Standoff detection of chemical and biological threats using miniature widely tunable QCLs

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ABSTRACT

Standoff detection and identification of chemical threats has been the "holy grail" of detection instruments. The advantages of such capability are well understood, since it allows detection of the chemical threats without contact, eliminating possible operator and equipment contamination and the need for subsequent decontamination of both. In the case of explosives detection, standoff detection might enable detection of the threat at safe distances outside the blast zone. A natural extension of this capability would be to also detect and identify biological threats in a standoff mode and there are ongoing efforts to demonstrate such capability.

Keywords: Chemical detection, standoff detection, biological threats, chemical threats

1. INTRODUCTION

In response to this strong need for standoff detection, Block MEMS, LLC ("Block") has developed such products for decades and today some of its standoff chemical detection systems are protecting our nation's critical infrastructure, such as the Pentagon. Recently, a critical technology that has enabled even more standoff applications has been introduced that is based on a new class of lasers, the Quantum Cascade Laser (QCL), which significantly extends the capability of well-known and proven Mid-Infrared Spectroscopy. Block is the leading company in using QCL-based mid-infrared spectroscopy for standoff detection applications and has demonstrated this capability through several new product offerings [Ref. 1, 2]. These applications were enabled by several key technical accomplishments, as described below.

2. TUNABLE QUANTUM CASCADE LASER (QCL) MODULE

One of the key Block capabilities in this area is the development of a miniaturized QCL module, the **Mini-QCL™ Module**, that is used as the "engine" inside all Block's QCL-based products. Such system architecture provides excellent flexibility, because it allows the product development team at Block to tailor the product to each application and match the specific application requirements with minimized effort and short development cycles. Figure 1 shows the Mini-QCL as compared to a US quarter coin. Inside the module, Block has used an External Cavity tuning configuration

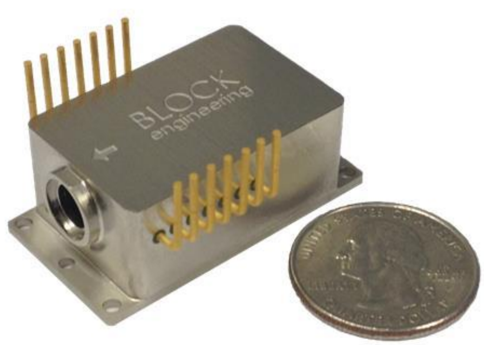

Figure 1. Block's Mini-QCL™ Module, based on an External Cavity Configuration.

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to tune across the Mid-Infrared Spectrum. The module presents several key features that have enabled the development of critical applications as described later in this paper. Table 1 summarizes the performance specifications of the Mini-QCL. However, there are some key features, which make this module a unique and world-leading product. First, each module covers a wide spectral range essentially anywhere in the 5.2-13 µm range of the mid-infrared spectrum. The range for each module typically exceeds 250 cm^{-1} and several user-selectable options are available from Block. Block's standoff products are designed to accommodate up to four such modules, so the users can easily match with their

Table 1. Mini-QCL™ Module Performance Specifications.

Mini-QCL™ MODULE PERFORMANCE SPECIFICATIONS

- Ultra-compact: approximately 1 cubic inch in size; weight 75 grams
- Industry-leading wide tuning range of over 1100 cm^{-1} (with multiple combined modules)
- Can be configured in specific spectral ranges of >250 cm^{-1}
- Eye-safe laser poses no personnel or combustion risk in industrial settings
- Tuning speed 25 cm^{-1}/msec
- Pulse lengths from ~30 to 300 nsec
- Repetition rate up to ~3 MHz
- 2 x 4 mm collimated, vertically polarized beam
- 2 cm^{-1} spectral linewidth typical
- Average Power of 0.5 – 15 mW over 95% of 1100 cm^{-1}
- Pulse Stability: < 5 % pulse to pulse typical
- Power Variation: < 0.05% over 10msec @ 1MHz
- <1 mrad pointing stability

application requirements. At the maximum system level of four modules, a range exceeding 1100 cm^{-1} is offered, enabling detection of most chemicals in the "fingerprint" region of the mid-infrared spectrum, i.e. 5.2-13 µm. Such capability is important when detection systems are needed that can be easily reconfigurable to detect changing lists of chemical and biological threats by simply upgrading the built-in libraries of these systems without changing any of the hardware. Second, the modules offer the fastest tuning speed in the world today for the achieved very wide spectral range, covering the designated spectral range in milliseconds. For example, if a 1000 cm^{-1} range is selected, then the QCLs tune across this range in about 40 msecs or at a speed of 25 cm^{-1}/msec. Such rapid scanning capability enables the acquisition of spectra at that rate and it is very critical when handheld applications of standoff detection are needed. In these cases, typical hand-shake could smear the measurements, but this ultra-rapid tuning essentially "freezes" in time the target-to-detector relative location and provides reliable measurements. Third, the QCL beam has excellent pointing stability (<1 mrad), which is critical for applications that involve long standoff distances. In addition, this capability applies across the complete spectral range, which is typically difficult to achieve due to the very wide range of wavelengths (5.2-13 µm) that the Block systems cover. Fourth, the Mini-QCL is packaged in a sealed miniaturized enclosure with built-in thermoelectric coolers (TECs), which provides a highly reliable, rugged and stable system. Well-known manufacturing and packaging techniques, which have been developed over the past 15 years for tough telecommunications applications, have also been used for these modules at Block's manufacturing facilities. Finally, it is quite important to point out that the Mini-QCL modules are driven by very compact, fast, custom designed and built electronics, which offer flexible options and alternatives to the end-users or OEM customers. The electronics have been designed in a modular architecture and the users can select the board or combination of boards that match their specific applications. This design philosophy has allowed Block to use the same boards, not only for all its end-user products, but its OEM configurations as well. Software Development Kits (SDKs) are typically provided to the OEM customers, so that they can develop their own interfaces and system controls.

3. STANDOFF APPLICATIONS

Mid-Infrared Spectroscopy is the fundamental technology that is being used in all the proposed applications. It is a technology that has been applied for more than a hundred years to analyze substances and it has been very-well understood and documented. Well-known instruments, such as Fourier Transform Infrared (FTIR) Analyzers, or Non-Dispersive Infrared (NDIR) sensors, have been used for many decades for detection and identification of chemical and biological threats. However, essentially all these instruments require physical sampling of the target, hence “standoff detection” is practically impossible. The commercialization and maturity of today’s QCLs have removed this limitation and have now opened numerous applications previously not possible for both government/military, as well as commercial markets.

Block has worked under several government contracts for applications such as standoff detection of Chemical Warfare Agents (CWAs), standoff detection of Trace and Bulk Explosives and detection of disturbed earth for dismounted soldiers for buried IEDs. Commercial markets of Block’s QCL products are also vast and current customers include many Fortune 100 companies with applications such as detection of hydrocarbons and other gases in Oil & Gas, detection of residual surface contaminants prior to paint application in manufacturing, on-line, real-time analysis of coatings of medical devices and high-resolution, high-speed, infrared chemical 2D imaging for forensics, industrial quality control and medical research.

3.1. Standoff Detection of Surface Biological Threats

One of Block’s products, the LaserScan™ Analyzer, which utilizes multiple Mini-QCL™ Modules inside, was used by the University of Puerto Rico [Ref. 3], a DHS Center of Excellence, to detect and identify a variety of simulant bacteria on multiple substrates, such as luggage, stainless steel, wood, etc. Figure 2 shows the results of these measurements. Chemometric algorithms, such as Principal Components Analysis (PCA) and Partial Least Squares Discriminant

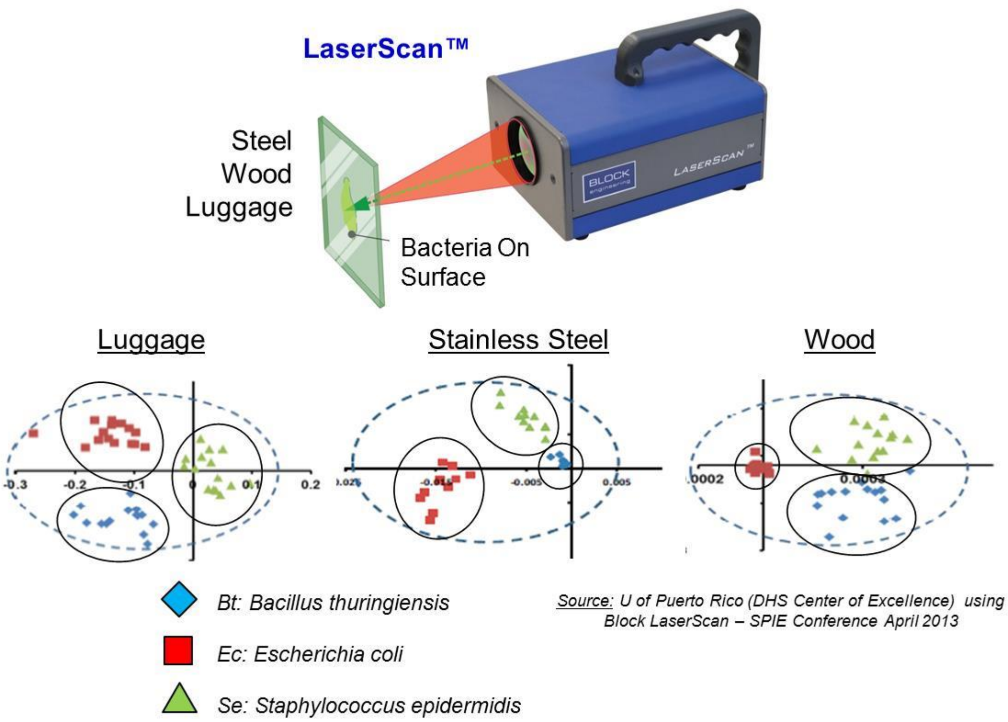

Figure 2. Standoff Detection and identification of simulant bacteria (*Bt, Ec, Se*), using the QCL-based LaserScan Analyzer. [3]

Analysis (PLS-DA), were used to extract and amplify the differences in the infrared spectra collected by the LaserScan and, after applying certain thresholds for detection, good separation was demonstrated, as shown in the figure. It is also important to point out that these measurements and detection can be carried out in real-time, since Block’s QCL systems provide complete infrared spectra in milliseconds, hence a final decision for detection and identification can be reached in a few seconds. Therefore, the key message from these results is that the QCL-based systems are able to detect the chemical differences between the various bacteria and provide good discrimination. Furthermore, the availability of miniaturized QCLs, is now allowing for these measurement to be conducted in real-time, in the field with handheld, lightweight devices, similar to the LaserScan used for these tests.

3.2. Standoff Detection of Surface Chemical Threats

Block has also applied its QCL-based standoff detectors to the detection of many surface chemical threats, including CWAs, explosives and simulants. Figure 3 shows selected results of tests conducted by Block for the detection of Methyl Salicylate (MeS), a CWAs simulant, and RDX, a military-grade explosive. Typical standoff distances for the LaserScan devices range between 6-12 inches, but longer distances can also be achieved with larger collection optics.

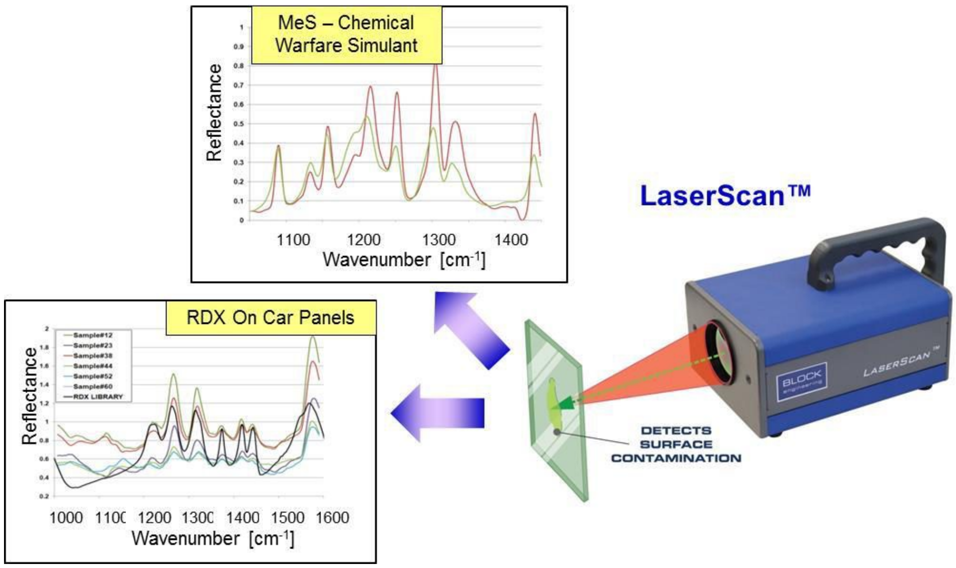

Figure 3. Standoff detection and identification of MeS and RDX, using the QCL-based LaserScan Analyzer.

The feature-rich spectra shown in Figure 3 indicate that the detection of such substances can be accomplished and low levels of detection can be achieved. It is important to point out that in these standoff measurements, complex interactions between the contaminant and the substrate can be observed, when trace amounts are to be detected. The following section describes these challenges in more detail.

3.3. Technical Challenges for Standoff Detection of Surface Threats

The detection of surface threats involves contaminants in droplet, film or solid forms. Depending on the amounts targeted, the surface contaminants could be in trace or bulk concentrations, creating layers potentially as thin as 1 µm or as thick as several mm. In the case of solids, the contaminants might be isolated particles scattered on a relatively large surface. In the case of thin layers or films of contaminants on surfaces the challenge is related to the fact that the spectrum reflected back into the detector contains spectral features that involve both the film and the substrate. Therefore the collected spectrum from the chemical in the film appears “distorted” or “mixed” and it does not typically match its absorption spectrum in the libraries, because it also contains spectral features of the substrate as well as refractive signatures from the various layer interfaces. The information for the trace deposits can be extracted from the mixed spectrum by applying Kramers-Kronig (KK) transforms. Block has developed sophisticated optical models that predict the shapes of the mixed signals and has developed custom algorithms, using Wavelets Transforms, Matched Filters, and other techniques that separate the effects and detect the trace deposits. As an example of the complexity of surface reflection spectra, Figure 4 shows the results of a simulation using the Block Models for thin films on surfaces. Polymethylmethacylate (PMMA) was used as the simulant contaminant substance and glass was the selected substrate for this modeling simulation. The spectrum transitions from no deposit on the bare substrate (glass) spectrum (black line) to the thick target spectrum (shown at 250 µm – blue line), which resembles the spectrum of pure PMMA, as the thickness of the film grows. During this shape transition, the spectrum appears “distorted” and different from the pure PMMA, requiring “correction”, using the Block Models, in order to utilize standard libraries.

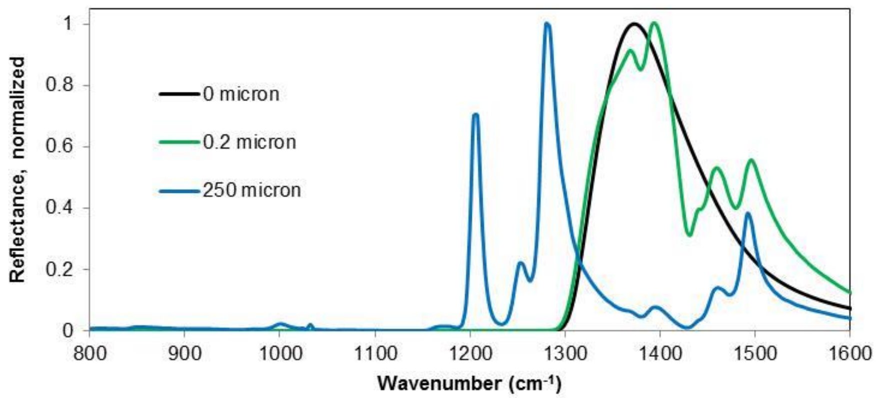

Figure 4. Simulated reflectance of a Polymethylmethacylate (PMMA) film on glass with increasing film thickness.

3.4. Standoff Protection of Critical Facilities against Chemical Attacks - LaserWarn™ Detector:

Chemical Warfare Agents (CWAs) and Toxic Industrial Chemicals (TICs) have been identified as potential threats to critical state and government facilities in the US. The potential release of “chemical or toxic clouds” over these facilities could result in numerous casualties among our forces, civilians and other personnel. Furthermore, the recent violation of international laws against the use of CWAs in Syria has amplified the potential for such threats at the hands of our enemies. Control and State Emergency Centers, State Agencies Buildings, Transportation Terminals, Embassies, Forward Operating Bases (FOBs), Intelligence Facilities and other critical infrastructure are good examples of installations that need to be protected, as shown in Fig. 1. A **Persistent Surveillance** capability is needed to continuously scan the surroundings of a facility and provide real-time, 24/7, “early warning” of threats.

Block is offering a QCL-based capability, the **LaserWarn™ Detector**, for this application. The system is shown in Figure 5 and it utilizes an “engine” set of miniaturized Mini-QCLs, covering most of the atmospheric transmission window over 7-13 µm. Eye-safe QCLs are used and they can be transmitted to several kilometers, covering very large areas, such as stadiums or airport terminals. Built-in libraries are used to compare the measured spectra with the ones in the libraries, in order to provide real-time detection and identification of the chemical threat.

Figure 5. LaserWarn™ Detector for protection of critical, indoors and outdoors facilities

An example of how such as system can be used is shown in Figure 6, where a simulated release into a facility is shown. Using a set of low-cost mirrors and retroreflectors, the LaserWarn establishes an invisible, eye-safe mesh of laser beams. If the chemical cloud crosses any part of the laser mesh, instantaneous detection is made and security protocols are initiated to protect the people in the facility. This is essentially a "chemical tripwire" that gets tripped when the chemical crosses it. The LaserWarn has no consumables at all and can be operated unattended on a continuous, 24/7 mode.

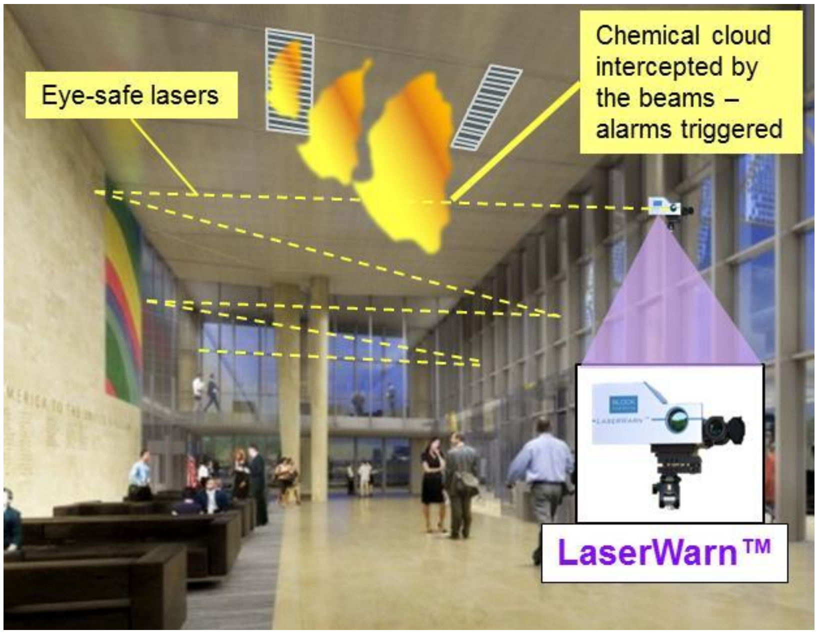

Figure 6. LaserWarn™ capability for 24/7 protection of critical facility against chemical attacks.

A typical installation of LaserWarn starts with a Threat Assessment Phase, which determines the pattern of the laser mesh, and then Block's engineers design an optimal layout of mirrors and retroreflectors for the final installation. The limit of detection of the LaserWarn system depends on the length of the chemical cloud. It is estimated that for a typical Table 2 presents an estimated Limit of Detection in parts-per-billion (ppb) of some of the common chemical threats, assuming a path of 50 m.

Table 2. Projected LaserWarn™ Limits of Detection for common chemical threats.

Agent Name and Type	Chemical Formula	Projected Limit of Detection with 50 m Path (ppb)
Tabun (Nerve)	GA	26
Sarin (Nerve)	GB	26
Soman (Nerve)	GD	26
Cyclosarin (Nerve)	GF	26
VX (Nerve)	VX	26
Mustard (Blister)	HD	157
Nitrogen Mustard (Blister)	HN_3	39
Lewisite (Blister)	L	174
Hydrogen Cyanide (Blood/TIC)	AC	2676
Cyanogen Chloride (Blood/TIC)	CK	5435
Phosgene (Blood/TIC)	CG	67
Hydrogen Sulfide (TIC)	H_2S	37267
Nitric Acid (TIC)	HNO_3	153
Ammonia (TIC)	NH_3	84
Sulfur Dioxide (TIC)	SO_2	2372
Chlorine (TIC) – as HCLO	HCLO	261

3.5. Standoff detection of Disturbed Earth using QCLs – LaserScan-DE

Block has also developed handheld systems, the LaserScan™-DE, for detection of disturbed earth, which might be an indication of a buried Improvised Explosive Device (IED). Dismounted (foot) soldiers can typically be the users of these devices, which can eliminate the subjective "visual" clues of a disturbed earth and operate day or night. Block has completed several field tests under government contracts and is currently implementing sophisticated algorithms for the analysis of the data. The results can be available to government agencies under the proper restrictions and controls.

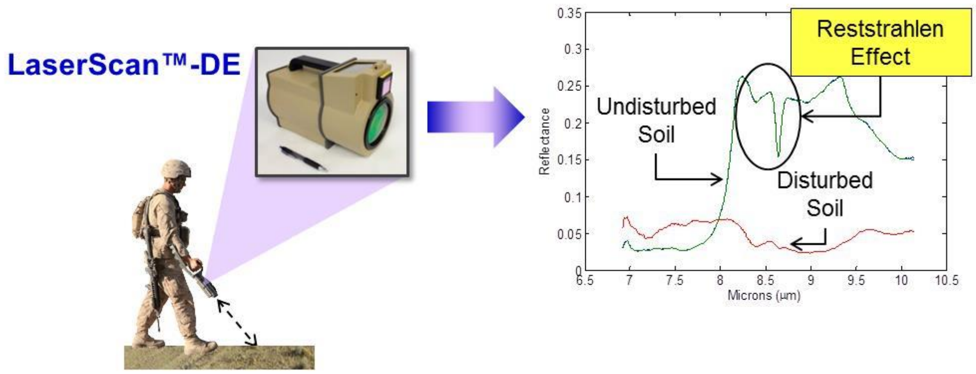

Figure 7. Real-time, standoff detection of Disturbed Earth for dismounted soldiers.

4. SUMMARY AND CONCLUSIONS

Standoff detection of chemical and biological threats has been demonstrated using the new class of QCLs, which offer wide tuning range and ultra-rapid scanning speed. The miniaturization of these QCLs by Block has also enabled the development of handheld, portable devices that can be used for field measurements, as well as fixed installations, in which case, more compact instruments can be used. Both surface and open air threats have been detected and a vast number of new applications for chemical and biological security are being evaluated.

5. REFERENCES

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