Abstract

A heated cell with optical access has been constructed to characterize spectroscopic parameters for various low-vapor-pressure contaminants of interest in the aerospace, power generation, and defense industries. Sarin gas (C₅H₈FO₂P) is a dangerous nerve agent used in chemical weapons of mass destruction. Due to the toxicity of Sarin gas, it is difficult for the experimenter wanting to develop reagents that help eliminate or mitigate its effects. Surrogates for Sarin, which have similar organophosphorus bonds but are much less toxic, are being studied at elevated temperatures and pressures to develop better chemical kinetics mechanisms to predict the behavior of Sarin destruction. Resolution of low-vapor-pressure species concentrations for sample surrogates is not trivial as gas dynamic effects during the experiment can lead to condensation of the species. Laser absorption spectroscopy offers a non-invasive diagnostic that is highly sensitive and allows for in-situ measurements of species concentrations. Measurements were made with a 2 mW 3.39 μm helium-neon gas laser in the infrared region that is sensitive to the C-H bond in hydrocarbons. The laser passes through a gas chamber with sapphire windows, heated to constant temperatures of up to 473 K, and is focused into an infrared-sensitive PbSe photodiode. Transmission was measured by the fractional attenuation of light through the cell at known conditions to record absorption coefficients and will be used to develop spectroscopic data for other species of interest.

Background

- Sarin Gas: Nerve Agent Being Used as a Chemical Weapon of Mass Destruction
- Research on Simulants to Understand Combustion Kinetics for Efficient Neutralization
  - Colorless
  - Odorless
  - Deadly

Problem

- Very Low Vapor Pressures
- Possibility of Condensing
- Hard to Accurately Record the Concentration in Studies

Approach

- Laser Absorption Spectroscopy
- Beer-Lambert Law

\[ T = \frac{I}{I_0} = e^{-k_v(P,T)P_{total}X_L} \]

- 3.39 μm Helium-Neon Infrared Laser

Results

- Absorption Coefficients for TEP at 473 K

Next Steps

- Take More Measurements at Different Temperatures
- Model the Coefficient as a Function of Pressure/Temperature
- Apply the Diagnostic to Other Species of Interest

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