RB.1 Multisensors Sensing Platforms: Detecting low concentrations of Chemical and Biological Threats (CBTs) Using Quantum Cascade Laser Spectroscopy (QCLS)

Soft Target Engineering to Neutralize the Threat Reality

Jorge Plata, *Priscilla Soler, Tatiana Serrano, Elvin Lebron PIs: Samuel P. Hernández-Rivera & José Centeno UPR-MAYAGUEZ*
jorge.plata@upr.edu, priscilla.soler@upr.edu, tatiana.serrano1@upr.edu, elvin.lebron1@upr.edu, samuel.hernandez3@upr.edu, jacenteno@comcast.net

SENTRY Challenge

Chemical and Biological Threats (CBTs) are dangerous to public health and safety. Threats can be intentional, as in the case of bioterrorism or chemical warfare agents, or unintentional, such as accidental releases. To prevent future attacks, early detection, and identification are crucial.

In this work, mid-infrared (MIR laser spectroscopy based on quantum cascade lasers (QCL) is being used to detect CBTs. The spectrometer will be mounted on an unmanned vehicle (UV) as a safe solution for remote detection.

Intentional or unintentional Chemical and Biological threats (CBTs) are dangerous to public health and safety. Detection is crucial to prevent future attacks. The possibility of detecting with a QCL spectrometer with different optical setups is studied.

Principal Component Analysis (PCA) models were developed with different preprocessing methods to determine the model that best discriminates CBTs. Results show that the Savitzky-Golay Second Derivative (SG2) + Standard Normal Variate (SNV) PCA model had the best separation between CBTs.

Accomplishments

The following analytes are examples of some of the CBTs that were analyzed using QCL spectrometers.

Spectra will be used to discriminate between the CBTs.

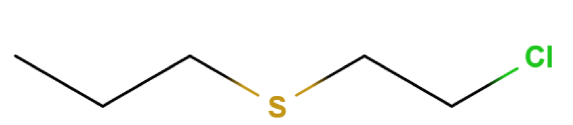


Figure 1. 2-chloroethyl ethyl sulfide (2CEES)

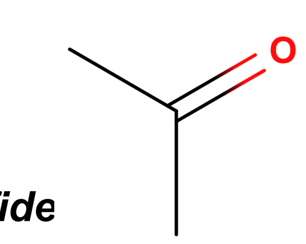


Figure 2. Acetone (ACET)

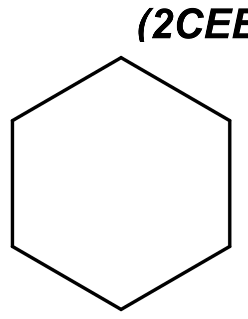


Figure 3. Cyclohexane (CYC)

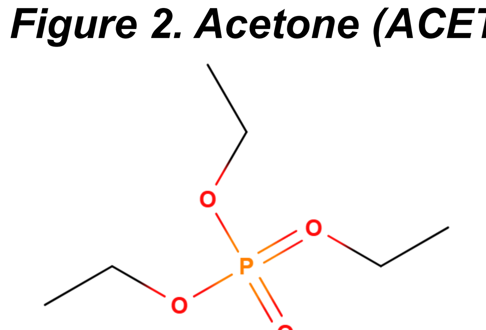


Figure 4. Triethyl phosphate (TEP)

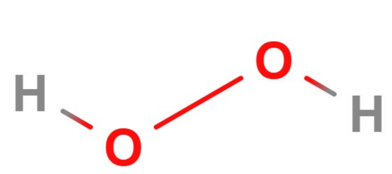


Figure 5. Hydrogen Peroxide (H_2O_2)

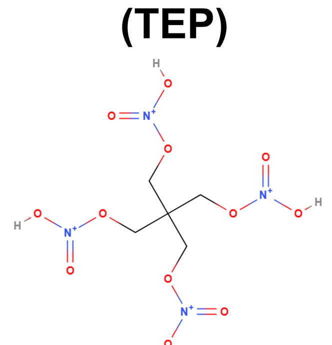


Figure 6. Pentaerythritol (PETN)

Addressing the Challenge

Spectra of CBTs simulants were acquired using QCL spectrometers. The objective was to characterize the vibrational spectroscopy markers (vib. bands) in the fingerprint region of the MIR. Several optical setups were used trying to reach low amounts (detection limits, DL) by depositing 12 μL on sample slides. The low concentrations of the CBTs used are in the range (5 μg/cm^2 to 500 μg/cm^2). This way we can train our Artificial Intelligence (AI) and Machine Learning (ML) models to detect CBTs and send warnings as soon as a CBT is within reach.

A polycarbonate box was designed to perform tests in controlled environments. This box has all the needed accessories to generate aerosols and vapors, and to control temperature (T), pressure (P), and Relative Humidity (RH). Maximum length that spectra is being acquire is 10m due to laboratory space. After acquiring spectra, CBTs were discriminated by developing PCA models. PCA scores show that each CBT contains its cluster. The distance between clusters was quantified to determine the data preprocessing (DP) method that best discriminates the CBTs.

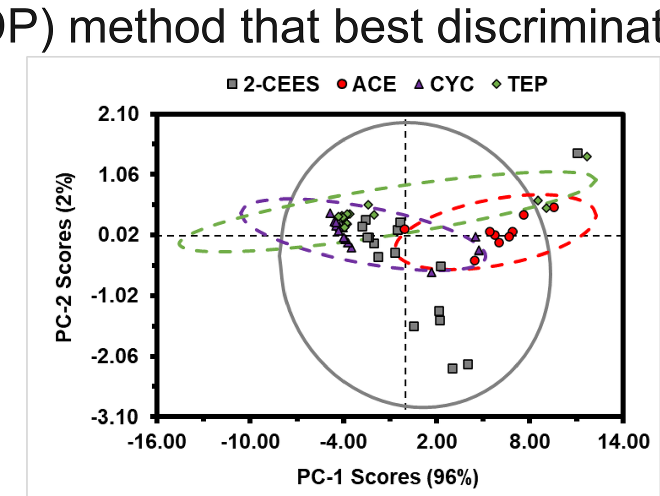


Figure 7. RAW PCA scores of QCL spectra for 2-CEES, ACE, CYC, and TEP

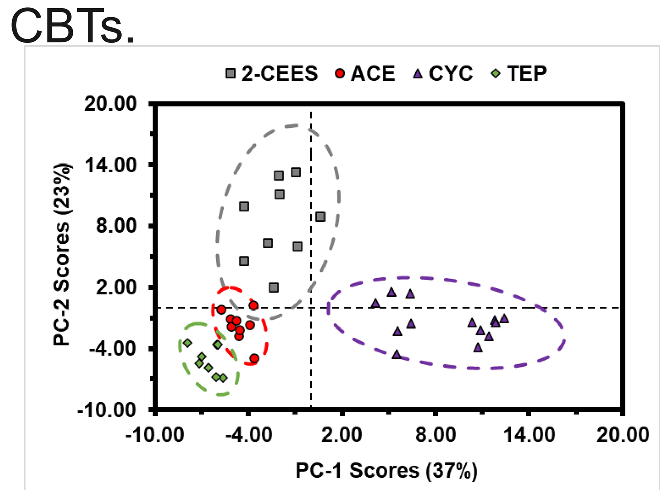


Figure 8. SG2+SNV PCA scores of QCL spectra for 2-CEES, ACE, CYC, and TEP

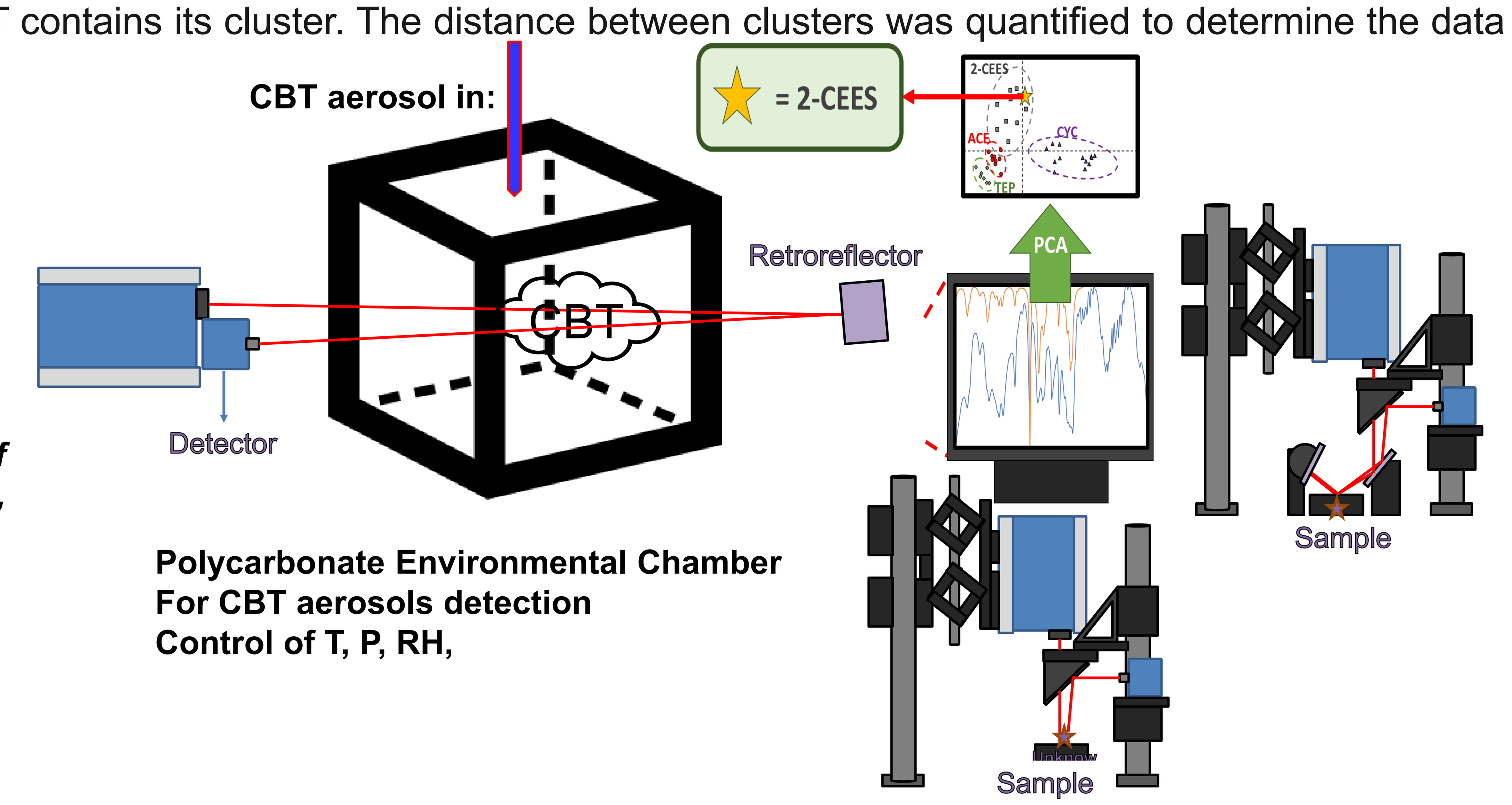
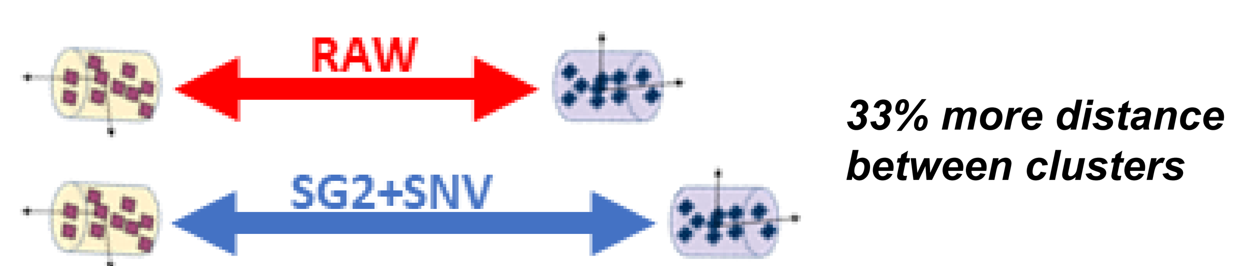


Figure 9. Example of some of the optical setups used to acquire spectra

CBTs were discriminated by developing PCA models that explain their spectral variation when using QCL-Grazing Angle (GA). PCA scores show that each CBT contains its cluster. Quantifying the distances between the clusters shows that SG2+SNV is the best DP method for discriminating CBTs. Figure 11 shows each cluster for the SG2+SNV model with their own 95% confidence ellipse having better discrimination in contrast to the RAW model in Figure 10. These results show that discrimination between CBTs is possible with QCL-GA.

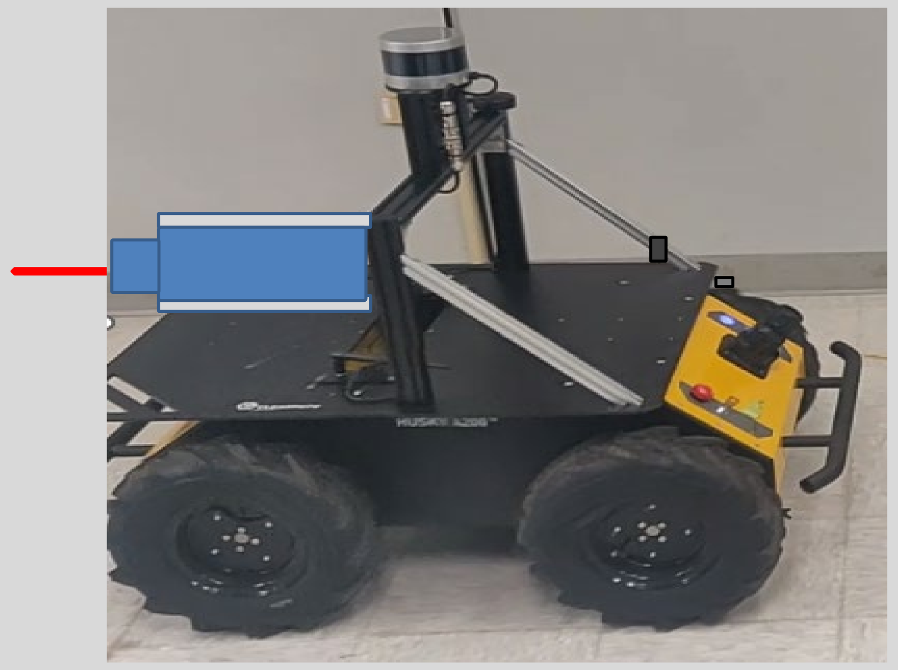


These QCLs have external detectors (Mercury-Cadmium-Telluride, MCT) that allow the versality of the optical setups, but even the QCLs that use an internal detector can be used to take long range measurements. There are commercial, tunable QCL-based spectrometers that can be used to monitor: detect, identify, and quantify gas phase CBTs at distances of > 300-500 m. What we can do is work to train these instruments using Artificial Intelligence (AI) and Machine Learning (ML) in various environments. These sensors promise to be of great interest to government entities such as EPA, DA-NIFA, TSA, CBP, DARPA, IARPA, and others. Private companies & security vendors are also potential partners to transition.

Next Steps

Ground Vehicle for Autonomous Sensing

Clearath Robotics Husky-A200™ Rover
Incorporated Garmin GPS and LiDAR 3D Velodyne Puck
for future autonomous operation



Aerial Vehicle for Autonomous Sensing

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