Validation of Model Predictions for the Dispersion of Reactive Chemical Releases in a Sub-estuary of the Chesapeake Bay

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Abstract:

Predicting the transport, dispersion, and fate of reactive chemical releases in dynamic estuarine systems is challenging. The System for Hazard Assessment of Released Chemicals (SHARC) is a waterborne chemical modeling tool developed for the U.S. Defense Threat Reduction Agency (DTRA) to predict the transport, dispersion, and fate of chemical agents introduced to aquatic systems. There is a need to validate SHARC model outputs in estuaries. On October 4, 2011, *in-situ* data on water column parameters and discreet water samples were collected for metals analysis from the tidal-fresh Potomac River estuary near the outfall of the Blue Plains Advanced Wastewater Pollution Control Plant (BPWPCP). Comparison of SHARC model predictions for the dispersion of a simulated release of radio-cesium (^{137}Cs) from BPWPCP to measured concentrations of reactive metals (Rb, Ni) introduced to the Potomac by BPWPCP showed that SHARC accurately predicted the general dispersion plume for ^{137}Cs in the tidal-fresh Potomac River. Plume shape was largely controlled by bathymetry and hydrological and meteorological forcing but differences in ^{137}Cs dispersion were also likely influenced by fine-scale spatial variations in temperature and pH. Results demonstrate a baseline capability of SHARC as a tool for waterborne chemical transport modeling in a dynamic estuarine system.

Study Area and Methods:

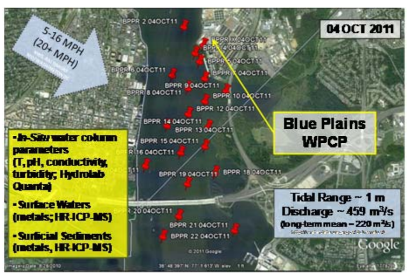

Figure 1. Google Earth view of a 2 x 1 km portion of the tidal-fresh Potomac River with the red pins denoting the random sampling plan (Stations BPPR 1-22) followed on October 04, 2011. Note: Station BPPR X indicates the BPWPCP outfall site. Station BPPR 1 is located mid-channel, ~3 km north of area shown.

Figure 1 shows the Potomac River study area near the outfall of the BPWPCP and local meteorological and hydrological conditions on October 4, 2011. The BPWPCP is a point-source for reactive constituents (metals, organics, nutrients, radioisotopes). *In-situ* data on water column parameters (T, pH) were collected using a Hydrolab Quanta and surface water samples were collected for metals analysis by HR-ICP-MS (**Fig. 2**).

SHARC was used to simulate an input of 50 kg of ^{137}Cs over 5 days starting on Oct 1, 2011. SHARC is designed to model and predict the fate and transport of Chemical Warfare Agents (CWAs) and Toxic Industrial Chemicals/Industrial Materials (TIC/TIMs) in natural waters. The model run included hydrographic data (tides, flow, and coarse bathymetry) and chemical reactivity constants specific to Cs. The 50 kg value was chosen to result in dissolved concentrations of ^{137}Cs in the Potomac River on same order as expected concentrations stable proxies (Rb, Ni).

Figure 2. Surface water collection on the Potomac River, October 4, 2011.

Results:

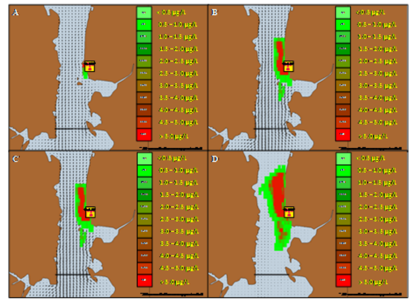

Figure 3. Output of SHARC Model run simulating input of 50 kg of ^{137}Cs from BPWPCP over 5 days (01-06 OCT 2012) for (**A**) 1200 01 OCT 2012; (**B**) 1200 02 OCT 2012; (**C**) 1200 03 OCT 2012, and; (**D**) 1200 04 OCT 2012. Red (darker color) denotes higher concentrations, green (lighter color) are lower concentrations. The velocity and direction of net (tidal and river) flow is indicated by arrows.

The results of the first four days of the SHARC model run, simulating an input of ^{137}Cs to the tidal-fresh Potomac River are shown in **Figure 3.** Note the dispersion of the plume along the eastern side of the river. **Figure 4** shows show modeled plume dispersion for a portion of a tidal cycle (5 hours) coincident with field sample collection. Note the influence of net circulation on the plume distribution.

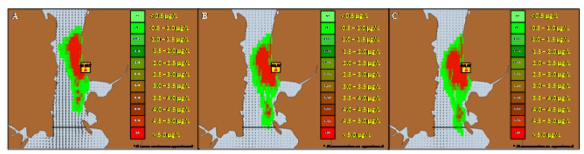

Figure 4. Output of SHARC Model run simulating input of 50 kg of ^{137}Cs from BPWPCP over 5 days (01-06 OCT 2012) for (**A**) 1300 04 OCT 2012; (**B**) 1500 04 OCT 2012, and; (**C**) 1700 04 OCT 2012.

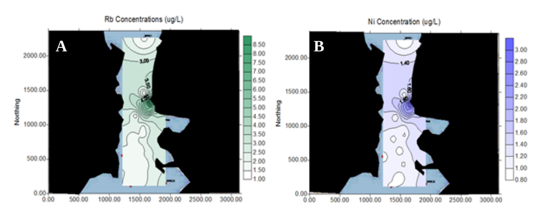

Figure 5. 2-D Contour plots of (**A**) Rubidium (Rb) and (**B**) Nickel (Ni) concentrations on October 4, 2011 based on measurements of surface water samples.

Comparing BPWPCP-sourced Rb distributions on October 4, 2011 (**Fig. 5A**) to SHARC-modeled ^{137}Cs dispersion (**Fig. 3 & 4**) shows that SHARC does a good job predicting plume but misses fine-scale focusing . Cesium and Rb both in (Group 1) on the periodic table so they should behave similarly in the environment. **Figure 5B** shows measured BPWPCP-sourced Ni (Group 10) distributions on October 4, 2011. Differences between Ni, Rb, and SHARC-modeled ^{137}Cs distributions are likely due to differences in the reactivity of the metal influenced by variable environmental conditions.

Discussion:

Figure 6. Blue Plains WPCP Plume Dye Study (USGS, Callender et al., 1984).

A BPWPCP Plume Dye Study by USGS (**Fig. 6**; Callender et al., 1984) concluded that plume dynamics are largely controlled by physical and geophysical factors such as bathymetry, morphology, river flow, tidal flow, and wind speed and direction. The SHARC model outputs for ^{137}Cs (**Fig. 3 & 4**) and measured Rb distributions (**Fig. 5A**) support these conclusions. Tidal and river flow, coupled with strong winds from the NW on October 4, 2011 (**Fig. 1**) and the shallow shoal on the eastern side of the Potomac River study area (**Fig. 6**), likely had the strongest influence on modeled and observed plume shape/dispersion.

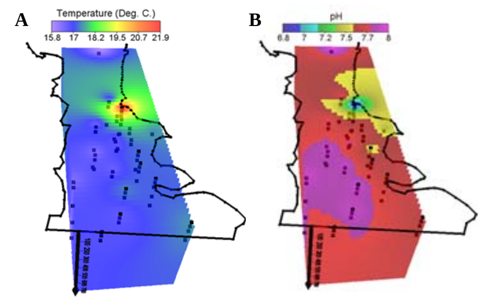

Figure 7. High-resolution, 3-D contour plots of (**A**) Temperature and (B) pH based on data collected with a Hydrolab Quanta on October 4, 2011.

Differences between measured Rb and Ni distributions (**Fig. 5A & B**) and SHARC-modeled ^{137}Cs distributions (**Fig. 3 & 4**) are likely due to spatial variability in environmental factors that can influence the reactivity of different metals. A high degree of fine-scale spatial heterogeneity was observed in temperature and pH (**Fig. 7A & B**) in the BPWPCP Plume. Temperature and pH are "master variables" that determine the partitioning of metals and other reactive constituents in aquatic systems.

Conclusions:

• SHARC does a good job predicting plume the dispersion of reactive constituents such as ^{137}Cs in the tidal-fresh Potomac River study area.
• High-resolution hydrographic and meteorological data will improve SHARC predictions.
• Further research is required to quantify variability in key water column parameters (T and pH) and their impacts on the partitioning and fate of specific reactive constituents.

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