Savannah River National Laboratory®

We put science to work.™

Recent strides in a 3D aqueous fate and transport model

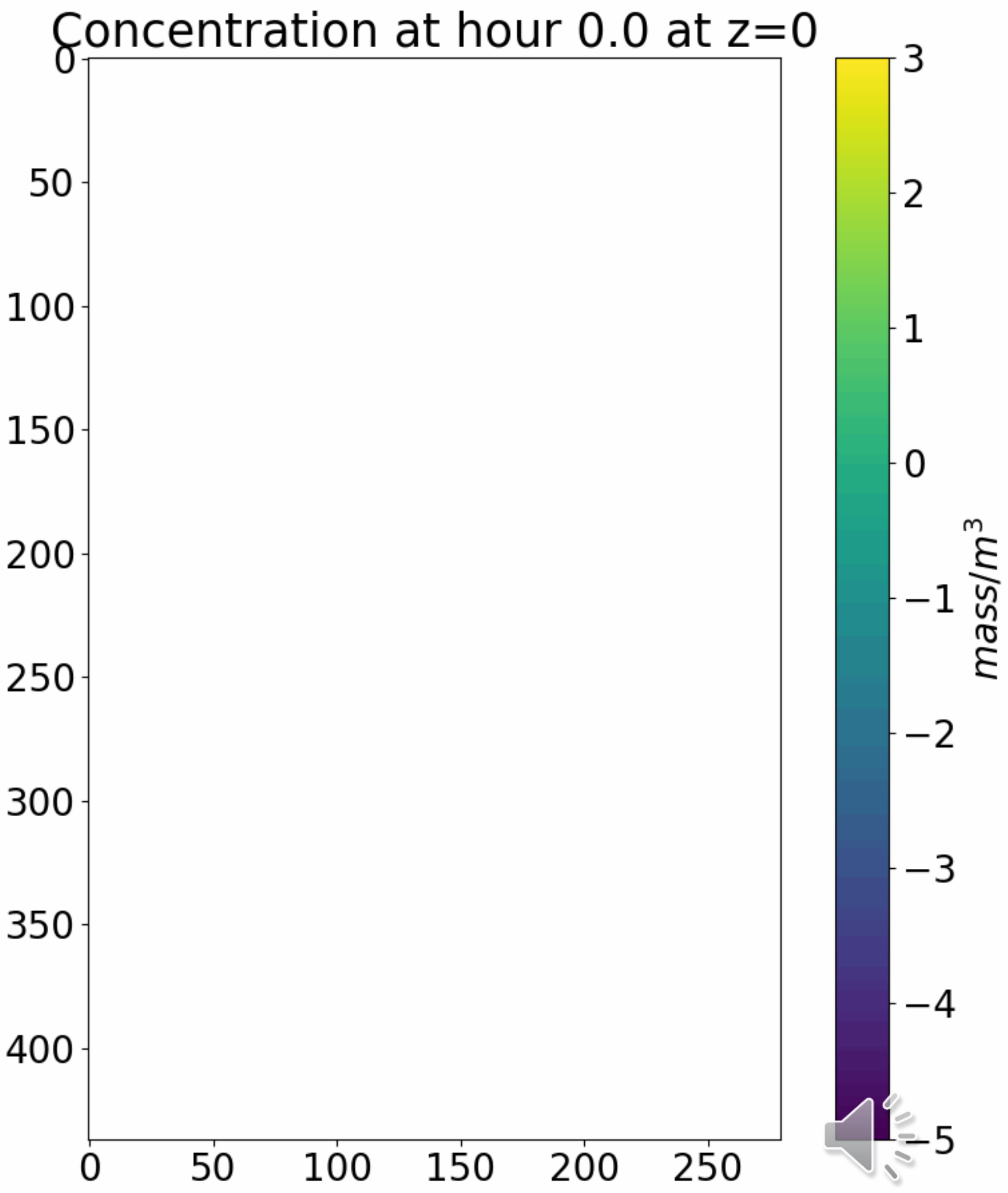
T1.4 Multidisciplinary Studies of the Earth's Subsystems

Vivian Turner

SnT 2025

What is ALGE?

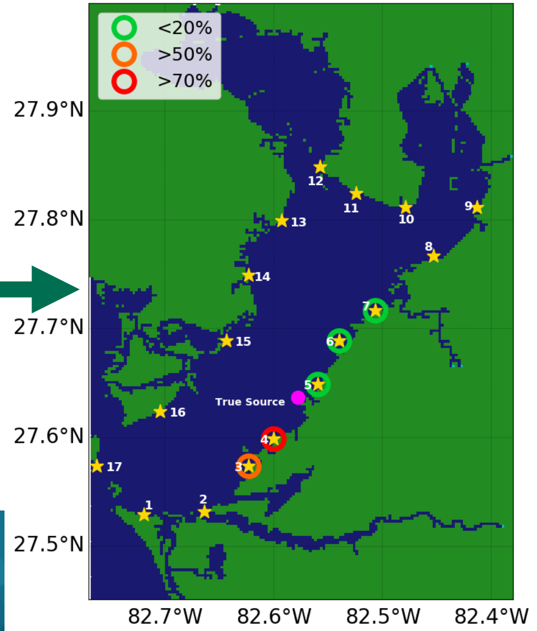
- ALGE is an in-house 3D aqueous fate and transport model, initially developed to examine thermal plumes on site
- Solves the mass, momentum, and energy conservation equations for sediment, particulate(dissolved tracer sorbed onto sediment), and dissolved tracer releases in predetermined lakes, rivers, coastal bays, and estuaries
- ALGE also considers wind stress effects, sensible and latent heat transfer, shortwave and longwave radiation transfer (including effects of clouds) tidal effects, and buoyancy forces.
- This makes ALGE unique compared to other aqueous transport models as it both 3D and considers complex atmospheric effects for dissolved, sediment and particulate tracers

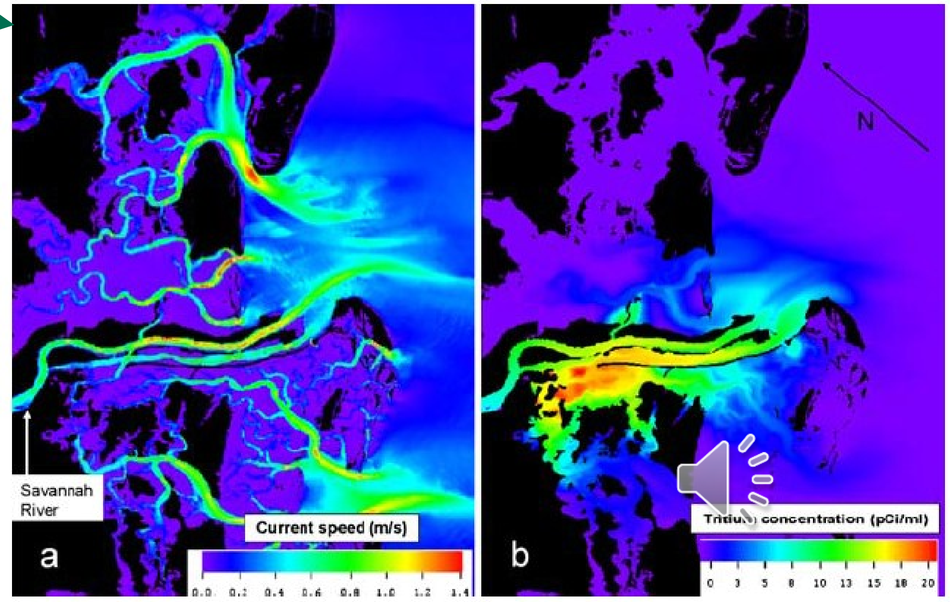


ALGE Previous Work

- Previous validation work includes:
  - Chlorine gas deposition into nearby bodies of water after a train collision in Graniteville, SC (Buckley et al, 2012)
  - Simulating flow rate of a creek as it enters Clinch River in Tennessee (Garrett et al, 2000)
  - Fate and transport of tritiated water from an accidental release at the Savannah River Site in 1991 (Blanton et al., 2009)

- Recent development includes:
  - A new backtracking capability-to determine potential sources of a pollutant should material be detected but a source cannot be found (Turner et al., 2023)





Continuation of ALGE as a robust model

- Recent work has created new capabilities/applications to improve or further validate ALGE
  - A pilot study to simulate microplastics
  - The addition of the physical process of sediment coagulation and breakup
  - The ability to use runoff to understand urban heat island effects due to urbanization

Recent Additions to ALGE- Microplastics

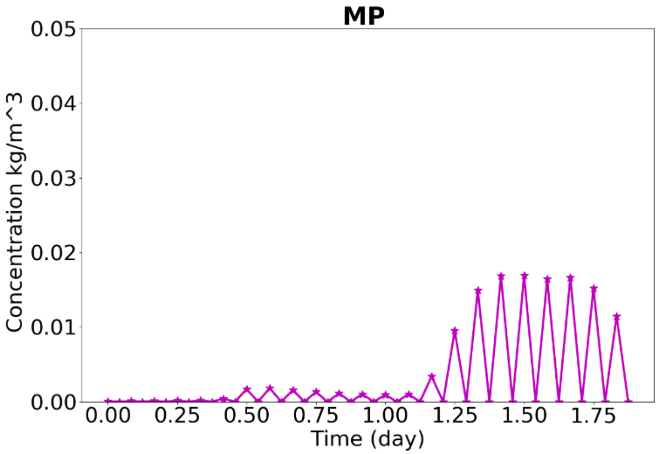
- Microplastics (MPs) are an emergent and ubiquitous contaminant capable of adsorbing material and leaching said material downstream in an aqueous system
- Literature has shown MPs interact with radionuclides and can act as potential carriers in the environment (Ioannidis et al., 2022; Ioannidis et al., 2023; Yadav et al., 2024)
- Can we simulate MPs in ALGE?

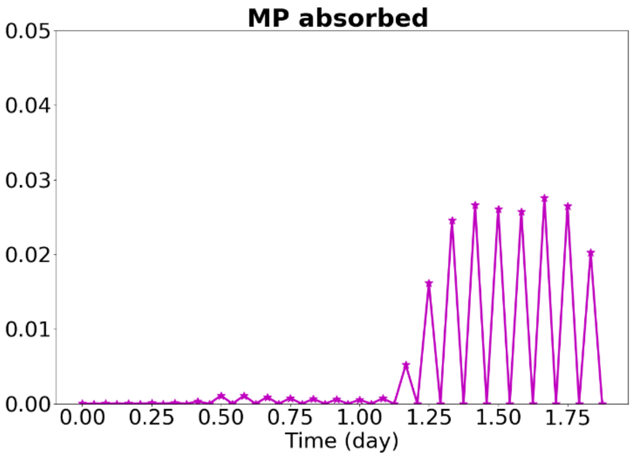
Microplastics

- 48hr simulations were performed with a release concentration of 10 kg/m^3

- Properties to simulate sediment were substituted for MP properties

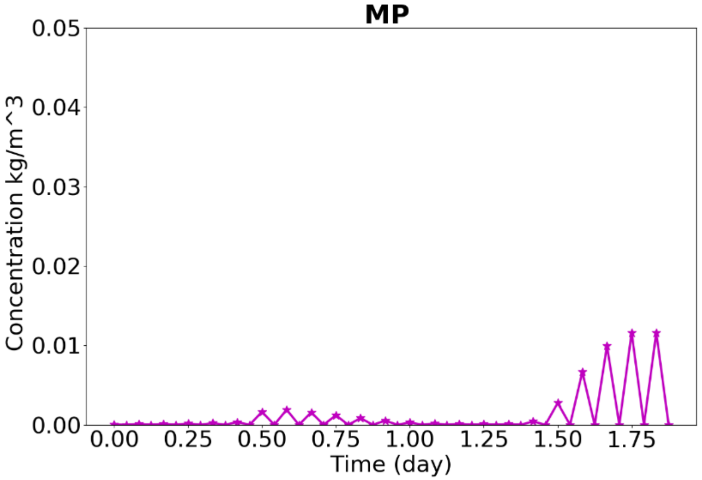
Radio/plastic	Plastic diameter (m)	Plastic density (kg/m^3)	Absorption coeff (K_d)	Decay constant (lambda)
PE U 232	4e-5	1390	3.4482758 [4]	6.118668e-06
PE U 235	4e-5	1390	0.8[6]	3.11936E-17
PE Sr 90	4e-5	1390	40,000[8]	2.8240082647238734e-06
PE Cs 137	4e-5	1390	80000 [5]	2.635741047075615e-06
PE H3	4e-5	1390	100 [3]	6.325778512981476e-06

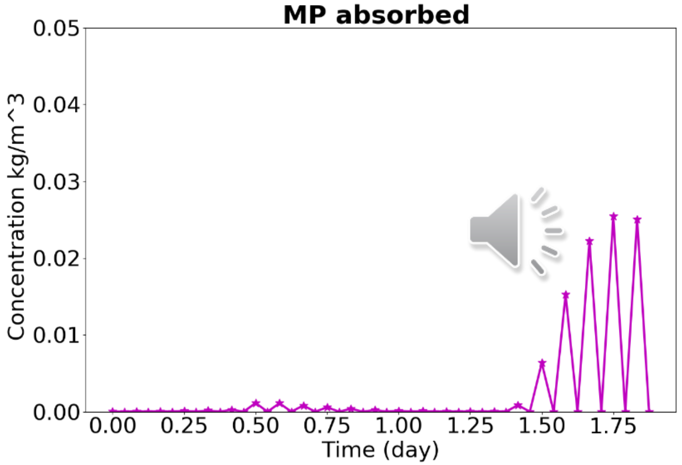




Preliminary results showcase ALGE can simulate MPs along with the potential capability to absorb/desorb various radionuclides

Future work to better understand how radionuclides interact with MPs can be incorporated into the ALGE model.





Savannah River National Laboratory®

Recent Addition to ALGE-Coagulation and Breakup

- Recently published work examines the addition of the complex movement of sediment coagulation and breakup:

1. What is the behavior of suspended clay coagulation and breakup in a freshwater environment produced by ALGE, and how does this compare to the literature?

2. How does this change with a salinity driven environment in ALGE?

3. Does the addition of turbulence (via Reynolds number) affect these results and lead to a significant change in floc size distribution and overall transport?

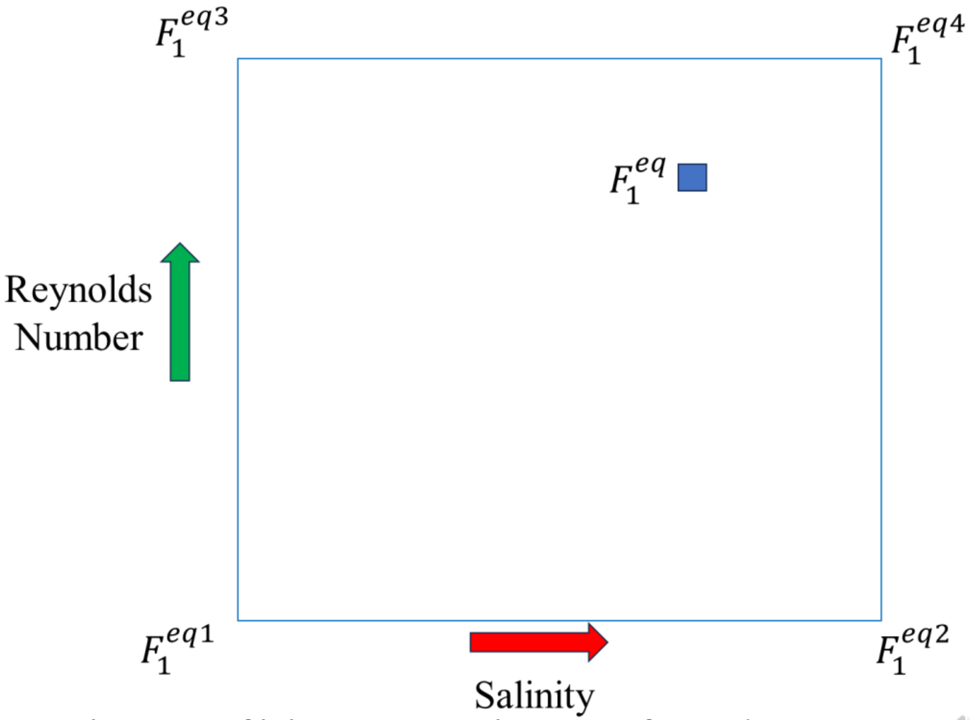
Create new additions to the model → Develop and run a series of experiments → Perform a statistical analysis

[Sensitivity analysis of a parameterization of coagulation in an aqueous transport model - ScienceDirect]

Coagulation and Breakup

- ALGE solves the 3D hydrodynamic equations for dissolved contaminant, sediment, and particulate (contaminant adhered to sediment) contaminant.
  - We first divided the sediment and particulate contaminant into three size bins

- $CT = C1 + C2 + C3$
- and we must then determine the fraction of mass in each bin (*F1*, *F2*, and *F3*). This is accomplished by 'relaxing' the fractions in bins 1 and 2 toward a respective equilibrium
- $dF1/dt = -k\ (F1 - F1eq)$
- where $F1eq$ is the fraction at equilibrium, and k is the decay rate. A similar equation exists for $F2$, and $F3$ is then solved as *1-F1-F2*. The 'equilibrium' value can vary with the surrounding environment (e.g., salinity).

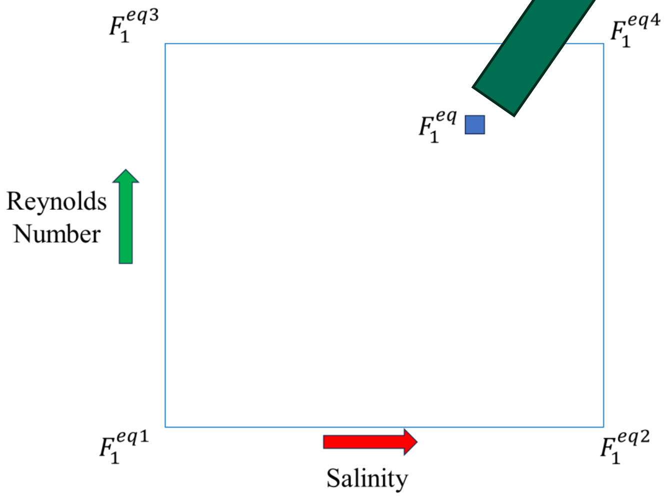


Schematic of bilinear interpolation performed in ALGE. Bin sizes are made a function of both Reynolds number and salinity

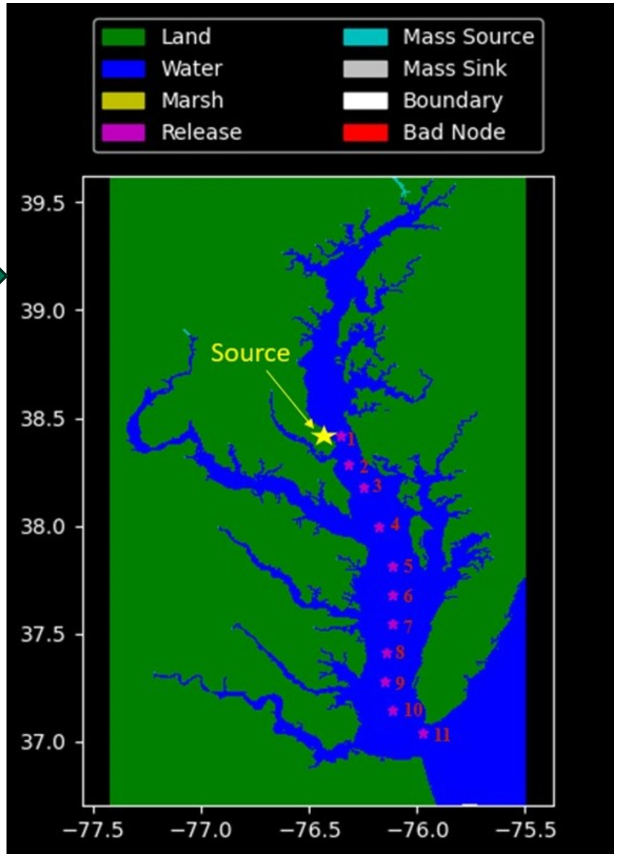
Coagulation and Breakup

Develop and run a series of experiments

Exp (#)	Diameter (μm)			Density (g/cm^3)			F_1^{eq1}	F_1^{eq2}	F_1^{eq3}	F_1^{eq4}	F_2^{eq1}	F_2^{eq2}	F_2^{eq3}	F_2^{eq4}
	Bin1	Bin2	Bin3	Bin1	Bin2	Bin3								
1							.30	-	-	-	.17	-	-	-
10	60	185	325	1.46	1.12	1.07	.30	.43	-	-	.17	.49	-	-
19							.30	.43	.11	.52	.17	.49	.082	.01
2							.28	-	-	-	.18	-	-	-
11	60	185	325	1.14	1.04	1.02	.28	.42	-	-	.18	.50	-	-
20							.28	.42	.093	.52	.18	.50	.08	.009
3							.31	-	-	-	.17	-	-	-
12	60	185	325	1.71	1.20	1.11	.31	.45	-	-	.17	.48	-	-
21							.31	.45	.12	.53	.17	.48	.08	.01



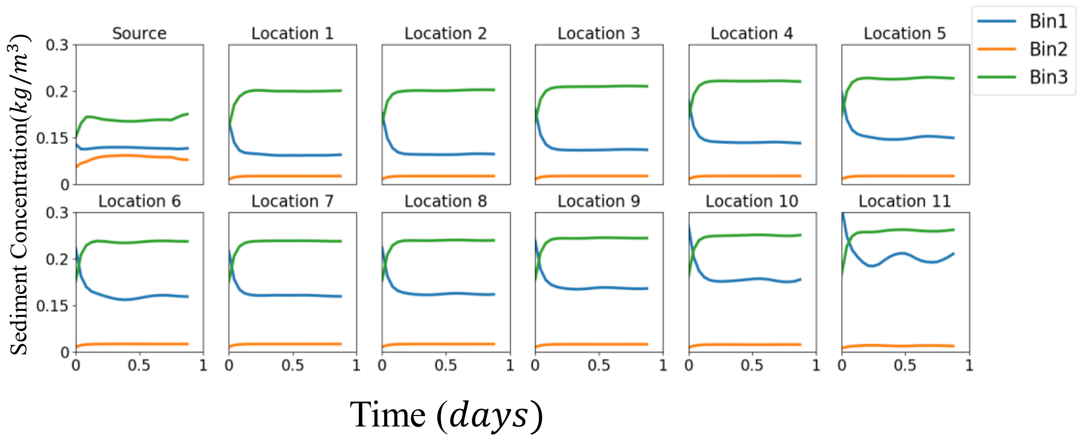
- 28 simulations were performed with various sediment diameter and densities and bin fractions.
- A time series and t-test was performed at 12 locations along the Chesapeake Bay to determine if significant differences in the results (spatial and temporal) are present due to these changing parameters.
- The Chesapeake Bay was chosen as our test sight as it is a well studied body of water-vast data and literature available for comparison

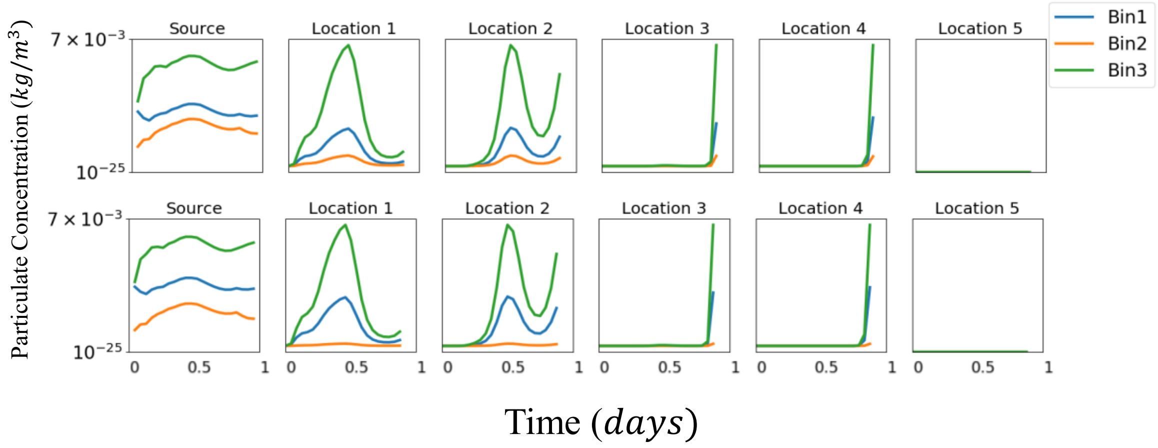


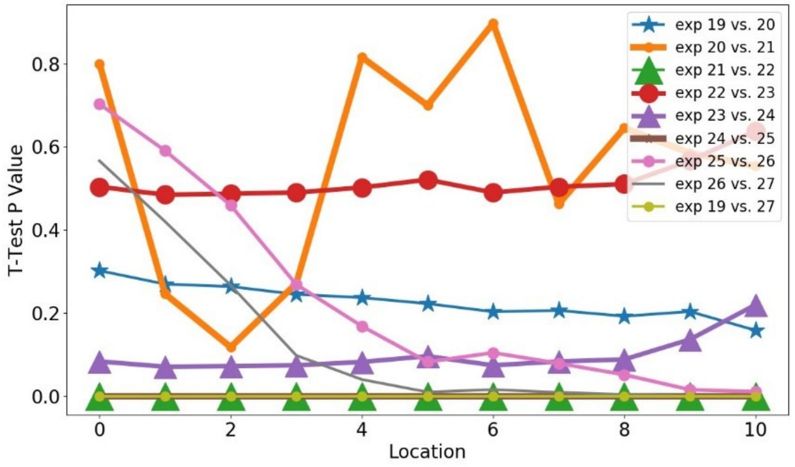
Map of Chesapeake Bay with list of locations where time series and t-test were performed

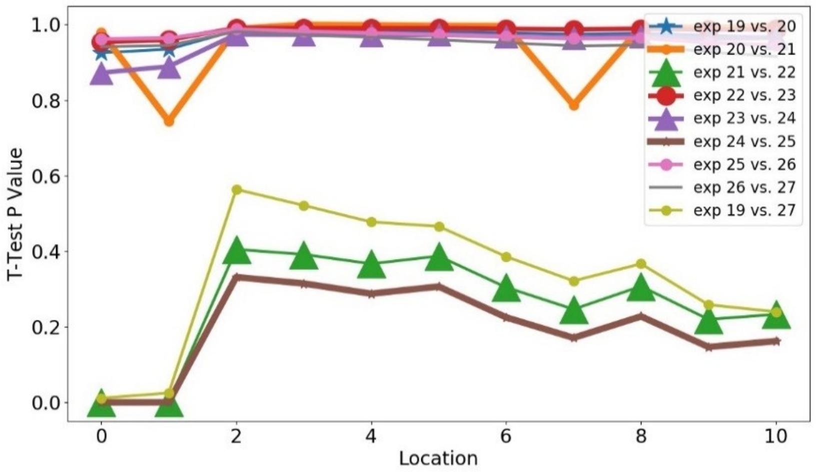
Coagulation and Breakup

Perform a statistical analysis



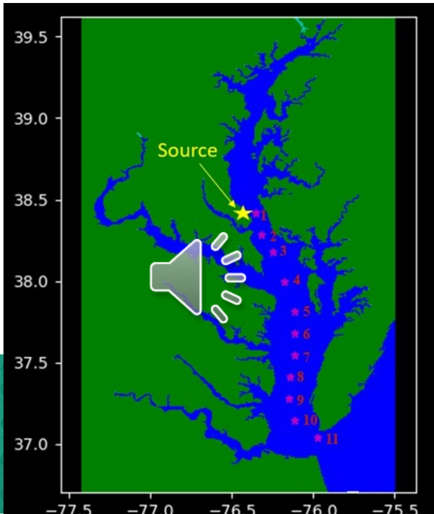






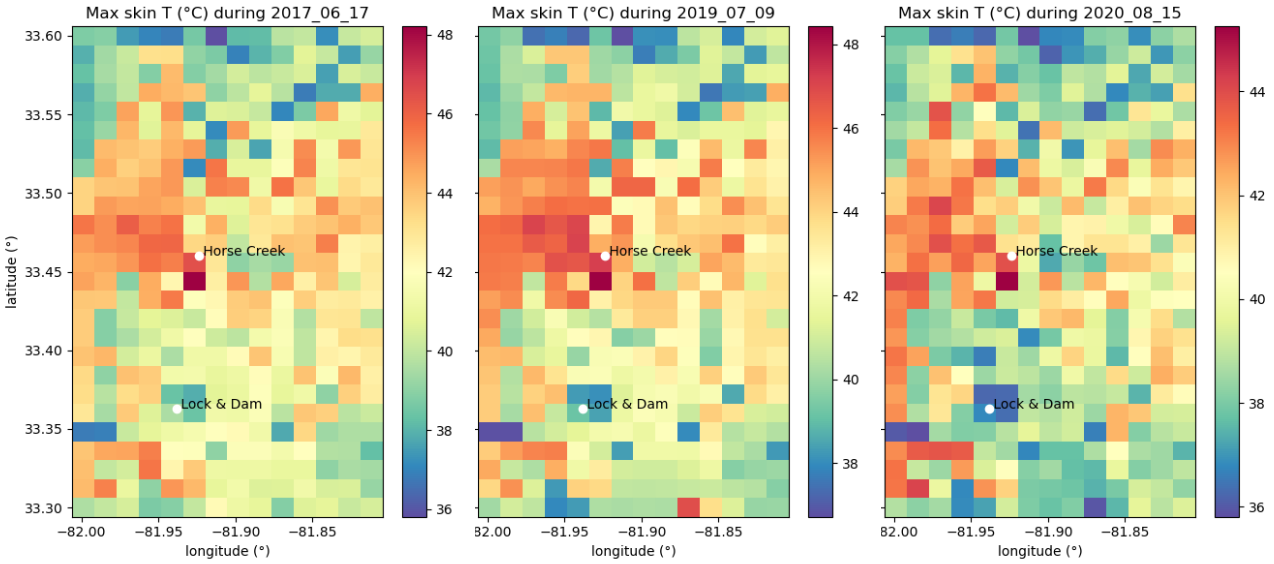
Concentrations reach equilibrium but majority of concentration is comprised of either bin1 or bin3

T-test results present more consistent p-values compared to experiments where only salinity is considered

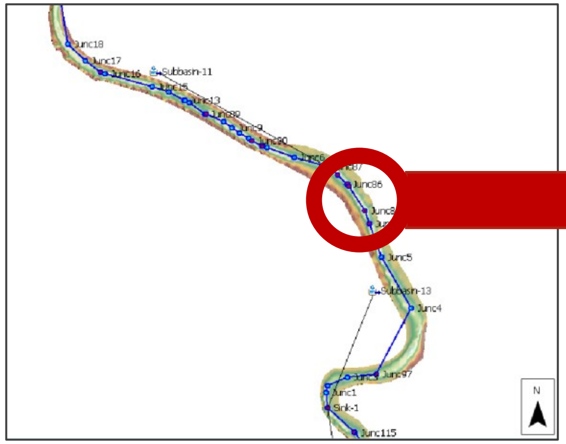


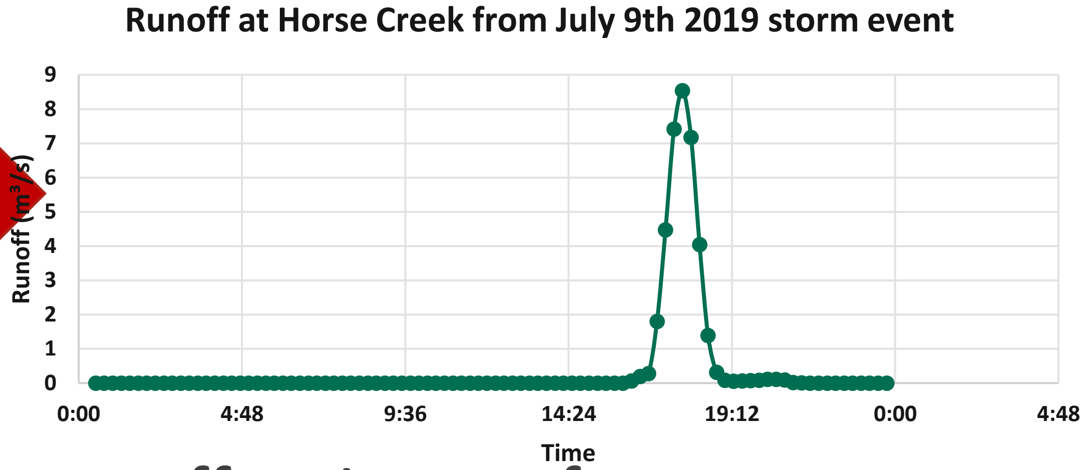
Recent Addition to ALGE-Aqueous Urban Heat Island Effects

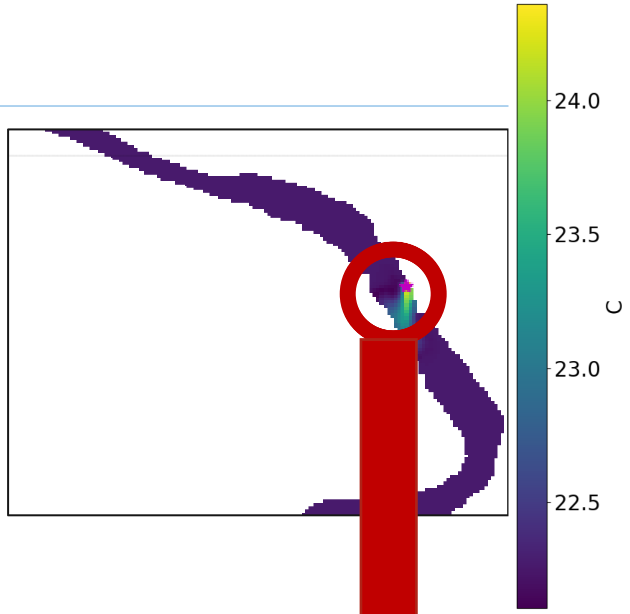
- The hydrological urban heat island (HUHI) effect describes thermal impacts to streams due to urbanization
- Recent literature suggests that warming of nearby bodies of water are a result of several factors such as connections to impervious surfaces, amount of canopy cover, and runoff due to rainfall events (Reza et al., 2020; Zahn et al., 2021).
- Can we use skin temperature, HEC-HMS, and ALGE to examine aqueous UHI effects in a developing city (Augusta, GA) after mild rain events?



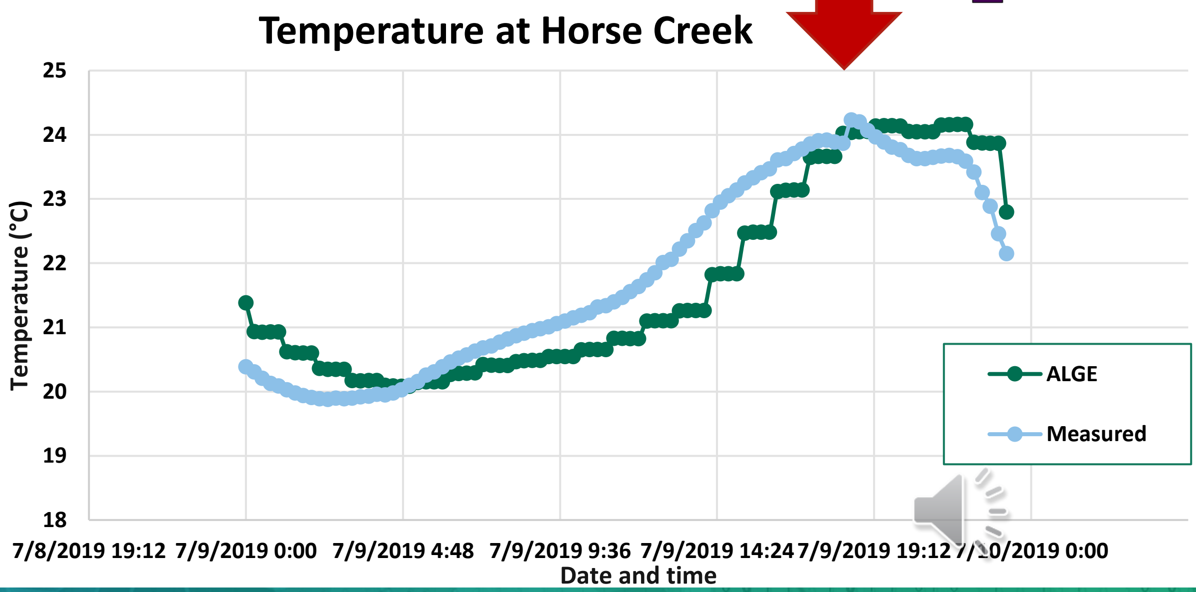
UHI simulations in ALGE







- HEC-HMS simulates runoff estimates from smaller streams that directly connect to the Savannah River
- ALGE uses runoff from HEC-HMS and skin temperature as input
- Runoff appears to not be properly accounted for



Summary

- Recent work has developed new capabilities and potential new applications for ALGE
- We can account for MP in an ALGE simulation by substituting sediment characteristics
- We added the physical process of coagulation and breakup of sediment by performing a bilinear interpolation
- We examined potential of using ALGE for simulating aqueous UHI effects

- Future work includes incorporating other models as input into ALGE (i.e. atmospheric models to account for deposition into bodies of water, oceanic/wave model), incorporating experimental data to better account for interactions of radionuclides and MPs, and technical/app development

Thank You!

Vivian Turner

vivian.turner@srnl.doe.gov