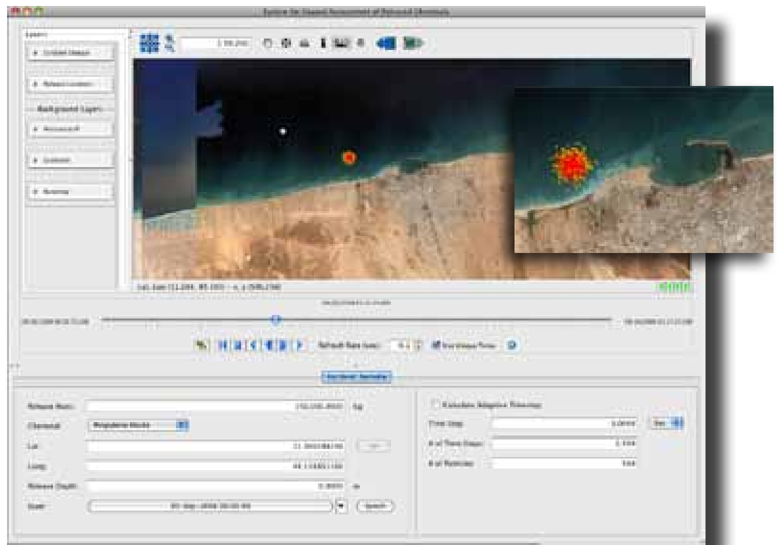
System for Hazard Assessment of Released Chemicals

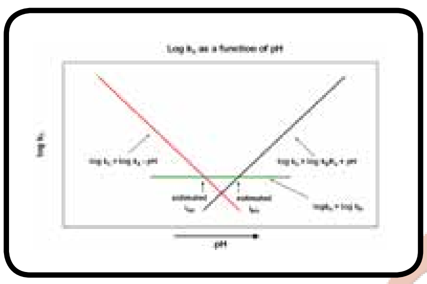
SHARC is a rapid modeling and analysis tool for calculating and visualizing the fate and transport of waterborne chemical releases. SHARC allows the user to quickly create and display chemical release incidents with a single intuitive interface. SHARC's chemical kinetics combine high temporal resolution with chemical-specific algorithms to produce near real-time results for chemical spill tracking. By including degradation product tracking, SHARC extends basic chemical kinetics to provide enhanced accuracy in modeling the overall persistence of released chemicals in both water and sediment matrices.

SHARC Features:

Near-real time chemical kinetics. SHARC's chemical kinetics were developed to provide enhanced waterborne modeling capabilities for Chemical Warfare Agents (CWAs) and Toxic Industrial Chemicals and Toxic Industrial Materials (TIC/TIMs). Designed to utilize time-varying environmental data for chemical spill forecasting, SHARC's kinetic algorithms encompass the impacts that changes in salinity, temperature, pH, alkalinity, and suspended material concentration have on degradation rates and chemical transport. SHARC's fate and transport pathways include dissolution, evaporation, volatilization, hydrolysis, photolysis, biodegradation, sorption, and sediment preservation processes. The rates of these processes are controlled by the physical and chemical environment. By including these properties as dynamic inputs to chemical fate algorithms, SHARC provides model results which have near real-time temporal resolution.



Degradation product tracking. SHARC features degradation product tracking for accurate determination of instantaneous local pH. Hydrolysis, the main degradation pathway for reactive chemicals released into aqueous environments, is strongly affected by variations in temperature, salinity, and pH. SHARC tracks the generation of acidic degradation products from hydrolysis to determine the effective local pH as a function of time. Natural waters have an inherent buffering capacity (alkalinity) which moderates the impact that the addition of acidic materials has on the pH in a non-linear fashion. SHARC contains an acid dissociation model which determines the local pH using dissolution and dispersion to track degradation products. By tracking the concentration and speciation of degradation products, SHARC provides a modeling capability that incorporates both chemical specific and environmental variability on the local chemistry as a chemical release incident evolves. The result is a more accurate tool for assessing the fate and transport of waterborne chemical releases.



Deterministic and stochastic analysis modes. SHARC has both deterministic and stochastic modeling capabilities. Users can select either analysis mode for waterborne chemical fate and transport modeling. Stochastic capabilities employ ranges of empirical observations for salinity, pH, alkalinity, and total inorganic carbon, as well as temporal variability, allowing the SHARC user to visualize probabilistic chemical fate and transport results that encompass both chemical and physical variability.

SHARC was developed as part of a U.S. Defense Threat Reduction Agency (DTRA) Small Business Innovative Research (SBIR) project focused on the development of an advanced waterborne chemical transport modeling capability.

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