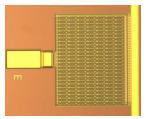
# PRECONCENTRATION, DETECTION, AND IDENTIFICATION OF CWA AND CWA SIMULANTS

SEACOAST SCIENCE, INC
A CHEMICAL SENSOR COMPANY

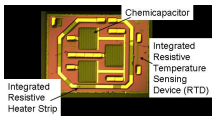
## ABSTRACT


Point detection of Chemical Warfare Agents (CWAs) and Toxic Industrial Chemical (TICs) is crucial for the protection of military personnel and fixed facilities. A preconcentration step is often required to deliver a sufficient quantity of analytes to the sensor surface for detection because of the toxicity of many CWA's and TIC's at low concentration. Seacoast Science reports on the development of a prototype system consisting of a preconcentrator, sensor, and identification algorithm. The sensor technology uses polymer filled micromachined capacitors to measure the dielectric constant of an array of selectively absorbing materials. The interaction between target analyte and polymer modifies the dielectric properties (capacitance) of the polymer. The polymer array consists of polysiloxanes, polycarbosilanes, organic bridged polysilsesquioxanes, and organic polymers. A small preconcentrator system capable of adsorbing target analytes at ambient temperature and desorbing at elevated temperatures allows for the detection of CWA simulants at low ppb levels. CWA simulants can be identified from the array response using selected algorithms to process the data. As a result, a hand-held detector capable of detecting nerve agent and vesicant vapor in the presence of water or hydrocarbons has been completed.

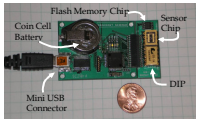

## SENSOR TECHNOLOGY



Micrograph of a Seacoast Science interdigitated electrode sensor element (~500 µm x 350 µm).




Micrograph of a Seacoast Science sensor chip with three chemicapacitors and an integrated heater and temperature sensor (RTD).



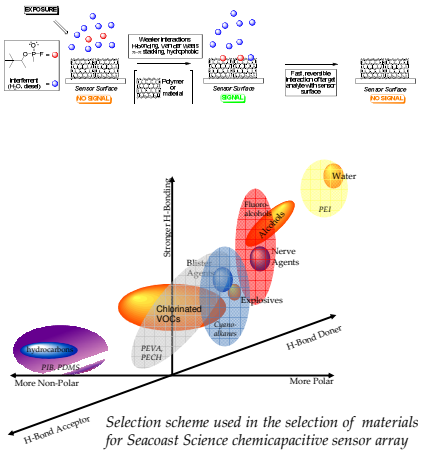

Seacoast Science's SC210 Prototype (6.5 x 4 x 1.5 cm), uses USB for fast real-time data collection directly to a computer or can be remotely located and powered by the coin cell battery for weeks of unattended data logging (stored on flash memory).


Seacoast Science's integrated preconcentration/chemicapacitive MEMS detector system.

- Circuit board controls timing and temperature profiles.
- LabVIEW-based software controls set-points and measures chemicapacitors
- Connects to Computer via USB
- Can be battery operated

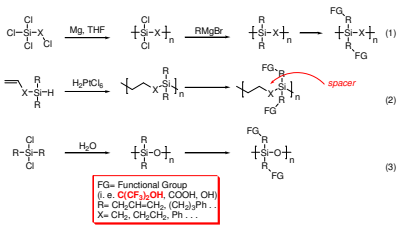
## RESULTS AND DISCUSSION

### Chemicapacitive Sorptive Sensor

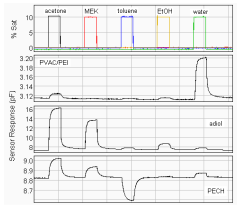



*Selection scheme used in the selection of materials for Seacoast Science chemicapacitive sensor array*

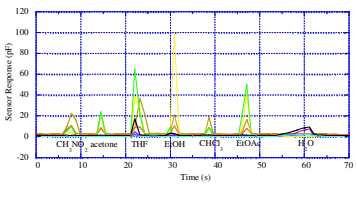
### Material Synthesis



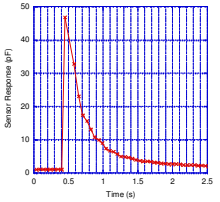

### Sensor Performance




Response of 3 coated sensor elements in Seacoast Science's chemicapacitive array to Acetone, MEK, Toluene, Ethanol, and water.




Seven exposures-detections of common solvents in less then a minute. Each color represents the response of a different material to solvent



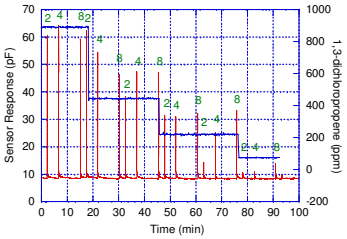

Sensor response to monomethyl hydrazine. Full scale sensor response in ~50 ms, recovery in ~1s.

### CWA and CWA Simulant Detection Limits

| CWA (2003) | LOD (ppm) | LOD (mg/m³) | $LCt_{50}$ (mg•min /m³) |
|---|---|---|---|
| AC | 0.07 | 0.08 | 2500 - 5000 |
| HD | 1.0 | 6.3 | 1500 |
| GA | 0.06 | 0.05 | 400 |
| GB | 0.008 | 0.5 | 100 |
| GD | 0.006 | 0.05 | 50 |

| CWA Simulants | LOD (ppm) | LOD (mg/m³) |
|---|---|---|
| CEES | 2.0 | 5.1 |
| MeS | 0.1 | 0.025 |
| DMMP | 0.001 | 0.004 |
| DIMP | 0.0005 | 0.005 |
| DFP | 0.0005 | 0.004 |

### Preconcentration



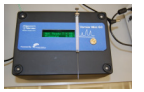

2, 4 and 8 minute collections of *E*/*Z*-1,3-dichloropropene (1,3-DCP) at 900, 450, 225 and 70 ppm. The effective sensitivity of the system increased 30x

### Interferrents

| Analyte | LOD (ppm) | Precon LOD (ppm) | Increase |
|---|---|---|---|
| $CH_2Cl_2$ | 7.8 | 1.6 | 4.9 |
| 1,3-DCP | 14 | 0.5 | 30 |
| MeOH | 15 | 0.06 | 250 |
| EtOH | 10 | 0.05 | 200 |
| $PhCH_3$ | 26 | 1.1 | 24.5 |
| *n*Butyl acetate | 1.1 | 0.005 | 210 |
| Cyclo hexanone | 0.10 | 0.007 | 15 |
| 3-pentanone | 1.4 | 0.003 | 466 |
| 2-heptanone | 0.03 | 0.007 | 4.3 |
| $CH_3NCS$ | 3.6 | 0.4 | 8.5 |

| Analyte | LOD (ppm) | Analyte | LOD (ppm) |
|---|---|---|---|
| $CH_2Cl_2$ | 7.8 | α-pinene | 11 |
| TCE | 22.1 | MeOH | 14 |
| THF | 3 | EtOH | 5 |
| $Et_2O$ | 34.5 | *i*-PrOH | 8.9 |
| DMF | 0.03 | *n*-BuOH | 0.9 |
| NMP | 0.004 | formaldehdye | 1.0 |
| benzene | 2.1 | heptanal | 0.4 |
| toluene | 6.5 | acrolein | 11 |
| xylene | 2.8 | acetone | 1.5 |
| naphthalene | 0.15 | MEK | 1.9 |
| hexadecane | 0.04 | methyl isothiocyante | 3.6 |

## PRODUCTS

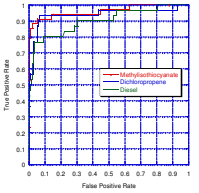


Seaport II Mini-GC with direct injection sampling

SC-BDG Badge Detector (7 x 4 x 0.5 cm, 50 g , coin battery)

Seaport Mini-GC: with integrated computer. Sample introduction by air sampling or direct injection.

### Analyte Identification




| A | B | C | None | Class |
|---|---|---|---|---|
| 21 | 0 | 0 | 9 | A |
| 0 | 27 | 0 | 7 | B |
| 0 | 0 | 23 | 7 | C |
| 6 | 1 | 6 | 89 | None |

Ada boost.m1 (logistic model tree) Confusion Matrix. κ = 0.71

Receiver Operator Curve for Diesel (A), Methylisothiocyanate (B) and 1,3-(*E*/*Z*) Dichloropropene. ROC areas of diesel, methyl isothiocyanate, and dichloropropene are 0.90, 0.86 and 0.94.

### References


Patel, S. V.; Hobson, S. T.; Sabina Cemalovic, S.; Mlsna, T. E. Detection of methyl salicylate using polymer-filled chemicapacitors." *Talanta*, **2008**, *76*, 872–877.

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