**Inverse Aqueous Transport Modeling for Emergency Response**

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Key Points:

* Aqueous Transport Model developed at the Savannah River National Laboratory has a new capability to back-track a pollutant to its source.
* A three step process is used to inverse model and results are compared to the 2021 Piney Point spill in Tampa Bay, Florida.
* Bayes Theorem was used to narrow down a source location based on overlap of multiple inversion runs.

Abstract

ALGE3D is a three-dimensional, finite-differenced aqueous transport model that simulates pollutant fate and transport in lakes, rivers, bays, and estuaries by solving the mass, momentum, and energy equations. Current modeling capabilities include sediment, dissolved, and particulate tracer transport for a series of predefined locations across the continental United States. Recently, an inversion method (also known as backtracking) has been added to ALGE3D, to provide a possible source of a pollutant, should one be detected by a sensor in a body of water and a source cannot be found. This inversion method is a 3 step process that uses an algorithm to inverse the time step and flow. An example of the model’s recent developments is described herein through simulating the 2021 Piney Point Spill in Tampa Bay, Florida (USA), where Bayes Theorem was computed on the inverse runs to reduce the area at which the true source could be located.

**Plain Language Summary**

The Savannah River National Labratory developed a model that tracks pollutant transport for multiple bodies of water across the United States. This model is capable of tracking various forms of pollutant transport three-dimensionally, providing a more accurate result of pollutant transport for emergency response capabilities. Recently, we have developed the capability to model pollutant transoprt backwards in time and space, which could provide the ability for emergency responders to find the source of a pollutant, should one not be found immediately. This new capability is a three step process, and we compare the model’s results to data collected from the 2021 Piney Point Spill in Tampa Bay, Florida (USA). A statistical method, Bayes Theorem, was used to narrow down the area which the source could be located.

1 Introduction

Hydrological models are important for environmental risk and emergency response, however the complexity of these models are limited by simulation time and computational resources (Herrera et al, 2021; Atkinson et al, 2002; Freeze & Harlan, 1969; Beven, 2002; Kuffour et al, 2020). ALGE3D, or ALGE, is a 3D aqueous transport model capable for emergency response that solves the conservation equations for mass, momentum, thermal energy and turbulent kinetic energy, particle mass, sediment mass, and dissolved and adsorbed tracer mass (Garrett & Hayes, 1997). An assessment of aqueous contaminant fate and transport models for emergency response was performed by Savannah River National Laboratory (SRNL) in 2018 (Maze, 2018) at the request of the National Nuclear Security Administration’s Office of Nuclear Incident Response, which revealed that ALGE was the only model in the Department of Energy or commercial nuclear complex capable of supporting fully 3-D assessments of radionuclide fate and transport in dynamically driven water systems such as lakes, bays, harbors, and coastal estuaries. Previous validation studies of ALGE include fate and transport of tritated water from an accidental release at the Savannah River Site in 1991 (Blanton et al, 2009), Chlorine gas deposition into nearby bodies of water after a train collision in Graniteville, SC (Buckley et al, 2007), and simulating flow rate of a creek as it enters Clinch River in Tennessee (Garrett et al, 2000). An inital description of ALGE’s modeling capabilities can be found in Garrett & Hayes (1997).

Inversion modeling has been commonly used atmospherically for pollution detection and emergency response (Zhang et al, 2021; Uliasz, 1993; Uliasz and Pielke, 1992). For hydrological purposes it has been used for a variety of research such as characterization of aquifers and ocean floor geological processes (Ghorbanidehno et al, 2020). Recently, SRNL has developed an inversion process for ALGE, which can be used for both research and emergency response. This paper will discuss ALGE’s inversion capabilities for emergency response by recreating the Piney Point wastewater spill that occurred in Tampa Bay, Floridia in 2021.

2 Data

In late March of 2021, a leak was discovered from a wastewater pond at an abandond Piney Point phosphate fertilizer plant. A total of ~237 million gallons of wastewater discharged into Tampa Bay via Port Manatee. An initial study by Beck et al. (2022) of the spill’s aftermath resulted in a series of blooms, ending with a bloom of red tide (*Karenia brevis*). This red tide led to a large fish kill where over 1600 metric tons of dead fish was extracted from the bay (Beck et al., 2022). Water quality data was collected by the Florida Department of Environmental Protection shortly after the detection of the leak. 27 water quality monitoring stations were place along the bay, with 4 placed at ports near the phosphate plant. This water quality data was collected from March 30th 2021 through October 14th 2021. Nutrients measured include Ammonia, Orthophosphate, Nitrate/Nitrite, Chlorophyll, total Nitrogen and total Phosphorus for all stations. These samples were not collected continuously and are considered one-time grab samples, therefore reports note that collection of these nutrients for some days were either not detected or, between the laboratory method detection limit and the laboratory practical quantitation limit. To ensure an accurate comparison between ALGE and the sampled data, results produced by ALGE are compared to total phosphorus measurements collected at stations 7,8,9,18,19, and 20. We also look to the recent publication by Beck et al. (2022) for comparison of total nitrogen and total phosphorus values to ensure the flow field produced by ALGE is valid prior to inversing the flow.

To simulate the Piney Point spill in ALGE, 270m resolution bathymetric data was used to accurately recreate the bay’s geometry. The model computed the mass, momentum, and energy equations for two forward runs: one starting from March 29th 2021 for 360 hours, and another beginning at April 1st 2021 for 3650 hours (~5 months) with a release concentration of 0.16 kg/m³ based on reported concentrations of total phosphorus. The flow rate was set to 1.39 m³/s, based on the volume of Tampa Bay and the total release of wastewater from the pond. Tidal forcing is considered with these calculations. Atmospheric, temperature, and salinity inputs were based on buoy data at the time of the spill.

3 Methods

Inverse modeling for an aqueous release is accomplished in ALGE by creating the flow field, inversing the flow field, and using the inversed flow field as an input to run backwards in time from a detection point. The flow field reversal is accomplished by using a simple algorithm that reverses the advective terms:

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in which u(x,t) is the velocity and c(x,t) is the concentration. We establish a 1-dimensional ‘grid’ with a spacing of 10m and a total length of 16km, along with a prescribed flow. We then run a full 360 hour transport simulation (with a 1s time step) using that flow and a prescribed tracer release from the location closest to the wastewater pond that we can resolve for (the edge of Port Manatee), resulting in a ‘pulse’ of tracer that moves downstream to a hypothetical detection point, for this study we used the sampling stations. As the forward run progresses, the entire (one-dimensional) flow field is written to an external file at each time step. After the program is complete, a second program, similar to the one executed for ALGE, is then run to read in this data and create a new file that contains the inverse flow - reversed in both the direction and the order of the timesteps. Finally, a third program is run to read in the inversed flow and advect tracer released from the detection point, toward the source. The results yield an area of influence, or an area of potential sources. Running ALGE inversely multiple times from different detection points, or stations, provides a map of where these areas of influence overlap, thus narrowing down the location of the true source.

To reduce the area of influence in a quantifiable manner, we proposed using Bayes Theorem to determine where the source could be located geographically. The result of Bayes Theorem yields a conditional probability of event B based on the occurrence of event A (Herrera et al., 2021) or in this case what is the likelihood that one of the potential sources located in the bay is the true source based on where the inverse runs overlap:

Where is the posterior probability, is the prior probability, or the probability that the hypothetical source with the maximum concentration overlap is the true source, is the conditional likelihood, or the likelihood that the true source is located within the top 3 hypothetical sources with the highest tracer concentration, and is the total probability, or the probability that any of the hypothetical sources are the true source. The benefit of using Bayes versus a standard probability method is that we can use non-mutually exclusive events to determine where the source is located. This allows us to account for uncertainty in a complex hydrological system by using a probabilistic approach (Doherty, 2015; Fienen et al., 2013; White et al., 2020; Herrera et al., 2021). To use Bayes Theorem, a list of potential sources were selected randomly around the parameter of Tampa Bay. We computed the prior probability two ways to compare. The first method to compute the prior probability determines the overlap of inversion runs based on concentration values closest to the forward release concentration. From this overlap, the maximum is selected from the potential sources as the prior probability. The second method to compute the prior probability determines which potential source has the maximum overlap using the highest sum of concentration at each potential source. Both posterior probabilities were compared to determine which method is most viable for use.

4 Results

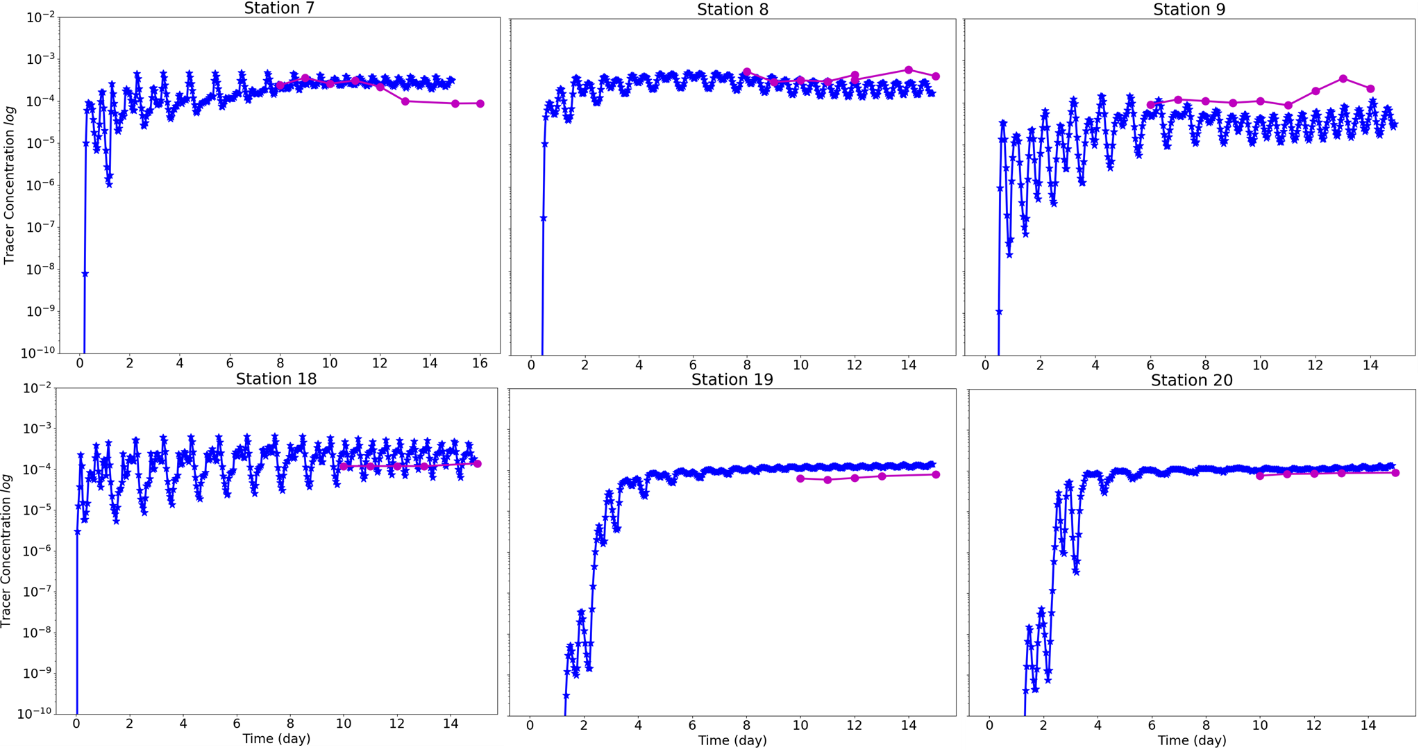
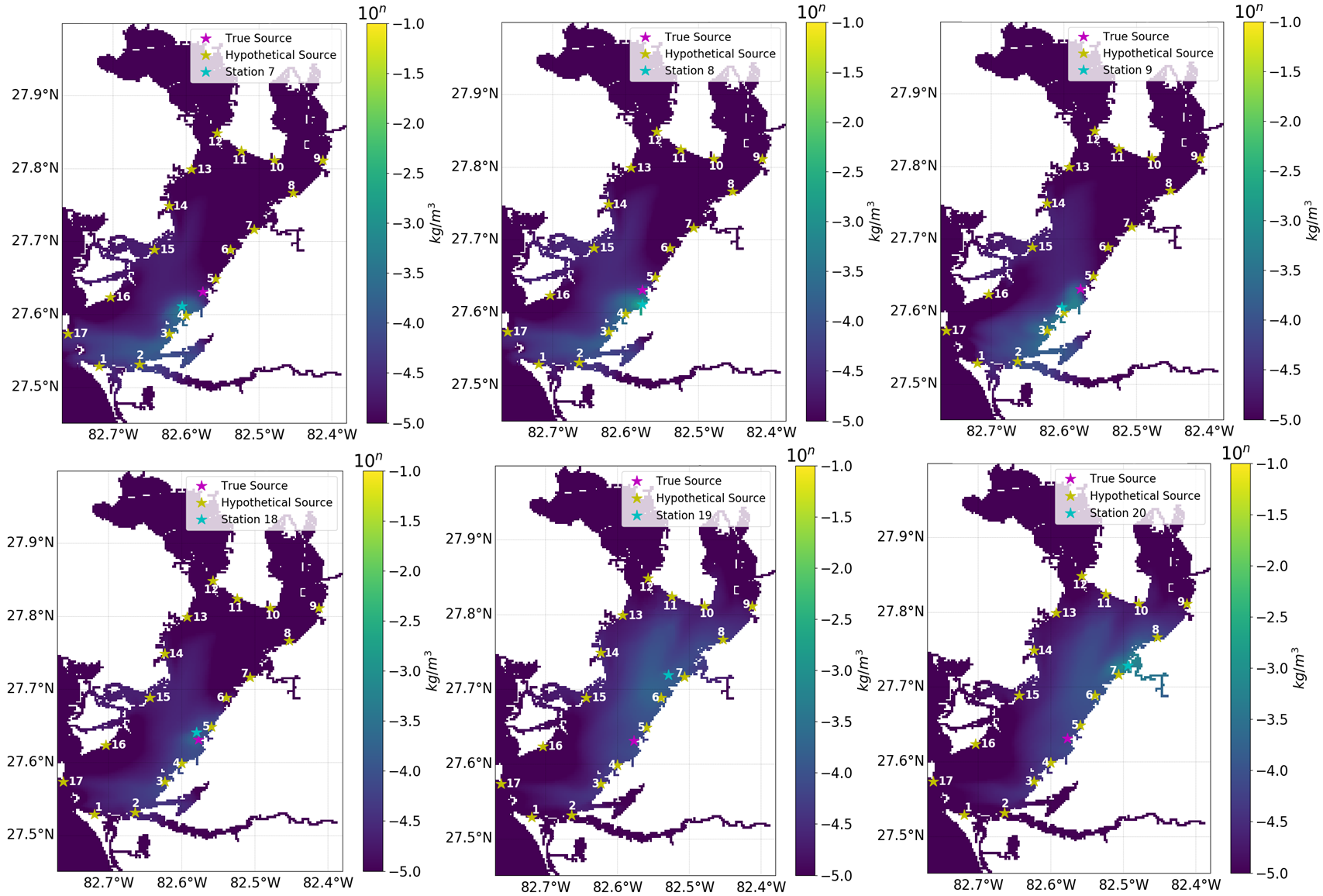
Total Phosphorus concentrations produced by the forward run in ALGE were compared to sampled data from the Piney Point spill. A time series from ALGE and the sampled data at each monitoring station (7,8,9,18,19,20) shown in Figure 1 overall show good agreement (within 1 order of magnitude). Fluctuation of Phosphorus concentrations in ALGE represents tidal changes, and the lack of tidal influence represented in the sampled data is a result of a one-time sampling technique that was used. An inversed run was performed with the detection point set to stations 7,8,9,18,19, and 20 respectively, and the corresponding area of influence can be seen as the corresponding map for each inversion run in Figure 2. Within each of these inversed runs the tracer concentration appears as a lighter blue color (roughly around an order of magnitude of 10¯³ kg/m³). From this visual it appears that much of the eastern part of the Bay could be considered the area of influence.

Figure1. Time series plots of tracer concentration (log) vs. time (days) at each sampling station for grab samples from Florida’s DEP and ALGE3D produced data. ALGE3D simulated data is represented in blue, while sampled data is represented in magenta.

However, it is important to note that the true source of the release can be found within the area of influence for all six inversion runs.

Figure 2. Dissolved tracer concentration maps for each inverse run. The yellow stars are numbered and represent the hypothetical sources randomly selected for comparison, the magenta star represents the true source, or the actual source of the release from the forward run, and the cyan star represents the detection point, or station, at which the inverse run source is selected to run backwards in time. After completetion, these maps show an area of influence represented by the area where concentrations is ~10¯³ kg/m³. This provides evidence that the true source can be found within the area of influence for each inversion run.

To narrow down the area of influence and quantify these results, we computed Baye’s theorem based on the area of overlap from the inversion results to reduce the area of influence. We are basing the likihood that a potential source is the true source based on the series of inversion runs that were completed. Therefore our series of inversion runs are considered event B which will influence the likihood of event A (likihood that a potential source is the true source). The posterior probability that hypothetical sources 3,4, and 5 are the true source were each computed to determine validity of inversion results. Potential sources 3,4,5 were selected based as they are the top three locations closest to the true source. Table1 lists the probibilites and conditional likelihood for potential sources 3,4, and 5 using both proposed methods to determine the prior probability. While either method to determine prior probability yields a reasonable degree of belief (>50%) using the number of times a tracer reaches a potential source as the prior probability does not narrow down the area of influence, as other potential sources yield the same degree of belief of 52.94%. Results show using the sum of maximum concentration at each potential source will narrow down the area of influence. In this instance, results show that potential source 5 has a degree of belief 70.59% whereas potential sources 3 and 4 have a degree of belief of 52.94%. These results are deemed reasonable as potential source 5 is closest to the true source and therefore expect this potential source to have the highest degree of belief.

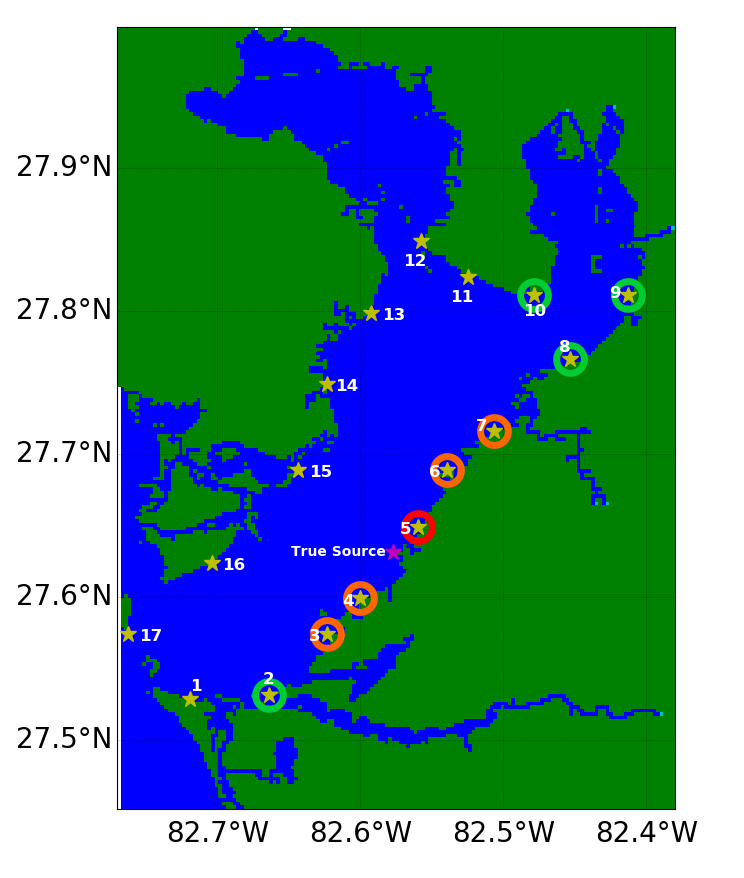


Figure 3. Map of results for Baye’s Theorem. The colored circles represent degree of belief that the numbered hypothetical source is the true source, with red as the highest degree of belief at >70%, orange at >50% and green at <20%. The yellow numbered stars are the hypothetical sources randomly selected, and the magenta star is the actual location of the release, or the true source.

5 Conclusions and Future Work

From the existing ALGE3D model we have developed a new capability to track pollutant transport inversely, should a pollutant be detetected in a body of water and a source cannot be determined. Using a three step process of running the model forward in time, inversing the flow field, and running the model again with the inversed flow field. Baye’s theorem has shown the capability of distinguinshing the true source from other potential sources. Therefore, the higher the degree of belief, the closer that location is to the true source. Streamlining the model by automating these new capabilities is needed prior to release for emergency response use. Once these developments are completed, this feature would take only a couple of hours to complete. It is important to note this capability is only efficient for short term runs (on the order of days to a few weeks) due to memory storage limitations to run the model inversely. Therefore, should a need to inversely run the model for a longer period of time arise, additional development would be necessary. For emergency response use, the user will need to run the model regularly, to ensure an up to date flow field is available for the possibility of an event to occur. It is also important to note that although the model can trace a pollutant back to the source, it cannot inform the user of the time the release occurred. This in part deals with the complexity of radioactive decay of a material. ALGE3D does compute radioactive decay, but only incorporates the half life of the material to compute the equations. Therefore, should the ability to estimate a time of release for radioactive material be needed, further developments must be made in terms of dealing with the chemistry of various materials.

(All figures and tables should be cited in order. For initial submission, please embed figures, tables, and their captions within the main text near where they are cited. At revision, figures should be uploaded separately, as we need separate files for production. Tables and all captions should be moved to the end of the file.)

References should use a name-date format, not numbers. Enclose citations in parentheses with authors in upright text (non italics) as in: (Smith et al*.,* 2009) or Smith et al. (2009). More information on in-text citations can be found in our [Brief Style Guide](https://publications.agu.org/brief-guide-agu-style-grammar/#reference),“Reference Formatting.”

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**Open Research**

Sampled data can be download at Florida’s Department of Environmental Protection website ([Tampa Bay Sampling Response and Results | Florida Department of Environmental Protection](https://floridadep.gov/dear/dear/content/tampa-bay-sampling-response-and-results)).

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