Multipath Extinction Detector for Chemical Sensing

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ABSTRACT

A novel multi-path extinction detector (M-PED) is being developed for point detection, identification and quantification of vapor phase chemicals. M-PED functions by pairing a broadband long-wave infrared (LWIR) quantum cascade laser with a novel sample cell, designed to simultaneously measure chemical absorption at multiple pathlengths and wavelengths. The pathlength samples are angularly separated in one dimension, such that a diffraction grating can be used to measure wavelength data in the orthogonal dimension using a compact, low-cost microbolometer array. The resulting data matrix is fit to Beer's Law in two dimensions to accurately quantify chemical concentration while rejecting common mode noise (e.g. laser amplitude noise). The design, characterization and a capability demonstration of the advanced prototype sensor are presented.

Keywords: chemical sensing, point detector, extinction, multipath

1. INTRODUCTION

Field-deployed point chemical detection systems typically employ ion mobility spectroscopy (IMS), gas chromatograph/mass spectrometry (GC/MS) or surface acoustic wave (SAW) architectures [1]. A common attribute of these designs is that they are closed systems, leveraging volumetric sampling of the ambient air via an inlet. These inlet lines are vulnerable to clogging or fouling, which their closed design makes difficult to diagnose. IMS systems have difficulty clearing after exposure to a high concentration [2]. SAW systems can detect, but cannot quantify the sample concentration, making the impact of a chemical detection more difficult to discern [1]. Finally, portable GC/MS systems cost over $100,000 and weight upwards of 30-40 lbs [1,3]. These shortcomings of prior art sensors limit their utility for wide spread deployment in threat detection and clearing missions, as well as for personal exposure monitoring. This motivated the development of a low-cost, portable, open-path optical sensor for the sensitive, quantitative detection of vapor-phase chemicals discussed in the remainder of this paper.

2. SYSTEM DESIGN

2.1 Design Overview

The multi-path extinction detector (M-PED) design was developed for the detection, identification, and quantification of chemical warfare agents (CWAs) and toxic industrial chemicals (TICs). Initial design efforts have targeted detection of vapor phase chemicals, with current efforts exploring expansion to aerosols. M-PED simultaneously captures snapshot extinction spectra of multiple pathlengths ranging from 8 cm to 4 m on a 14-bit microbolometer, thereby achieving five decades of dynamic range. The key facets of this design, shown in the gamma prototype (Figure 1), are:

- A broadband quantum cascade laser (QCL) providing continuous and sufficient spectral power density (>25 μW/cm $^{-1}$) across the relevant spectral range for CWAs and TICs;
- A multipass, fan-driven, open-to-air sample cell providing folded pathlengths up to 4 m in a compact volume (<150 cm^3);
- A partially transmissive sample cell exit window providing angularly separated feedback on sample extinction at select pathlengths;
- A reflective grating dispersing spectra for each sampled pathlength along the orthogonal spatial axis;

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- A low cost, 2D uncooled microbolometer to simultaneously record data along spectral/spatial dimensions at 60 Hz;
- Image processing algorithms to parse each frame into a matrix with pathlength samples along one dimension and corresponding spectral samples along the other dimension;
- A log-linear fit algorithm to calculate sample extinction using all pathlength samples within the linear range of the detection electronics at each wavelength of interest; and
- A spectral processing algorithm to identify and quantify chemical threats using those spectra.

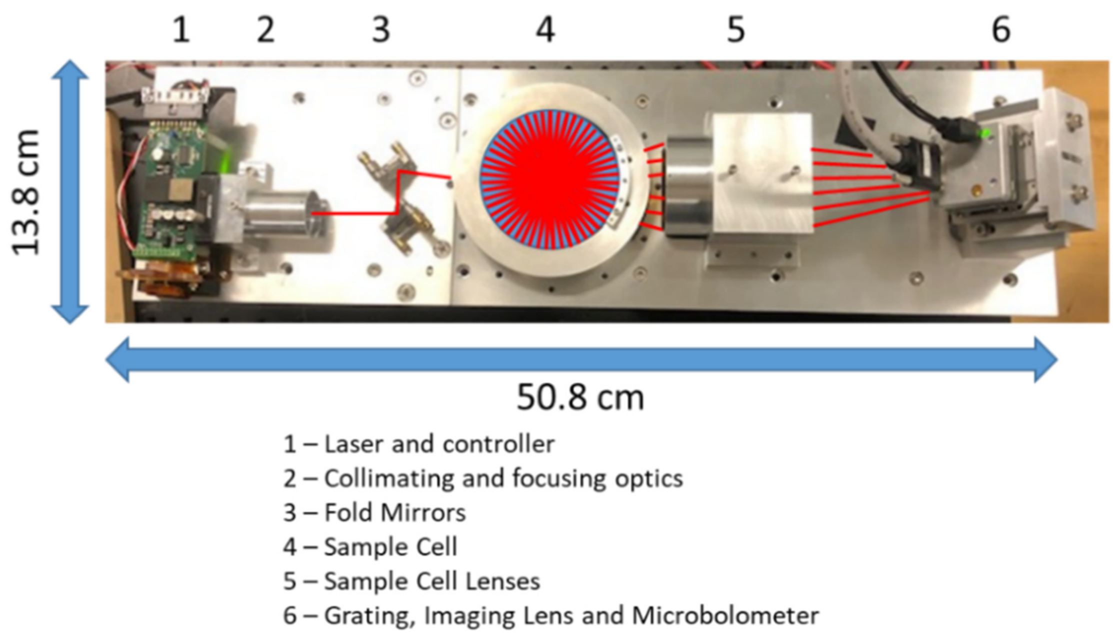

Figure 1. Gamma Prototype (volume - 6600 cm^3, weight - 2.5 kg) with significant room for size, weight and power (SWaP) reduction.

A key feature of this approach is the simultaneous acquisition of wavelength and pathlength data which mitigates noise arising from laser and sensor spectral/temporal instability; the result is detector-noise limited sensitivity (with a theoretical extinction equivalent noise floor of 1.76 x 10^{-6} m^{-1}). All processing will be conducted on-board, producing real time threat identification and quantification to the user with an alarm. In addition, the open path configuration enables immediate sampling of ambient air without the clear down issues which plague closed sampling detector designs. This approach has the following enabling attributes:

- Sensitivity due to the 4 m maximum pathlength, high power laser (>25 µW/cm^{-1}) and detector noise limited performance;
- Selectivity from its 10 cm^{-1} spectral resolution across the fingerprint region relevant for vapor phase CWAs and TICs;
- Broad dynamic range response owing to the 50x range of pathlengths used to characterize sample extinction;
- Compactness through novel sample cell design, elimination of the reference cell and use of an uncooled detector;
- Low power due to use of a high efficiency source and uncooled detector; and
- Low cost from component count minimization.

M-PED's key innovation is the use of spatially resolved, spectrally multiplexed multi-pass data to provide common mode noise rejection and dynamic range extension. The preliminary capability-specific Key Performance Parameters (KPPs) that guided the design of the M-PED sensor are listed in Table 1.

Table 1: Key Performance Requirements

Item	Parameter	Requirement
1	Sampling Method	Open path
2	Detectable Threat Agents	Aerosolized chemical threats: chemical warfare agents (CWAs), Toxic Industrial Chemicals (TICs) and Pharmaceutical-Based Agents (PBAs)
3	Detection Time	≤ 60 s [≤ 30 s]
4	Probability of Detection at LOD[1]	≥ 95%
5	Mean Time Between False Alarm at LOD[2]	≥ 168 Hr
6	Sensor Volume	≤ 0.013 m^3
7	Sensor Weight (including batteries)	≤ 4.5 kg
8	Battery Life	≥ 12 Hr [≥ 18 Hr]
9	Unit Cost (100s of units per year)	≤ $10,000

2.2 Key Components

The key elements in the M-PED design are: the laser, the multi-pass sample cell, the exit optics assembly, and the spatial and spectral algorithms. The key details of each component will be addressed in the sections to follow.

Laser

M-PED requires a low divergence laser source, supporting many non-overlapping laser bounces within the sample cell. This need is met using broadband QCL lasers with wavelengths targeting the fingerprint region necessary for CWA, TIC and PBA detection. PSI has used such lasers, produced by Thor Quantum Electronics, in early M-PED prototypes, where each laser spans up to 2 micron in the LWIR (Figure 2). Multiple lasers can be dichroically combined to cover the full range of interest, where the laser has minimal impact on system power consumption.

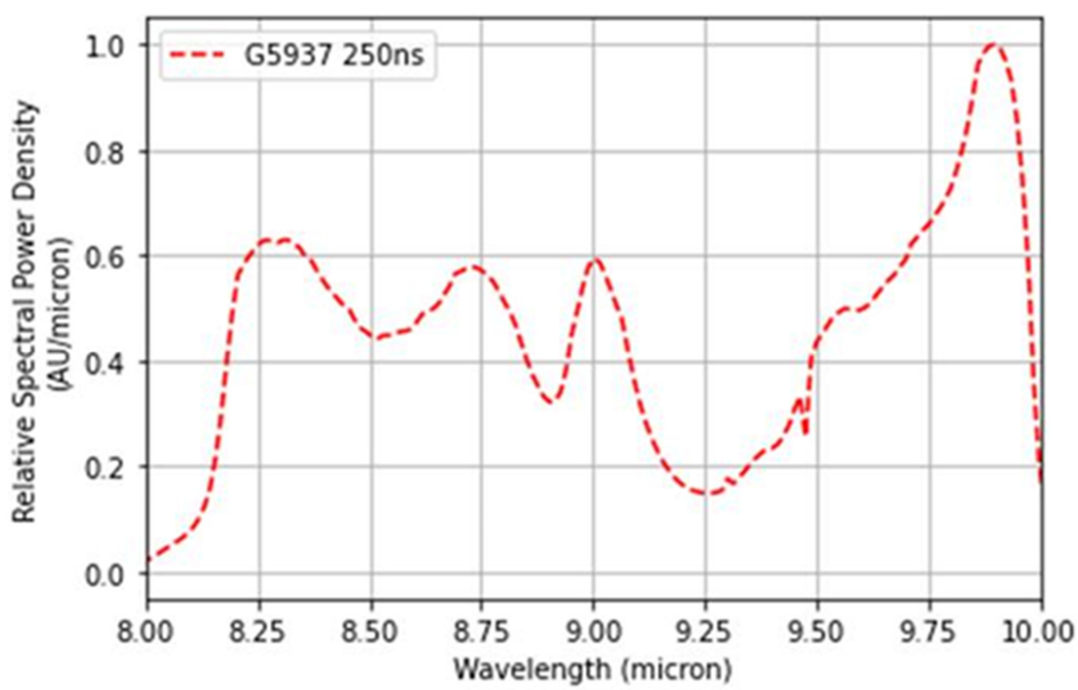

Figure 2. Gamma prototype laser power spectral density

1 Based on reported JCAD requirement across tests performed in 2005 and 2006. This probability of detection would also ensure more than 9 alarms over a 10 minute exposure at the ten minute negligible MEG.

2 Based on JCAD requirement as reported in DOD Programs Brief.

Multi-pass Sample Cell

The multi-pass cell is the key enabling technology of the M-PED design and builds on the IRcell design developed by IRsweep[i]. A focused laser beam is injected into the sample cell slightly off-axis, such that it traverses a chord through the cell. The cell is designed to support laser refocus each traverse. With this design, the laser processes around the perimeter of the mirror, such that the laser traces a star pattern, where each point represents a different pathlength through the aerosol sample. By breaking the cell into two elements (a metallic mirror and a dielectric mirror), light can be sampled from a plurality of these pathlengths to measure transmission through the chemical sample. The metallic mirror has a robust lasergold coating, providing 99% reflectivity and supporting field cleaning. The dielectric mirror has a reflectivity of ~96%, such that ~4% of the incident light will be transmitted to the exit optics for measurement. The gamma sample cell design has an 8 cm diameter, with facets supporting a 50 point star pattern. The first three and last three pathlengths are sampled at the dielectric mirror, supporting measurement of sample transmission over a 50x range of pathlengths (8 cm to 4 m), thereby providing enhanced dynamic range and Beer's Law fit stability.

Exit Optics Assembly

Figure 3 shows the gamma exit optics design. A 45 degree arc of the sample cell, encompassing the first three and last three pathlength samples, is filled by the dielectric mirror (or exit window). The light transmitted by the exit window is collected with a lens to form an aperture plane, acting like six distinct entrance slits into a grating spectrometer. A second imaging lens is then placed one focal length away to form a pupil for the diffraction grating, shown here in transmission for illustration purposes. The diffracted light from the grating is collected with an objective lens, imaging different wavelengths to different locations on the detector array in the dimension orthogonal to the pathlength samples (i.e. into and out of the page).

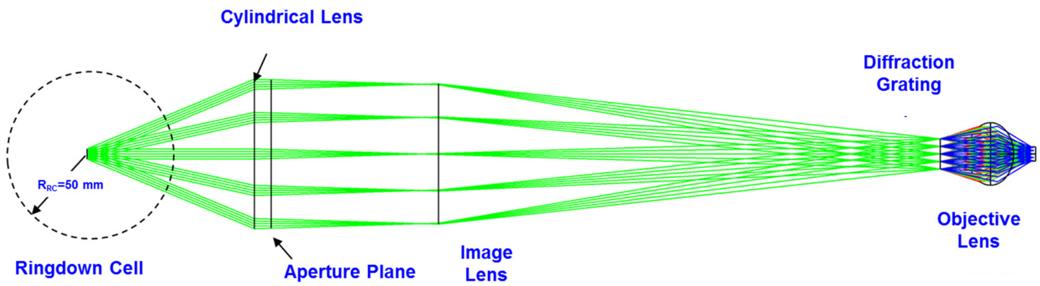

Figure 3. M-PED conceptual exit optics design

Algorithms

The images recorded by the microbolometer (Figure 4) are processed to parse them into a matrix of data with pathlength along one dimension and wavelength along the other. Threshold based segmentation is used to identify regions of interest. The spectral dimension is mapped using a series of spectral filters to anchor the wavelength scale. All pixels associated with a given pathlength and spectral resolution element are averaged and placed in the appropriate indexed location of the matrix. The result is a 6 pathlength x 25 wavelength matrix of data to be input into the log-linear fit algorithms.

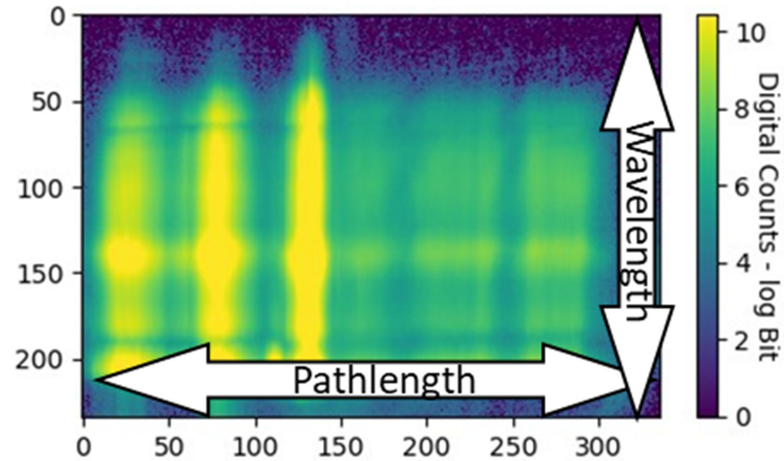

Figure 4. Beta prototype microbolometer output showing pathlength samples (horizontal axis) and wavelength samples (vertical axis). Sharper pathlength images and increased power levels in the final three samples is expected for the gamma prototype due to cell design refinement.

Measurement of sample transmission at multiple pathlengths enables a log-linear fit that can be used to identify the extinction of the sample at each wavelength independent of calibration variables. In more conventional designs, calibration variables like laser power output, detector response and mirror reflectivity are addressed through the use of a reference cell. The M-PED approach does not require a reference cell and therefore marks a significant SWaP-C benefit over standard multi-pass approaches. In the proposed design, calibration variables are separated from the quantity of interest (extinction) by performing a log-linear fit. As the laser light travels through the open path sample cell, a small amount of light will transmit the dielectric mirror each traverse. Referencing Table 2, the light transmitted each traverse can be modeled as follows:

$$S(N, L_N) = P_o \cdot (1 - T_{mirror})^{N-1} \cdot T_{mirror} \cdot (e^{-\kappa \cdot L_N}) \tag{1}$$

Table 2. Summary of Parameters for (1)

Symbol	Parameter Definition
P_o	Laser power
T_{mirror}	Mirror transmission
N	Number of round trips through the cavity
κ	Sample extinction coefficient
L_N	Pathlength through the sample after the Nth traverse
$S(N)$	Measured signal on the imager

If a series of these measurements are made after successive round trips using the spatially separated spots on the imager array, a log-linear fit can be performed to isolate calibration variables (e.g. laser power, mirror reflectivity, and detector response) from the parameter of interest (the extinction coefficient) as shown in 2-3.

$$\ln[S(N, L_N)] = \{ln[P_o \cdot T_{mirror}] + (N-1) \cdot \ln(1 - T_{mirror})\} - \kappa L_N) \tag{2}$$

$$y = b + mL_N \tag{3}$$

3. RESULTS

Several M-PED prototypes have been built and their performance has been characterized with respect to spectral range, spectral resolution, noise correlation across pathlength samples and slope temporal stability. The results of these investigations have been provided in the paragraphs to follow. In addition, measurements were made against several test chemicals to validate system algorithms and to provide a full capability demonstration.

Spectral Range and Resolution

Wavelength mapping was accomplished by tuning a Daylight Solutions MIRCAT to ten different wavelengths across the M-PED spectral range from 962 to 1162 cm^{-1} (8.6 to 10.4 micron) and directing it into the exit optics assembly. The relevant portion of the microbolometer frames have been provided as Figure 5, showing the laser spot shifting down the frame as the wavelength increases. It should be noted that the dimming of the laser in the vicinity of 9.6 micron is a function of the laser power (as independently verified with a laser power meter), rather than the response of the exit optics components.

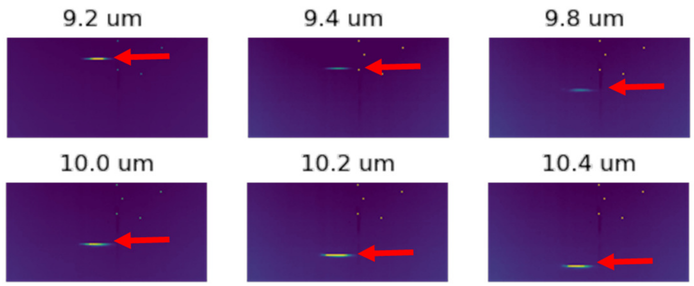

Figure 5. Microbolometer frames for a range of laser wavelengths showing the laser spot (highlighted with a red arrow) scroll down the image as the wavelength is increased.

These centroid locations were plotted against the commanded laser wavelength in Figure 6. The data closely tracks the anticipated linear trend for a grating spectrometer and verified that the full spectral range addressed by the M-PED QCL (Figure 2) would be captured on the microbolometer.

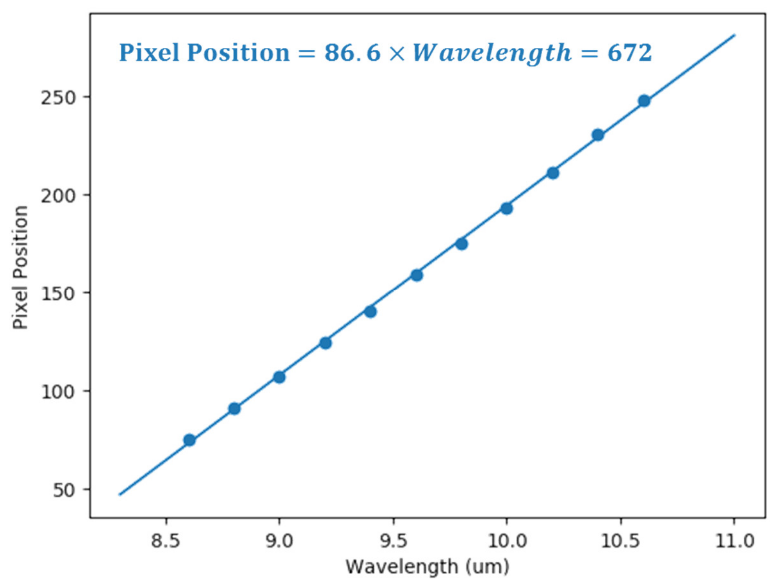

Figure 6. Linear wavelength mapping of the M-PED spectral range.

While the previous measurements are were taken in the absence of the toroid, the impact of that component on the overall spectral range and resolution is modest. Using the same wavelength mapping data set, the pixel spread of each spot was mapped to wavelength space using the calibration data presented in Figure 6. The results of this analysis showed a spectral resolution on the order of 15 - 30 nm, where the factor of two spread has been attributed to the spots spanning only 1-3 pixels (i.e. being under-resolved by the camera). This more than meets the system resolution requirement of 10 cm^{-1} (or roughly 100 nm in this spectral range).