



# System for Hazard Assessment of Released Chemicals (SHARC) Model Validation and Verification Studies: Improvement of Model Predictions for Chemical Releases in Dynamic Estuarine Systems



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The System for Hazard Assessment of Released Chemicals (SHARC) is an advanced waterborne hazard fate and transport modeling and analysis tool developed by Maritime Planning Associates, Inc. (MPA). Validation and verification (V&V) studies performed in the tidal-fresh Potomac River near Washington, DC from 2011-2017 under different forcing conditions revealed areas for SHARC model improvement, such as better integration of high-resolution hydrographic & meteorological model data into SHARC and refinement of SHARC chemical fate algorithms to better quantify how variability in key water column parameters impact the partitioning and fate of specific reactive, non-conservative constituents. Additional V&V studies are needed in more dynamic estuarine systems with a wider range of variability in physiochemical conditions to improve the capabilities of SHARC for predicting the transport, dispersion, and fate of conservative and semi-conservative chemical releases in estuaries. In 2019-20, follow-on data collection efforts and SHARC V&V studies are being performed in the mesohaline Chesapeake Bay and the Severn River, MD to investigate the potential for improving SHARC model predictions through the integration of high-resolution hydrographic and meteorological model data and physiochemical water column parameter predictions derived from field data run through machine learning algorithms.

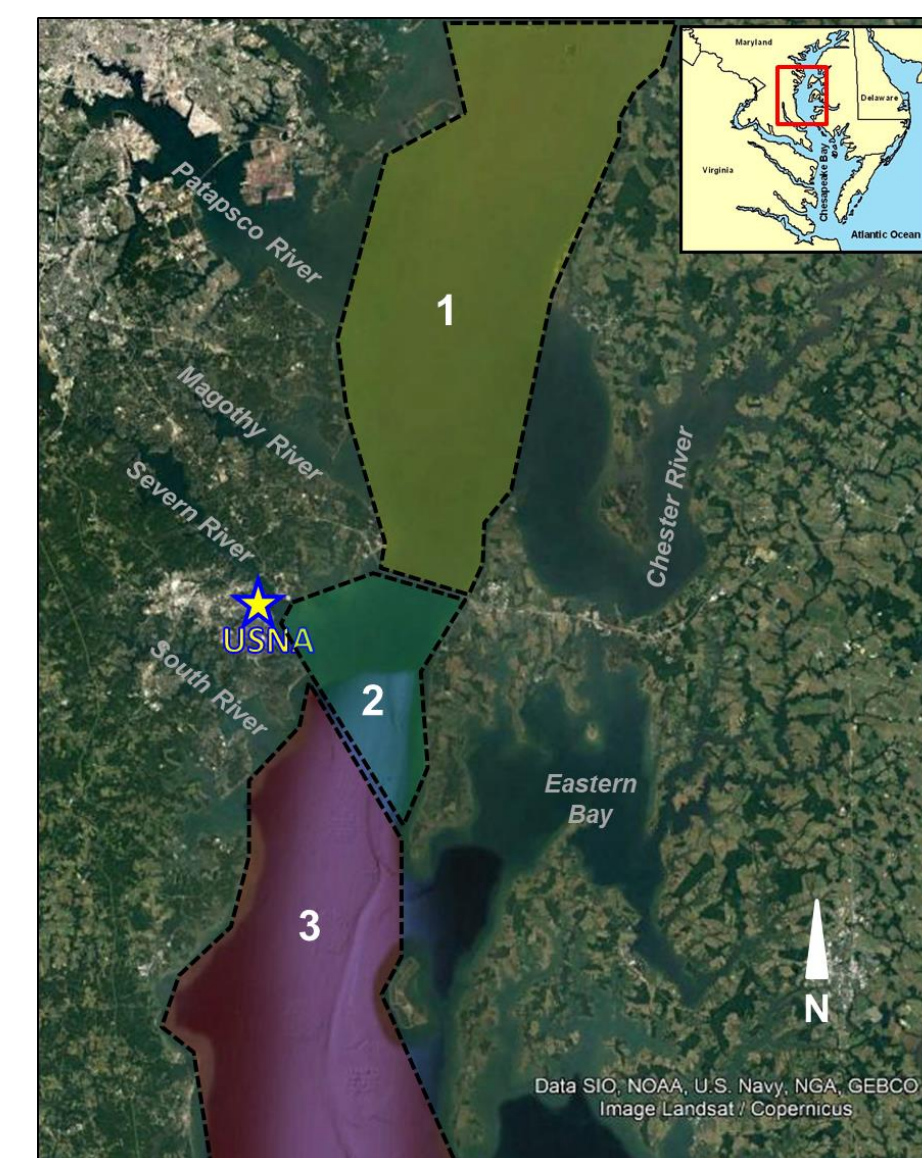
## Background:



**Figure 1.** Results of a 30-day SHARC (v 4.0.0) simulation starting on 01 October 2019 for an instantaneous polygon release of 10,000 gallons of a conservative agent into the mesohaline Chesapeake Bay near the mouth of the Severn River near the U.S. Naval Academy (USNA). Hydrodynamic forcing was downloaded from the SHARC Tidal Harmonic Database (THDB). No meteorological forcing was included. Water column parameters such as temperature, salinity, pH were determined from the SHARC seasonal profiles database (SPDB).

**Figure 1** shows the results of a 30-day SHARC simulation for the release of a conservative chemical agent into the mesohaline Chesapeake Bay at the mouth of the Severn River near the U.S. Naval Academy (USNA). In this simulation, plume spreading is a function of dispersion and advection (tides only) and since the agent released behaves conservatively, any changes in water column parameters would have little effect on agent fate. Accurate simulation of reactive chemical agents in dynamic estuaries like Chesapeake Bay requires high-resolution hydrographic and meteorological model inputs and better understanding of variability in water column conditions that affect chemical partitioning and speciation.

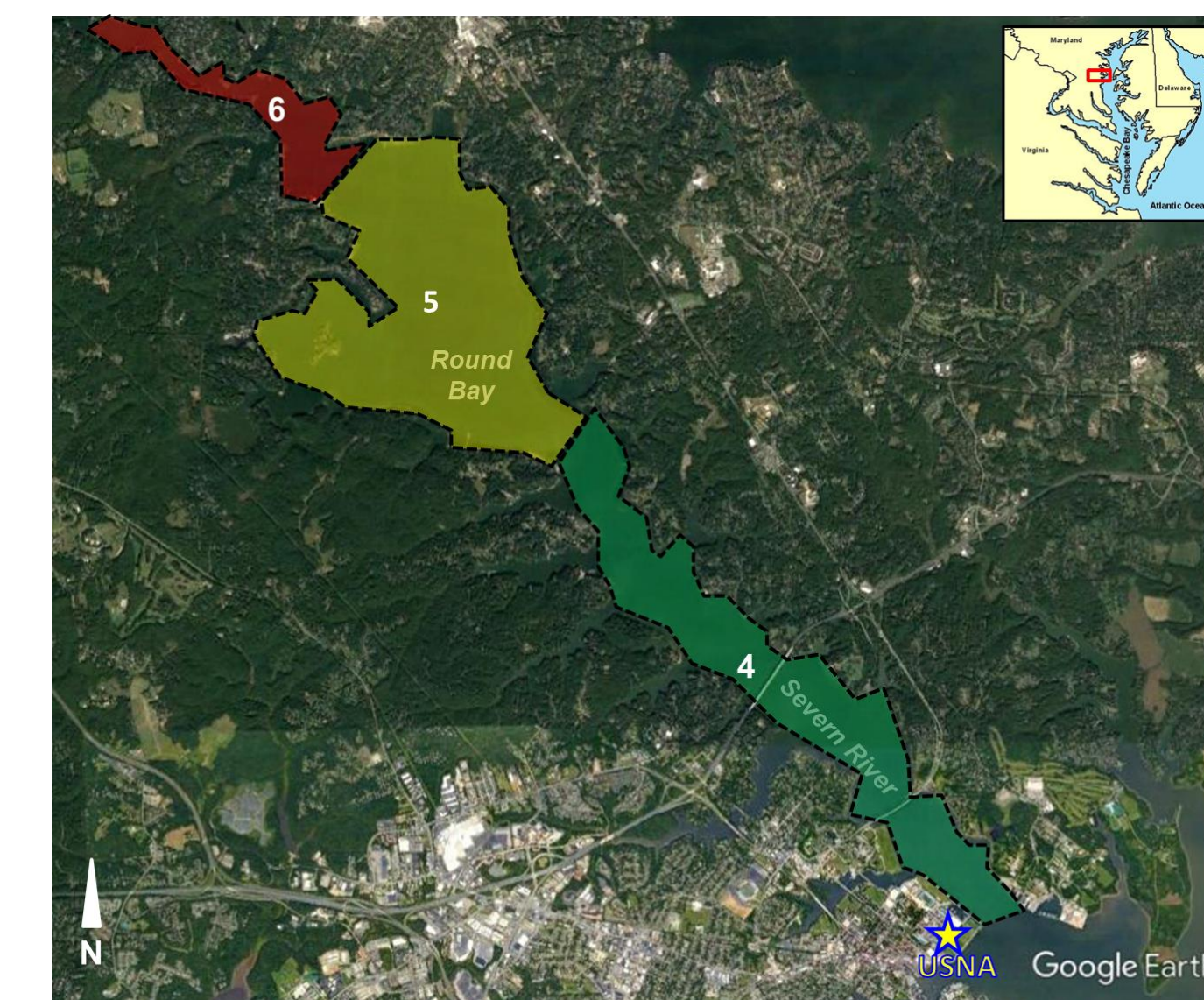
## Mesohaline Chesapeake Bay:



**Figure 3.** Map of the mesohaline Chesapeake Bay study area. The study area is broken down into three general sections (1-3) that are color coded based on the number/completeness of data records on surface water (0 - 1.5 m) physiochemical parameters collected by USNA from 2013 - 2017 (green = high number/good temporal coverage; yellow = medium number/some significant temporal gaps; red = low number/large temporal gaps). Section 1 is from the Chesapeake Bay Bridge to just north of the Patapsco River near Baltimore. Section 2 is south of the Chesapeake Bay Bridge to the mouth of Eastern Bay and includes the mouth of the Severn River where the U.S. Naval Academy (USNA) is located. Section 3 extends from Eastern Bay south to the mouth of the Choptank River (not shown).

**Figure 3** shows the study area of the mesohaline Chesapeake Bay. The Chesapeake Bay is a large, north-south aligned, ecologically-complex and dynamic partially-mixed estuarine system on the eastern seaboard of the United States. The Chesapeake Bay Watershed includes 6 States (and the District of Columbia) and is home to 17 million people and borders major urban centers like Washington, DC, Baltimore, MD, and Norfolk, VA. More than 150 rivers, streams, and tributaries drain into the Bay but freshwater flow is dominated by the Susquehanna River. The dynamic nature and complexity of the Chesapeake Bay system makes it an ideal system for conducting SHARC V&V studies. The USNA is located at the mouth of the Severn River in the mesohaline Chesapeake Bay and USNA has been collecting data on physiochemical conditions in the mesohaline Bay for over a decade.

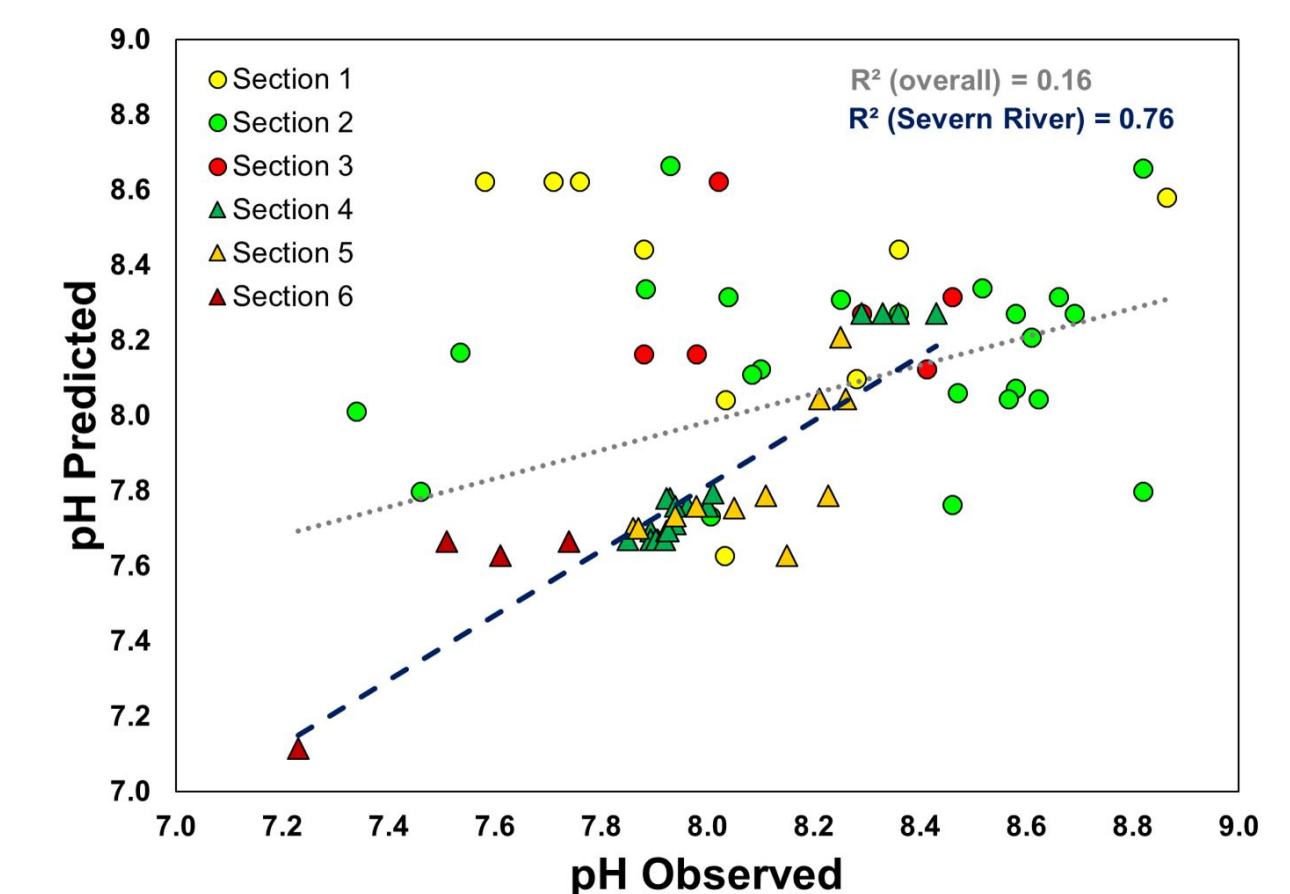
## Severn River:



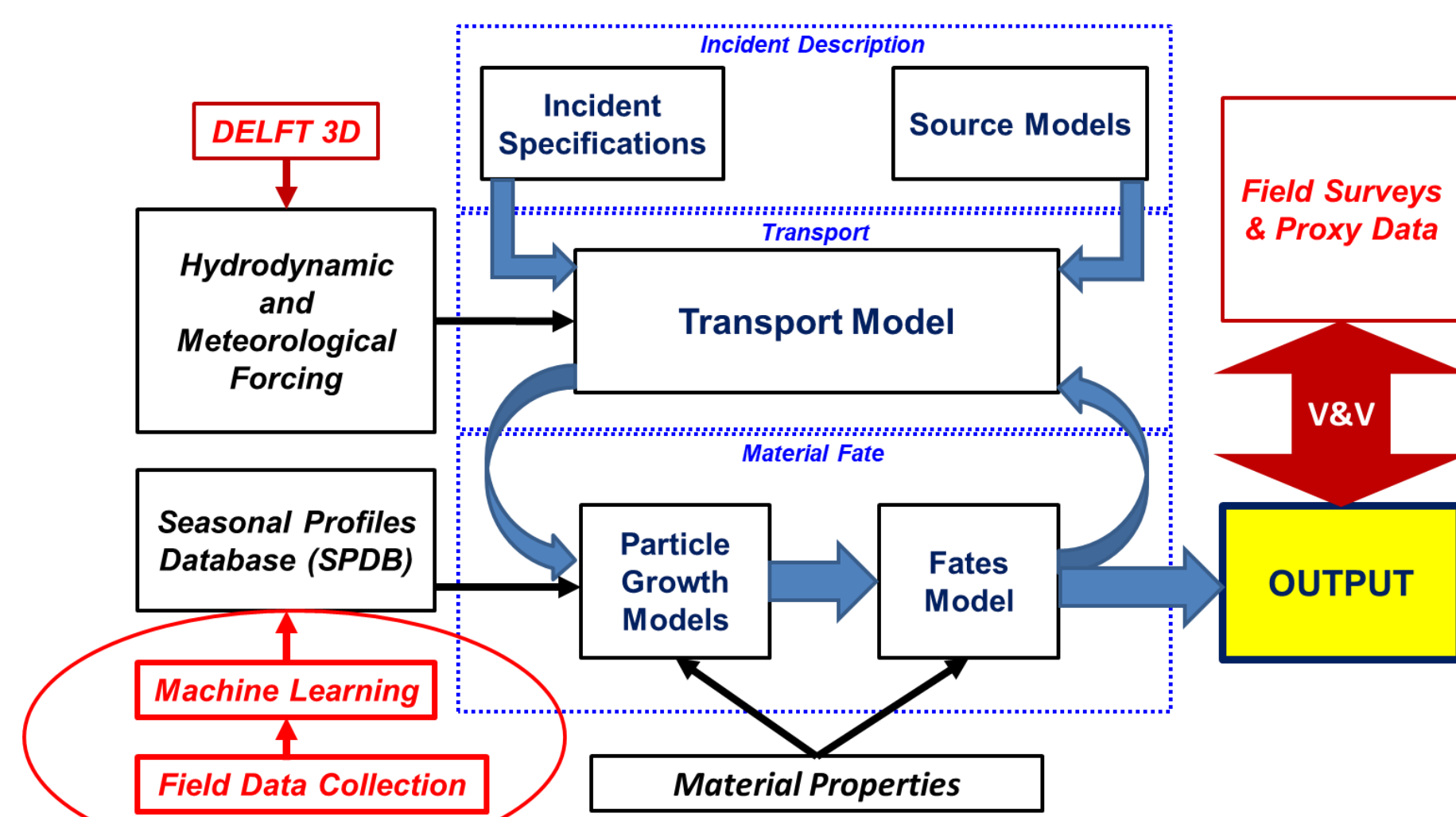
**Figure 4.** Map of the Severn River study area. The study area is broken down into three general sections (1-3) that are color coded based on the number/completeness of data records on surface water (0 - 1.5 m) physiochemical parameters collected by USNA from 2013 - 2017 (green = high number/good temporal coverage; yellow = medium number/some significant temporal gaps; red = low number/large temporal gaps). Section 4 is from the mouth of the Severn River near the USNA Triton Light to the mouth of Round Bay. Section 5 is Round Bay. Section 6 extends from Round Bay westward to Severn Run (not shown).

The Severn River (**Fig. 4**) is a small brackish tributary (sub-estuary) that empties into the upper, mesohaline section of Chesapeake Bay. The sub-estuary drains a watershed area of ~ 210 km<sup>2</sup>. Freshwater flow is limited to runoff inputs from the numerous small creeks and groundwater-fed streams that empty into the upper section of the river. Physical circulation, especially in the lower-estuary is dominated by tidal exchange with the Chesapeake Bay. Typical tidal range is ~ 0.3 m and salinity varies seasonally from about 3-15. The river is urbanized at the mouth near USNA and the City of Annapolis where it joins the Chesapeake Bay with a moderate degree of residential development lining the river further upstream. USNA has been collecting data on physiochemical conditions in the Severn River regularly since and it is continuously monitored by the USNA Oceanography Department Severn River Watershed Observatory (SRWO) in Section 4 since 2017.

Hourly-averaged meteorological conditions (air temperature (°C), wind speed (m/s), wind direction; NOAA KNAK weather station at USNA), SRWO surface water quality parameters (water temperature (°C), turbidity (FNU), dissolved oxygen (mg/L), salinity; **Fig. 5**), Susquehanna River Flow (m<sup>3</sup>/s; USGS 01578310 SUSQUEHANNA RIVER AT CONOWINGO, MD), and year, month, and hour of collection were used to train a complex-tree regression model to predict pH using the Regression Learner App in MATLAB R2017a (**Fig. 6**). **Figure 7** shows pH values predicted using the trained complex-tree regression model (**Fig. 5**) vs. observed pH in surface waters (0 - 1.5 m) of sections of Chesapeake Bay (1-3; **Fig. 3**) and the Severn River (4-6; **Fig. 4**) sampled by USNA from 2013 - 2017. The trained regression model does an adequate job predicting pH in the Severn River but fails overall. Additional predictors should be considered and additional model training should be conducted to better predict pH in the main-stem Bay and in data sparse areas.

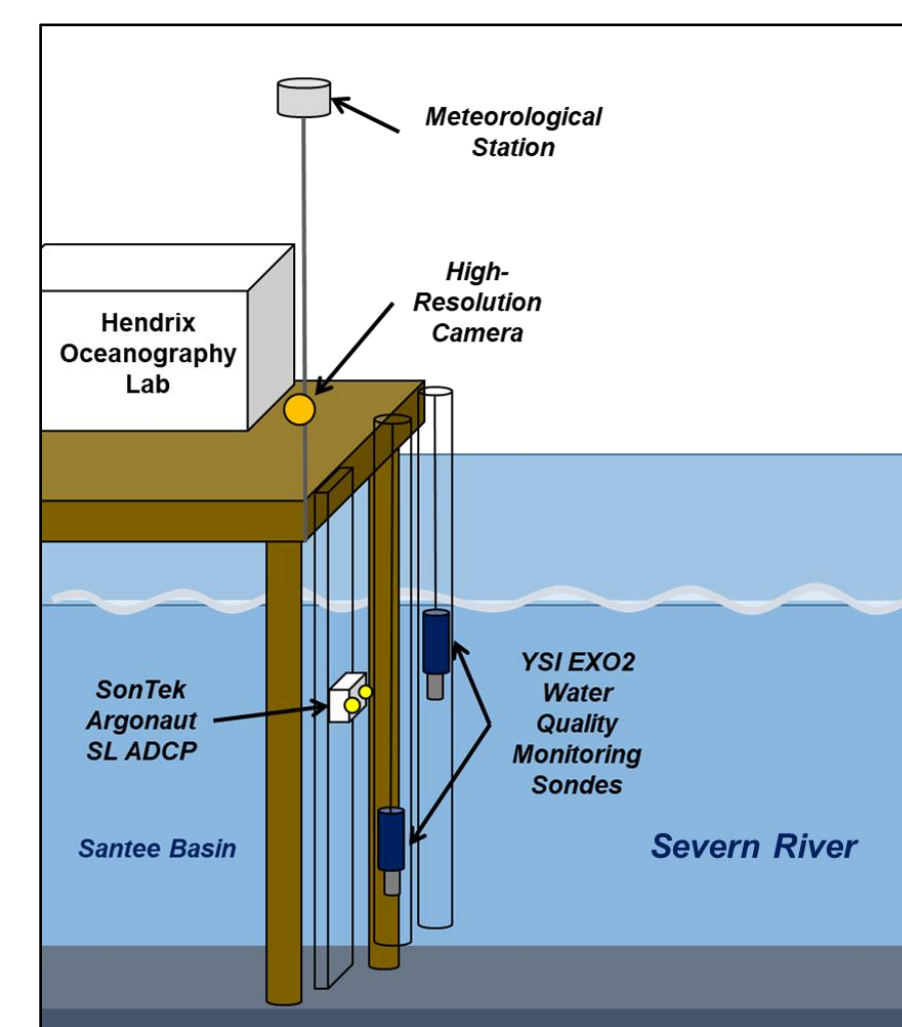


**Figure 7.** Predicted pH values (response) vs. observed pH in surface waters (0 - 1.5 m) of sections of Chesapeake Bay (1-3; **Fig. 3**) and the Severn River (4-6; **Fig. 4**) sampled by USNA from 2013 - 2017. The linear regression fit to predicted vs. observed pH data was poor ( $R^2$ ; grey dashed line) overall was poor but the model did an adequate job predicting pH values in the Severn River.

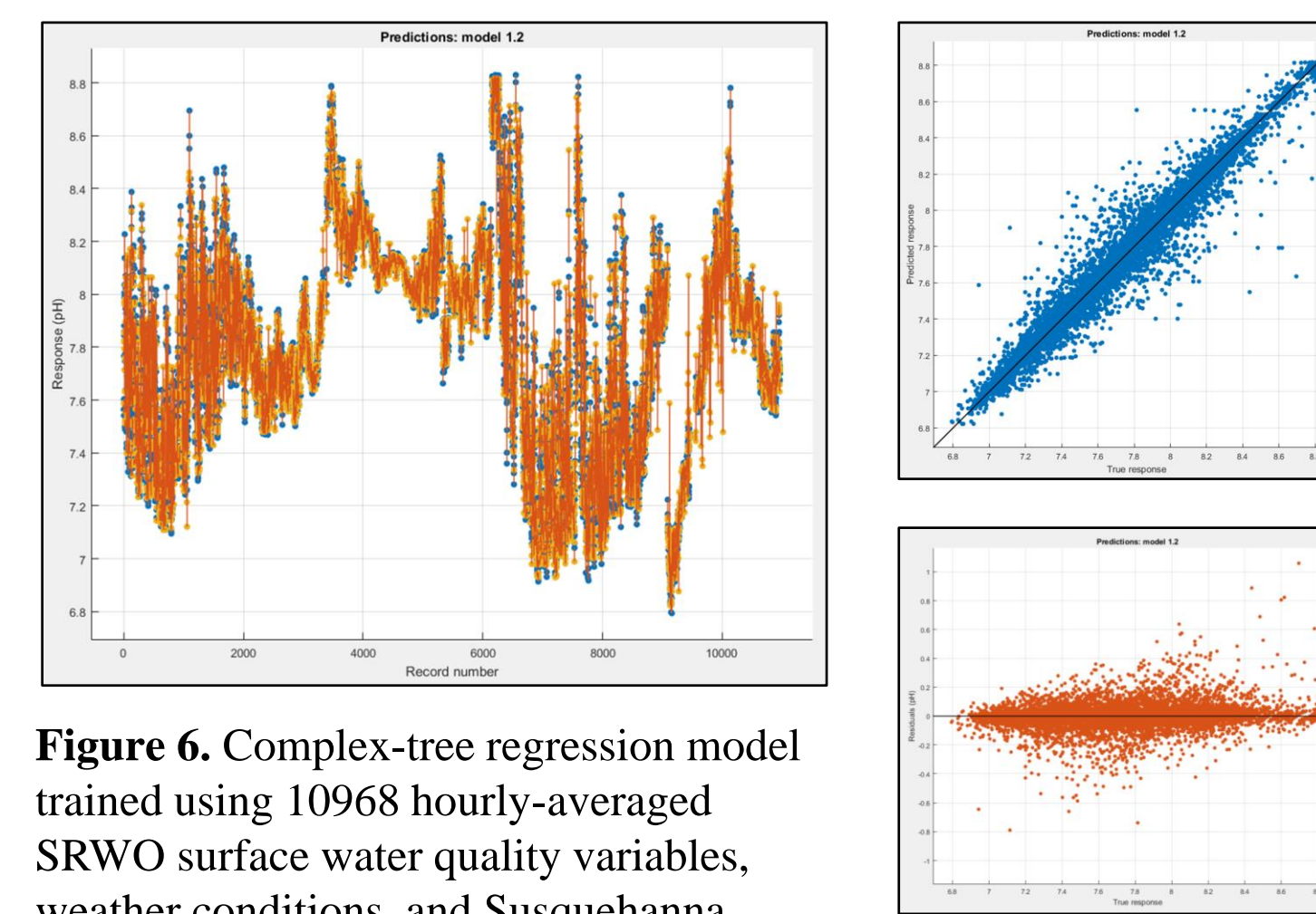


**Figure 2.** SHARC architecture schematic showing the four main components of SHARC: 1) the Incident Description; 2) Transport Model; 3) Material Fate Models; and 4) Output Interface. The SHARC Transport Model accepts external hydrodynamic and meteorological forcing model inputs. The Material Fate Models are a function of water column water column conditions derived from the SHARC Seasonal Profiles Database (SPDB). Items in highlighted in red are focus areas for USNA efforts (in red) to improve SHARC model simulations and validate & verify (V&V) model outputs.

**Figure 2** shows the general SHARC architecture schematic along with USNA efforts to improve SHARC model simulations and validate & verify (V&V) SHARC model outputs in two study areas: 1) the Mesohaline Chesapeake Bay and 2) the Severn River, a tidal sub-estuary of Chesapeake Bay. **This work (Phase I) focuses on assessing the utility of using field data on water column parameters run through machine learning algorithms to provide probabilistic inputs to the SPDB to feed SHARC Material Fate Models.** Phase II work will involve the conduct of field surveys using proxy data to validate & verify improved SHARC model outputs and will employ hydrodynamic modeling software like DELFT 3D to create custom, local-scale high-resolution hydrographic model inputs to the SHARC Transport Model.



**Figure 5.** Diagram of Severn River Watershed Observatory (SRWO) Node 1 located at the mouth of the Severn River at USNA (**Fig. 4**, Section 4).



**Figure 6.** Complex-tree regression model trained using 10968 hourly-averaged SRWO surface water quality variables, weather conditions, and Susquehanna River flow from June, 2017 - March 2019. Predicted pH (response; orange symbols with red lines indicating error) was based on 11 predictors using 5-fold cross-validation and was fit to observed pH values (blue symbols) with a  $R^2 = 0.96$  and RMSE = 0.08 (preliminary results).

*Results demonstrate the potential for using machine learning informed by field datasets to develop models to predict physiochemical water quality parameters such as pH in dynamic estuarine environments like the Chesapeake Bay and the Severn River. These models would provide inputs into the SPDB in data sparse environments and improve SHARC model predictions. Follow-on work will continue to compile data and develop and train models to inform the SHARC SPDB. Work will develop local-scale hydrographic models to improve SHARC model predictions in the Chesapeake Bay and the Severn River and increase the utility of SHARC as a decision support tool in estuaries.*



Ongoing and Future Work:



Improvements to be assessed in follow-on SHARC V&V studies...



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