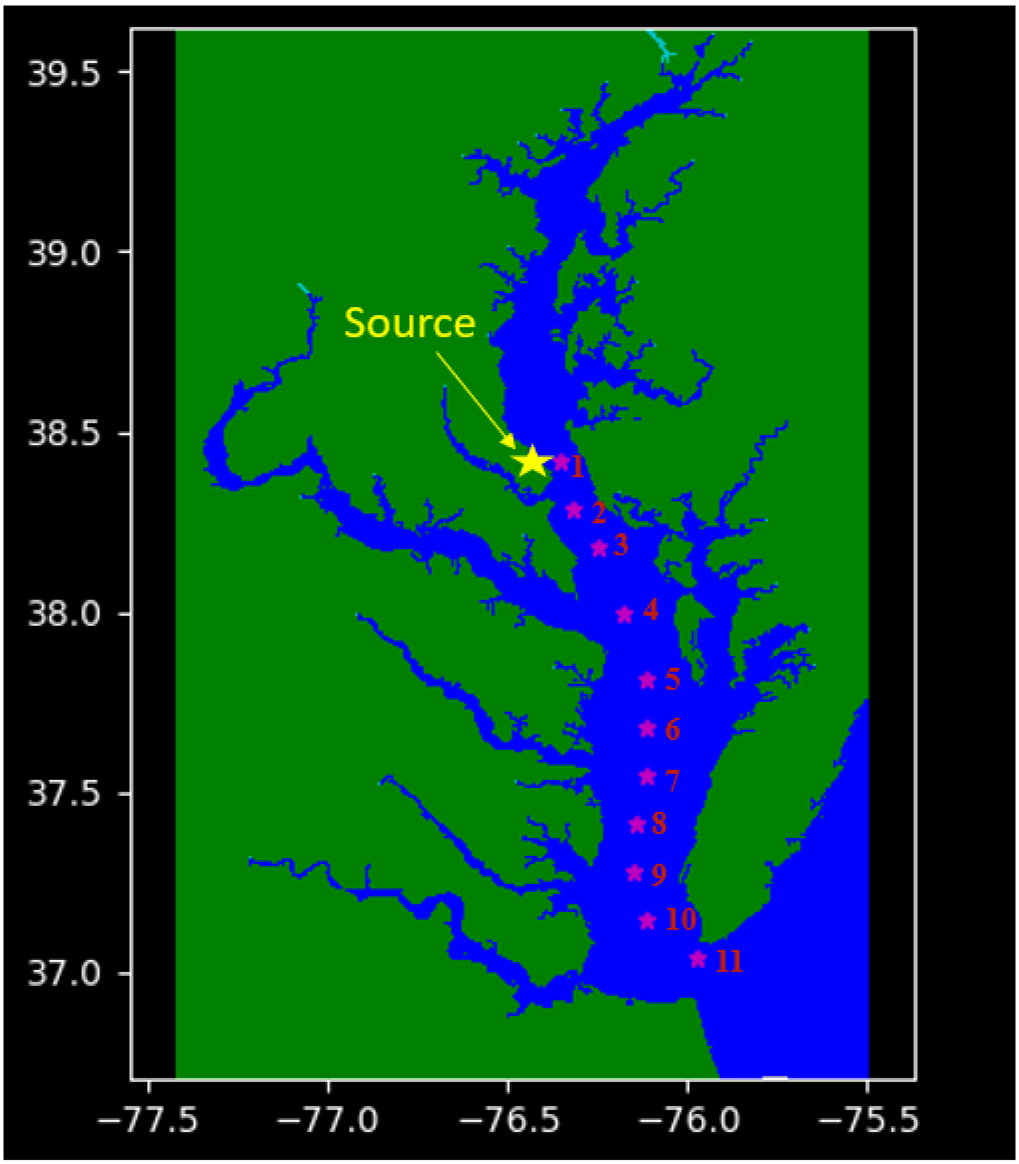

Figure 1. Map of the 11 tested locations and source within the Chesapeake Bay.

Nine simulations were computed to compare various parameter settings related to sediment and particulates. For each experiment, sediment and particulate concentrations are broken up into three size ranges, or bins and the following parameters were examined: diameter, density, F1eq0, F2eq0, and F1 and F2 slopes (Table 1). Where F1eq0 and F2eq0 are the percent of the total sediment concentration for bins 1 and 2, respectively. F1 slope and F2 slope denote the relation between coagulation and break up of sediment, in the presence of salt, over time. The salinity of this environment was set to 35 ppt.

An independent t-test was conducted between each experiment at every location along the Chesapeake Bay to determine significant or insignificant differences between the parameter settings .A t-test is a statistical test used to compare two sample means. An Independent t-test compares two sample means from two unrelated groups and outputs a p-value. A p-value ≤ 0.05 denotes there is significance between the values being compared. The independent t-test can be computed as:

$$t = \frac{\overline{x_1} - \overline{x_2}}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}} \quad (1)$$

Where $\overline{x_1}$ is the mean value of the first sample, $\overline{x_2}$ is the mean value of the second sample, n_1 is the total number of points in the first sample, n_2 is the total number of points in the second sample, s_1 is standard error of the first sample, and s_2 is the standard error of the second sample.

Table 1. Parameter values for each bin in the 9 experiments.

Experiment	Diameter (μm)			Density (kg/m^3)			F1eq0 (%)	F2eq0 (%)	F1 slope	F2 slope
	Bin1	Bin2	Bin3	Bin1	Bin2	Bin3	Bin 1	Bin 2		
1	60	185	325	1.46	1.12	1.07	0.3	0.17	0.004	0.009
2	60	185	325	1.14	1.04	1.02	0.28	0.18	0.004	0.009
3	60	185	325	1.71	1.20	1.11	0.31	0.17	0.004	0.009
4	70	240	400	1.39	1.10	1.05	0.41	0.44	0.011	-0.007
5	70	240	400	1.12	1.03	1.02	0.38	0.46	0.011	-0.007
6	70	240	400	1.6	1.15	1.08	0.42	0.43	0.011	-0.007
7	50	140	270	1.57	1.18	1.08	0.13	0.28	0.0001	0.011
8	50	140	270	1.17	1.05	1.03	0.11	0.27	0.0001	0.011
9	50	140	270	1.87	1.27	1.13	0.14	0.28	6.73E-05	0.011

IV. RESULTS

Time series plots for experiments 1 and 9 of sediment and particulate concentrations are shown in figures 2 and 3. Two of the nine experiments are shown to portray a comparison between the extremes of the parameter values (greatest and smallest values). Three locations in the Chesapeake Bay were chosen for comparison purposes between experiments. The source, location 3, and location 11 were chosen to show how the particle concentrations change over time as they travel across the bay. Each time series plots bins 1, 2, and 3 over a 24-hour period to visualize changes based on parameters set for each experiment (Table 1). T-test results are shown in table 2 to determine significant differences between experimental runs.

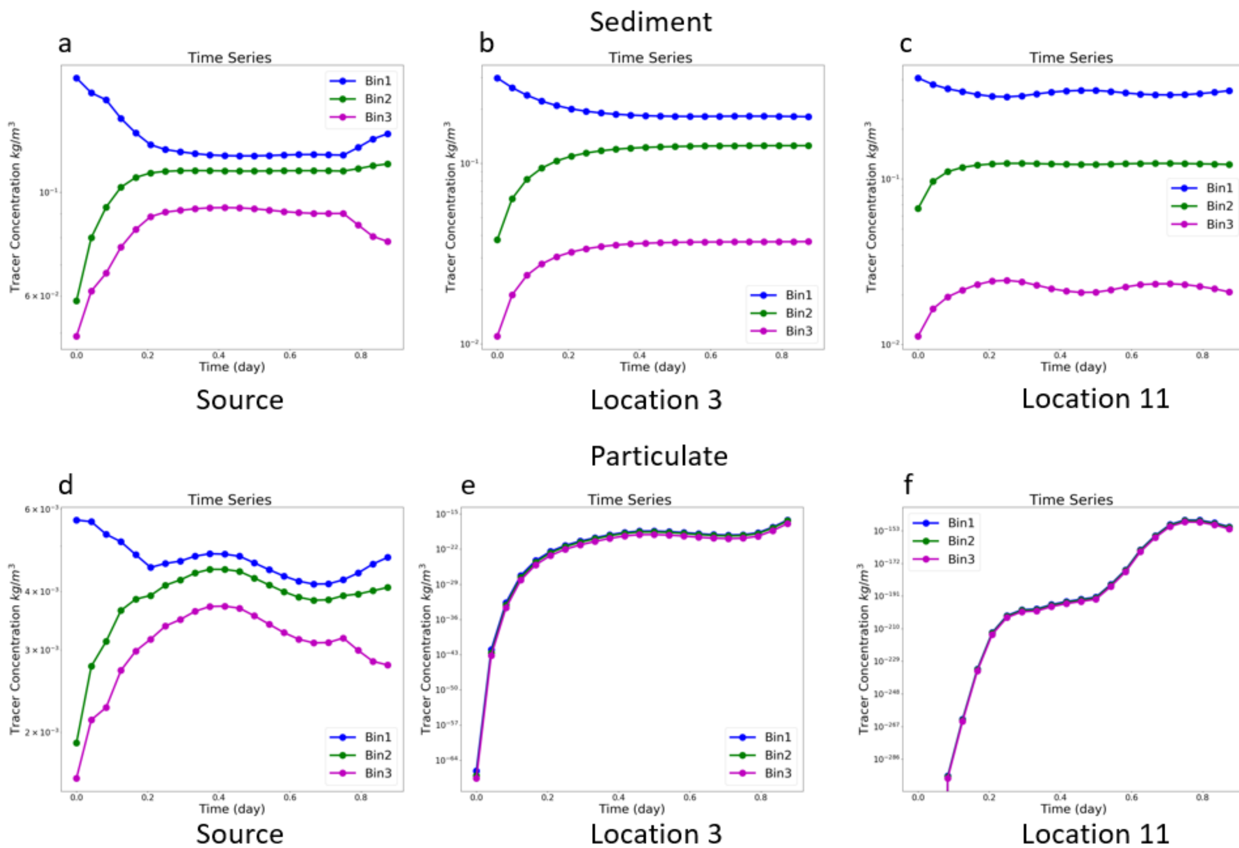

Figure 2. Sediment and particulate concentration time series for experiment 1.

Figure 2 shows the time series results from experiment 1. The sediment concentrations consistently show the same trend, where bins 2 and 3 increase in concentration until insignificant change, at 0.2 days (or around 5 hours). Whereas bin 1 decreases in concentration until insignificant change, at 0.2 days. When observing particulate concentration trends, the source compared to locations 3 and 11 differ. At the source, the particulate concentrations for bins 2 and 3increase , whereas bin 1 decreases in concentration. However, locations 3 and 11 show all three bins increase in concentration throughout the time series. It is important to note that particulate concentrations from location 3 to 11 are negligible, as values become greater than 10^{-40} (Figure 2e & 2f). Similar trends for all three bins in the time series can be seen in figure 3 for experiment 9 for both the sediment and particulate concentrations at all locations.

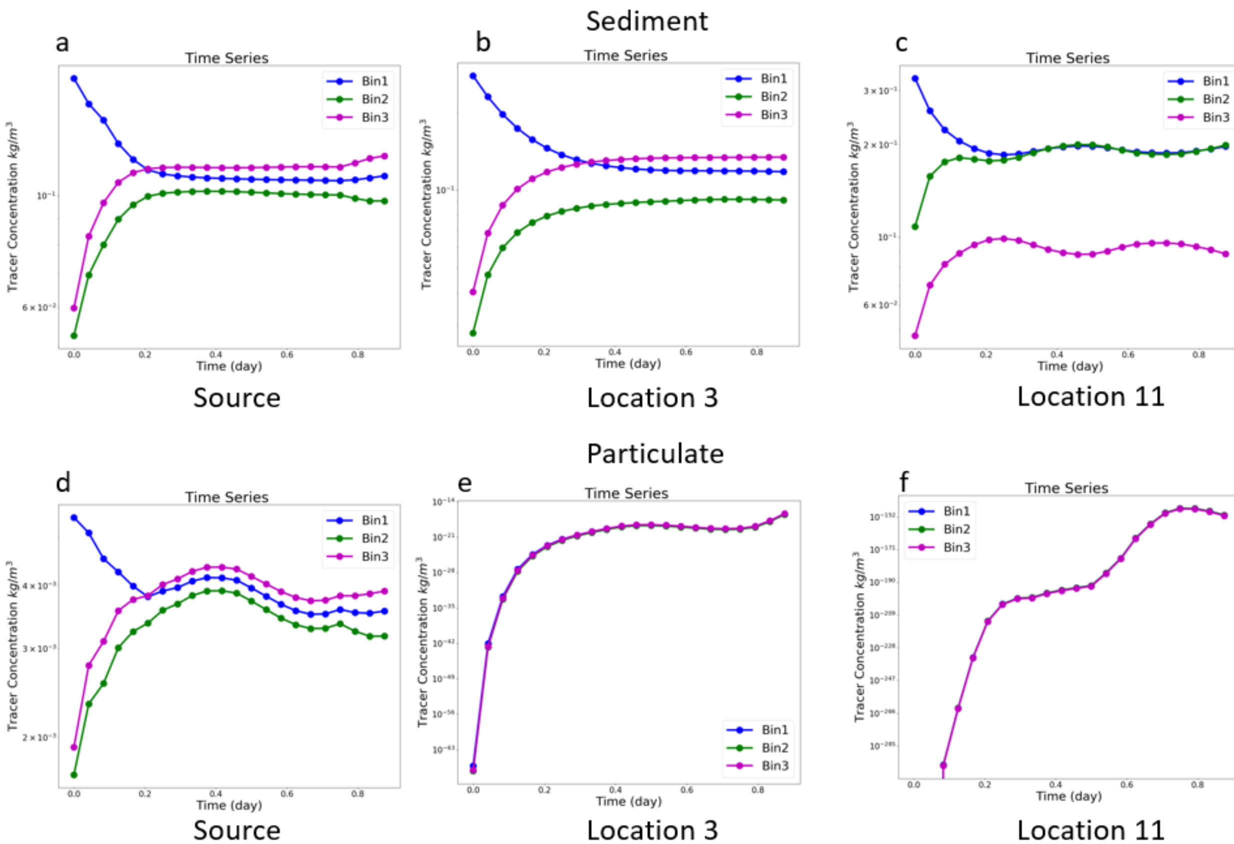

Figure 3. Sediment and particulate concentration time series for experiment 9.

P-values from the independent t-test are shown in Table 2. Sediment concentrations at each location show significant difference when comparing experiments 1 and 9, having values below 0.05. Whereas p-values from the particulate concentrations show insignificance between experiments 1 and 9 at the source and the 11 locations, having each value greater than 0.05. Based on these p-values, this means that the particles differ in sensitivity between sediment and particulate concentrations. Sediment concentrations are more sensitive to changes in parameters values from table 1 than the particulate concentrations.

Table 2. P-values from t-test conducted between experiments 1 and 9 at the source and each location. Highlighted cells denote the p-value shows significance.

Exp 1v9	Particulate	Sediment
Location	P-value	P-value
Source	0.1758454	0.009112
1	0.6835295	1.02E-06
2	0.9937939	2.19E-07
3	0.8450324	1.81E-07
4	0.5623051	2.20E-08
5	0.2960641	2.09E-09
6	0.3030144	1.12E-10
7	0.2045789	1.49E-09
8	0.1493675	3.56E-10
9	0.2051633	8.66E-11
10	0.1299985	8.66E-13
11	0.1509582	5.72E-13

V. CONCLUSIONS

After testing different values for the density, diameter, fractions and slopes of sediments and particulates (Table 1), there were noticeable changes in the concentration trends as the particles travel through the bay. The t-tests determined if significant differences exists between experiments , this provides insight to how sensitive the addition of coagulation and breakup of particles is in ALGE.

Results suggest that ALGE is more sensitive to changing the parameters for sediment concentrations compared to particulate concentrations. This could be because once the chemical adheres to the sediment and becomes the particulate, the different values chosen for particulates in the range between all nine experiments is negligible when using ALGE. The particulates are also confined within the bay as it is only simulated as part of the release. Whereas the sediment concentration has an input across the bay. It is important to note that chemical break-down processes are not taken into consideration (e.g., half-life or chemical stability of a contaminant), therefore radioactive releases or specific chemical reactions may adhere differently to sediment and should be considered for future work. Coagulation occurs faster when salt is present in water, therefore only coastal environments are accounted for in this study. Future work will recreate all nine experiments without salinity present to determine significant difference between parameters to account for freshwater systems. Time series analysis with depth could also be done to investigate if the particulates are settling out, leading to the negligible concentrations.

VI. ACKNOWLEDGMENTS

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VII. REFERENCES

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