

Dynamic Contaminant Identification in Water

Summary:

Locating contaminants in a large water system such as a lake or part of the ocean more quickly would allow faster and more effective emergency response. This paper proposes that Solid State Spectral Imagers (SSSI) attached to stationary buoys and/or mobile rovers capable of identifying chemical samples in the field would allow suspicious or interesting areas to be examined in real time. First the SSSI and its functions are described, then the methods employed for chemical analysis are detailed, followed by a section on the computer interface used for communication to the SSSI.

The SSSI design uses a laser-diode array that spans the spectrum from near-infrared to ultra violet and photodetectors to examine substances up to 10 m away and analyze them for chemicals of interest using a hyperspatial data analysis algorithm. The diodes are first activated using a Walsh-Hadamard encoding sequence. The contribution of each diode is demultiplexed from the resulting reflectance signal detected by the photodetector using an inverse Hadamard transform and then analyzed. If the data indicates that a chemical of interest might be present, the target is scanned using a CRISP encoding that approximates the spectrum of the chemical of interest. If the response is strong, the chemical is present in the target.

The proposed network of sensors will cover estuarine regions where water quality and environmental monitoring is critical. The initial planned test location is the Hudson-Raritan Estuary, which has already been modeled using a 2D Spectral Element Ocean Model. The SSSI's capabilities are used by a DDDAS to monitor the environment around each sensor in real time. If an interesting chemical is found, the simulation runs the appropriate application and requests that the SSSI look for other chemical traces of interest based on the current information obtained by the simulation.

The simulation will use incoming data to update its simulation of contaminant transport in the water body. As its sensors find contaminants, mobile sensors can investigate interesting regions more carefully and provide better information to further inform the simulation. Initial conditions are provided by a combined least squares and Bayesian approach

that gives a high acceptance rate based on sampling the sensor data from the known distribution, producing various realizations of initial data.

Chemical analysis is performed on a collected sample spectrum using the Bootstrap Error-adjusted Single-sample Technique (BEST). Spectra are stored as a point in a hyperspace with as many dimensions as there are wavelengths in the spectra. Chemicals of interest have the spectra recorded ahead of time and stored. Samples with similar spectra produce points in hyperspace that are near known points, indicating they are chemically similar. The computational costs of using the BEST algorithm can be reduced by approximating it using multiple linear regression.

For tracking oil spills, oil droplet size can be determined using light scattering information. Droplet size has a significant impact on its motion in a water body, so this information is important for simulating the transport of detected oil. Oil detection by the SSSI can be improved by placing a filter on the detector that converts it to a laser fluorosensor, allowing it to detect oil more effectively against a variety of background substances.

The current interface to the SSSI is provided by Matlab. The SCIRun-Matlab interface can be used for a specific problem solving application. SCIRun detects if Matlab is available at run-time and if so acts as a virtual shell to Matlab, providing an interface to the user and keeping Matlab running in its internal engine. Communication between Matlab and the user is transparent. SCIRun can thus be used to create a problem specific interface to the existing Matlab code controlling the SSSI.

Application of DDDAS:

The interaction between the simulation of contaminant transport and the SSSI sensor network is a clear application of DDDAS. The simulation reacts to the information that the sensors give it by running applications appropriate to the situation (for example, notifying authorities of the contamination) and instructing the sensors to better investigate the contaminant by looking for particular chemical traces and sending mobile sensors to areas that are currently believed to be future locations of contamination based on the current simulation data. As new information arrives from these sensors, the simulation is updated and the symbiotic cycle repeats.

Ways to Improve DDDAS Application:

The current prototype design for the SSSI's must be reprogrammed over the network to look for a particular chemical using CRISP encoding, as onboard storage does not currently allow enough space to store a large library of chemical information. The addition of more memory and an ability to do more preliminary analysis would reduce the network bandwidth used by the sensors, as they would be able to more effectively report only interesting samples to the simulation. The danger of allowing this is that it is possible that something important will be overlooked if it is deemed unimportant by the SSSI's onboard chemical analysis, which would not be as thorough as the simulation's more powerful computing ability and memory storage capacity.