# Threat Aerosol Characterization using Rotating Drum with Quantum Cascade Laser Cavity Ring Down Spectroscopy

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## Abstract

Aerosolized chemical warfare agents (CWAs) and toxic industrial chemicals (TICs) are potential threats for the warfighter, resulting in the need for aerosol identification and characterization for further developments in protection and mitigation. We have developed a new method for the interrogation of aerosols via the combination of cavity ring down spectroscopy (CRDS) and a rotating drum. Through the implementation of quantum cascade lasers (QCLs), CRDS is a highly sensitive technique that has the ability to investigate the mid-infrared (IR) fingerprint region. This experimental setup is a novel configuration that results in *in situ* investigations of chemical aerosols.

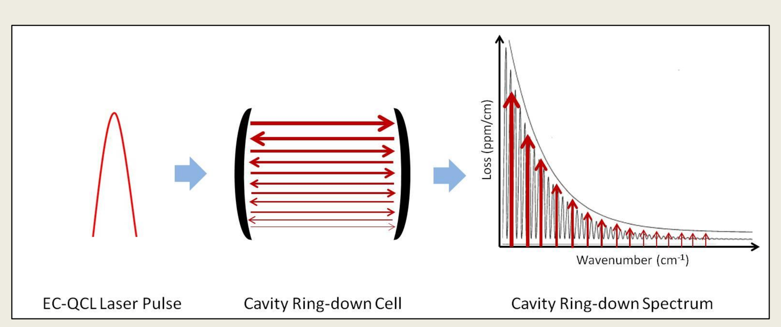
## Objective

The goal of this research is to obtain cavity ring down spectra for chemical warfare agent aerosols suspended in a rotating drum. The *in situ* spectra will provide more detailed knowledge of these compounds as aerosols in a realistic scenario (i.e., suspended in the atmosphere).

## Paired QCL and CRDS Capabilities

Once a laser pulse enters the optical cavity, the light bounces between the highly reflective mirrors and with each pass a fraction of the light is lost and the signal is collected by the detector. The result is a spectrum measuring the light absorption (loss of light) vs. excitation laser wavelength as shown in Figure 1.

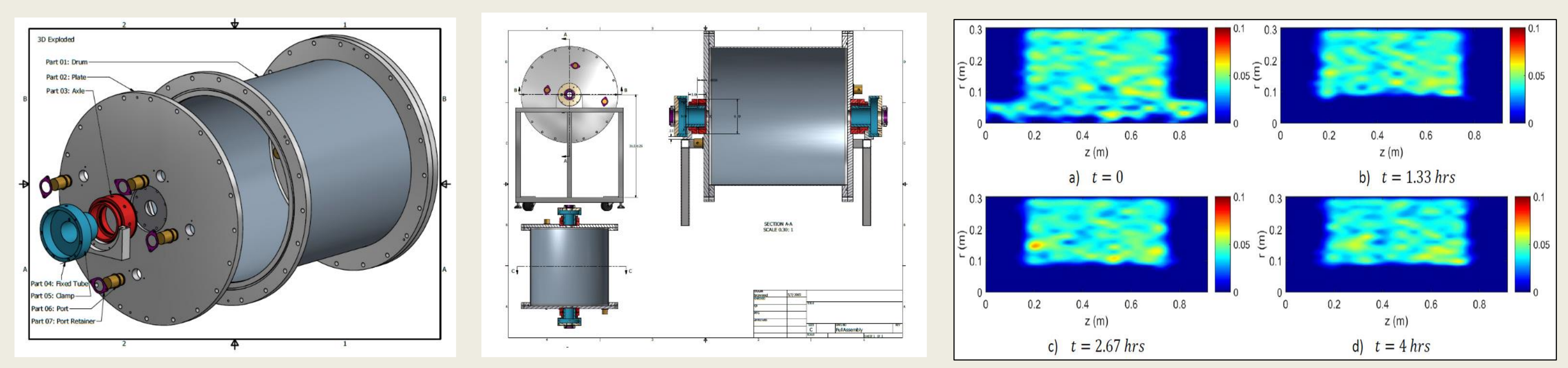
*Figure 1. Paired QCL and cavity ring-down process. The schematic representation of a spectrum shown is one of an empty cavity, i.e. a background scan. This spectrum is also characteristic for any IR inactive carrier gas such as nitrogen, $N_2$.*




High reflectivity mirrors and a cavity cell of approximately 1 meter length simulates a path length on the order of 10 kilometers. The sensitivity of the system is directly related to the path length.

## Rotating Drum Design

In aerosol research, the study of particles suspended over an extended period of time (~ 1 day) are essential for better characterization of the gas-particle or liquid-particle dynamics. However, gravitational settling is inevitably encountered in attempts to maintain suspension. Figures 2a and 2b illustrate our rotating drum design for elongating particle lifetimes. This is achieved through slow rotation of a horizontal cylindrical chamber about its axis.



(a) UNCLASSIFIED//FOR OFFICIAL USE ONLY (c)

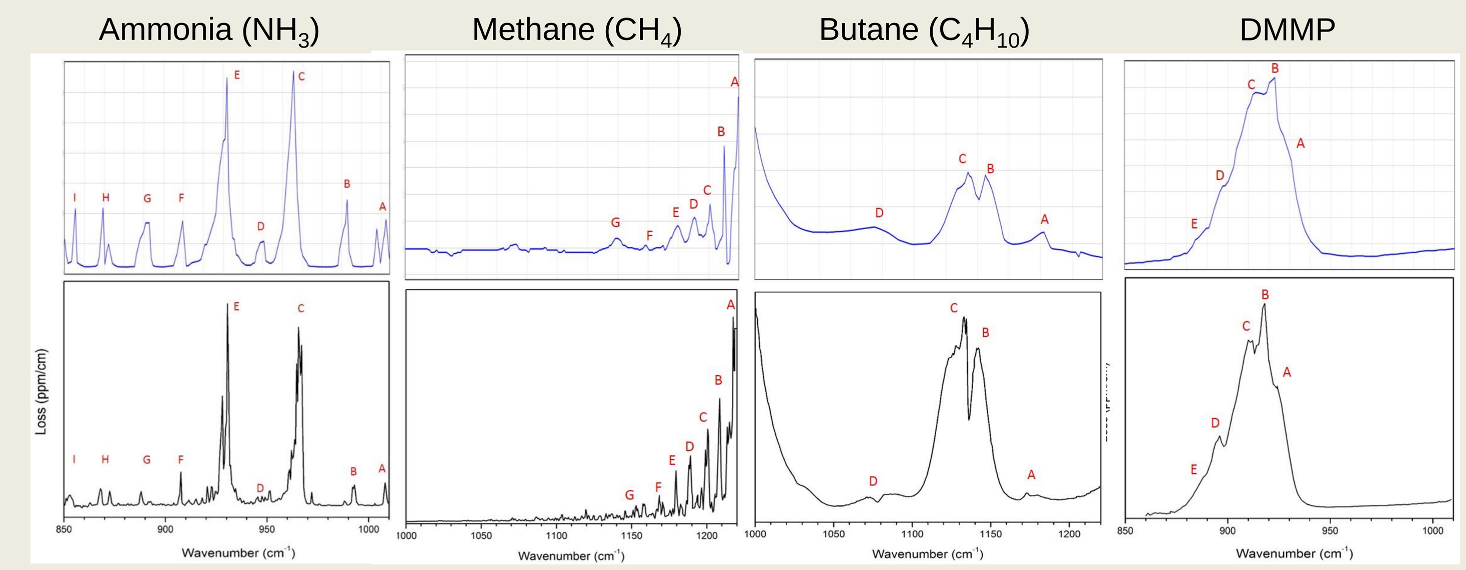
*Figure 2. a) side view and b) end flange views of the stainless steel rotating drum for aerosol suspension. This drum is 24" x 24" (not including extension tubes) and weighs approximately 300 lbs and c) particle concentration distribution contours for the final design.*

Particle flow modeling is needed to predict the radial and axial velocities that will affect the distribution of particles in the drum, and is shown in Figure 2c. CRDS requires that all optics remain stationary, therefore, tube extensions were designed to house the mirrors and to isolate resultant flow fields from penetrating into the main chamber. Particle flow modeling ensures the validity of this configuration and predicts the centerline will be evacuated for the optical path of the CRD spectrometer for vapor characterization. The completed rotating drum is shown in Figure 3.

*Figure 3. Completed construction of the rotating drum. Optical assembly and accessories include the CRDS high reflectivity mirrors, aerosol introduction and an aerosol evacuation end, each with 4 varying radial ports. At the introduction end are 3 VCR ports for reaction gas, mixing gas, and relative humidity (RH) introduction. At evacuation end are ports for an RH and temperature sensor, pressure gauge, and VCR fittings to evacuate the chamber for cleaning.*

## Vapor Characterization

The superior sensitivity of this system, compared to other absorption techniques, is illustrated by several spectra obtained for TICs and simulants in Figure 4.




(a) (b) (c) (d)

*Figure 4. Comparison of NIST** IR spectra (in blue) and our collected spectra (in black) for (a) ammonia, (b) methane, (c) butane, and (d) dimethyl methylphosphonate (DMMP).*

**P.J. Linstrom and W.G. Mallard, Eds.,NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, http://webbook.nist.gov

## Initial Aerosol Suspensions

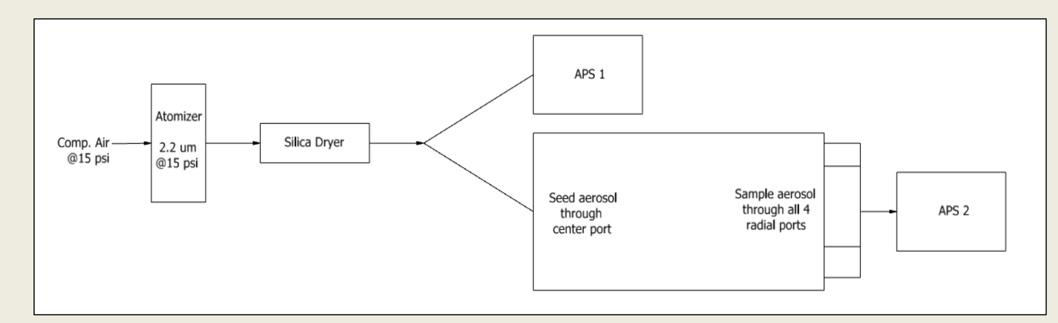



*Figure 5. Experiment set-up for initial testing of aerosol introduction and flow for a uniform concentration across the drum. APS 1 set upstream and APS 2 set up downstream.*

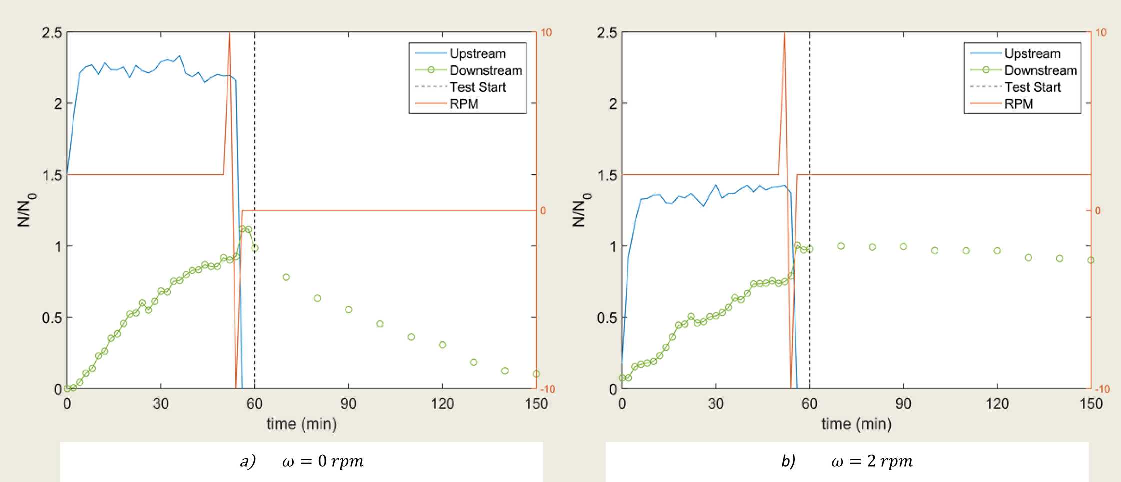



*Figure 6. Measurements of particle concentration upstream and downstream of drum vs. time. Also marked is the test start time for sampling the decay rate, and the drum rotation rate at a) 0 rpm and b) 2 rpm.*

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