



PRECONCENTRATION, DETECTION, AND IDENTIFICATION OF CWA AND CWA SIMULANTS



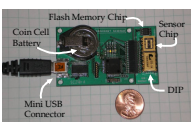
ABSTRACT

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 adsorbing 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 polysilsequioxanes, 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).



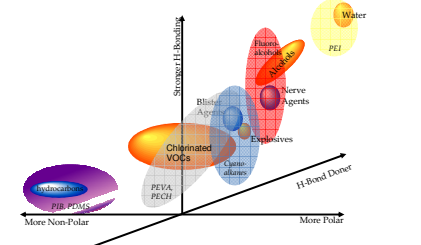
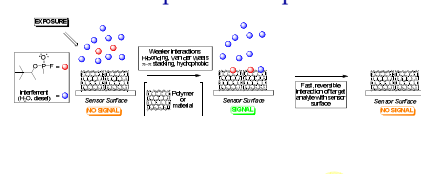
Seacoast Science's SC210 Prototype (6.5 x 4 x 1.5 cm), uses USB for fast real-time data collection directly to a computer or can be remotely located and powered by the coin cell battery for weeks of unattended data logging (stored on flash memory).

Seacoast Science's integrated preconcentration/chemicapacitive MEMS detector system.
• Circuit board controls timing and temperature profiles.
• Lab-VIEW-based software controls set-points and measures chemicapacitors
• Connects to Computer via USB
• Can be battery operated



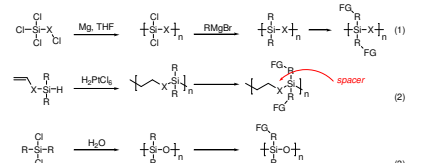
RESULTS AND DISCUSSION

Chemicapacitive Sorptive Sensor



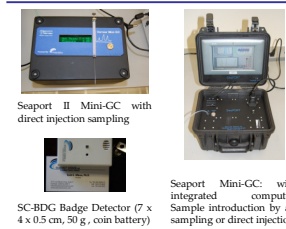
Selection scheme used in the selection of materials for Seacoast Science chemicapacitive sensor array

Material Synthesis



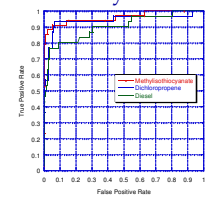
FG: Functional Group
 β: = C(CF₃)₂OH, COOH, OH
 R: CH₂CH₂CH₂, (CH₂)₃Ph...
 X: CH₃, CH₂CH₂, Ph...

PRODUCTS



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

Analyte Identification



A	B	C	Name	Class
1	1	1	None	B
2	2	2	B	B
3	3	3	None	B
4	4	4	None	B
5	5	5	None	B

Ada boost.m (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.

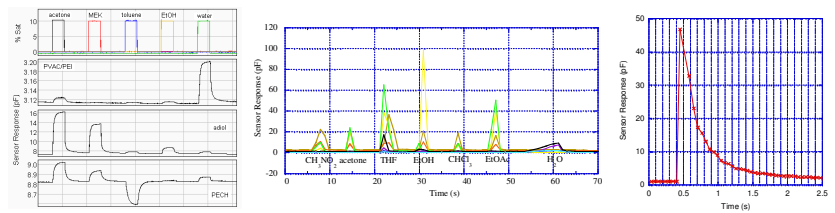
References

Patel, S. V.; Hobson, S. T.; Sabina Cemalovic, S.; Misna, T. E. Detection of methyl salicylate using polymer-filled chemicapacitors. *Talanta*, 2008, 76, 872-877.
 Misna, T. E.; Cemalovic, S.; Warburton, M.; Hobson, S. T.; Misna, D. A.; Patel, S. V. Chemicapacitive Microsensors for Chemical Warfare Agent and Toxic Industrial Chemical Detection. *Sensors and Actuators B: Chemical*, 2006, 116, 192-201.
 Patel, S. V.; Misna, T. E.; Frubberger, B.; Klassen, E.; Cemalovic, S.; Baselt, D. R. Chemicapacitive microsensors for volatile organic compound detection. *Sensors and Actuators B: Chemical*, 2003, 96 541-553.

Acknowledgements

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Sensor Performance



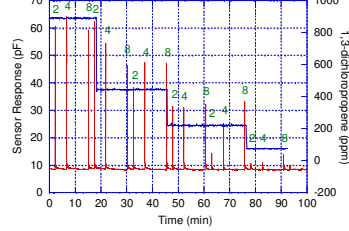
Response of 3 coated sensor elements in Seacoast Science's chemicapacitive array to Acetone, MEK, Toluene, Ethanol, and water.
 Seven exposures-detections of common solvents in less than a minute. Each color represents the response of a different material to solvent.
 Sensor response to monomethyl hydrazine. Full scale sensor response in ~50 ms, recovery in ~1s.

CWA and CWA Simulant Detection Limits

CWA (2003)	LOD (ppm)	LOD (mg/m ³)	LC ₅₀ (mg*min/m ³)
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/m ³)
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

Interferents

Analyte	LOD (ppm)	Precon LOD (ppm)	Increase
CH ₂ Cl 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
nButyl 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 ₃ NCS	3.6	0.4	8.5

Analyte	LOD (ppm)	Analyte	LOD (ppm)
CH ₂ Cl ₂	7.8	α-pinene	11
TCE	22.1	MeOH	14
THF	3	EtOH	5
Et ₂ O	34.5	i-PrOH	8.9
DMF	0.03	n-BuOH	0.9
NMP	0.004	formaldehyde	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 isothiocyanate	3.6