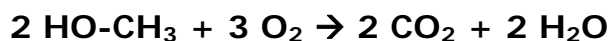


# 100 chemical pictures every second.

## Kinetics of Methanol Explosive Combustion Using EP-IR Emission Spectroscopy.



*Complete combustion of methanol. The stoichiometric equation seems to say it all! But what truly happens? How fast does it happen? Is the combustion continued? Sustained?*

*This short experiment was designed to demonstrate the ability of Encoded Photometric Infrared spectroscopy to record in detail (full spectrum information) all chemical information pertaining to an ultra-rapid chemical reaction. Although this particular example is proposing the use of an EP-IR spectrometer for emission spectroscopy measurement, the technology can equally be used for the monitoring of chemical kinetics in transmission and absorbance spectroscopies for the analysis of samples in solid, liquid and gas phase.*

### INTRODUCTION

Encoded Photometric Infrared (EP-IR) spectrometry is a novel technique allowing access to full spectrum information with a scanning speed of 100 scans per second (one complete refresh of the total chemical information every 10 milli-second.) EP-IR spectrometers rely upon the use of a single, non-hygroscopic part to generate an interferogram: a vibration insensitive proprietary encoder disk with an MTBF superior to 50,000 continuous use hours. This post-dispersive technology enables the design and implementation of many different sampling technologies for the analysis of gases, liquids or solids. Lastly, the same post-dispersive design allows for easy versatile use for emission, transmission and absorption spectroscopy techniques.

### MATERIALS & METHODS

An Aspectrics MC5000A 128-channels EP-IR spectrometer covering the 2.5 – 5.0  $\mu\text{m}$  (2,000 – 4,000  $\text{cm}^{-1}$ ) spectral range was used for this experiment. The EP-IR spectrometer was mounted on the Aspectrics multi-purpose sampling bench without accessories in the sample compartment. The Mid-IR source was continuously left on to provide baseline emission signal.

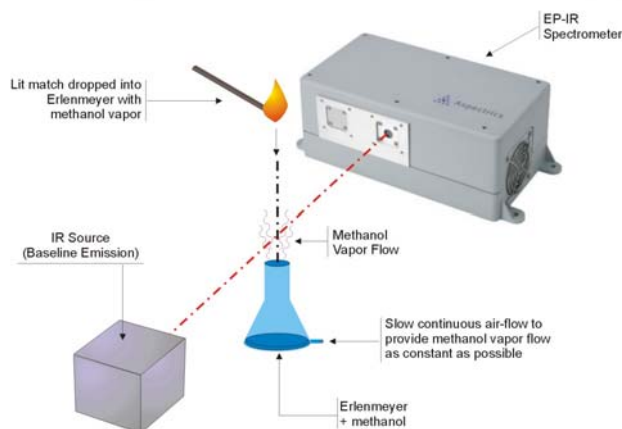


Figure 1: Experimental Set-Up

Approximately 2-3 mL of methanol ( $\text{HO-CH}_3$ ) was placed in an Erlenmeyer flask. A slow and continuous flow of air was injected at the bottom of the Erlenmeyer to ensure regular outflow of methanol vapor from the neck of the Erlenmeyer.

After a few minutes of air flowing into the methanol, a lit wooden match was dropped into the Erlenmeyer from above, eventually igniting the methanol vapor (*fig. 1*).

The EP-IR spectrometer was set to record full-spectrum intensity spectra at a rate of 1 every 10 milli-second.

Spectra were stored in real-time and later retrieved for display and analysis.

### RESULTS

*Fig. 2* represents 50 spectra collected over only 500 milli-seconds during the entire experiment. Spectra are plotted over the entire spectral range covered by the MC5000A. Please note that five very distinct phases can be observed over that 500 milli-second time span. As detailed on *Fig 3*, they are, in chronological order in the 2000-2300  $\text{cm}^{-1}$  region:

1. No emission. The only signal observed is the baseline emission from the IR source.
2. Emission caused by the lit match passing in front of the spectrometer as it is dropped in the Erlenmeyer (approx. 100 msec.)
3. Large emission observed when the accumulated methanol vapors are igniting (approx. 30 msec.)
4. Emission caused by the combustion of the remainder of methanol vapor, lasting approximately 70 msec. until combustion is complete.
5. Return to no emission signal when all the methanol vapors had been combusted.

In addition to the combustion energy information observed in detail over the 2000-2300  $\text{cm}^{-1}$  region, chemical information pertinent to the chemical oxidation of methanol is also visible, this time in the 3500 - 3900  $\text{cm}^{-1}$  region of the emission spectrum. Of particular interest are the water vapor information (wide band

$\sim 3600\text{ cm}^{-1}$ ) and the CO<sub>2</sub> overtone information (dual band  $\sim 3800\text{ cm}^{-1}$ ) which chronologically appears as follows (Fig. 4, 5):

1. Initial period. No water vapor nor CO<sub>2</sub> spectral information can be observed beyond ambient conditions (approx. 130 msec)
2. When the lit match passes in front of the spectrometer as it is dropped in the Erlenmeyer (approx. 100 msec.), some water vapor and CO<sub>2</sub> spectral information can be observed.
3. When the accumulated methanol vapors ignite, large (intense) water vapor and CO<sub>2</sub> spectral information appears for the short duration of the explosion (approx. 30 msec.)
4. During the combustion of the remainder of methanol vapor, significant water vapor and CO<sub>2</sub>

spectral information is still observed for approximately 70 msec. until combustion is complete.

5. When all the methanol vapors had been combusted, water vapor and CO<sub>2</sub> spectral information return to their original level.

### CONCLUSION:

This experiment clearly demonstrates the ability of EP-IR to capture ultra-fast (30 milli-second) reaction information over the entire spectral range. The advantage is two-fold; simultaneous real-time observation of information pertaining to the thermodynamics of the reaction and that of the formation of products of the reaction.

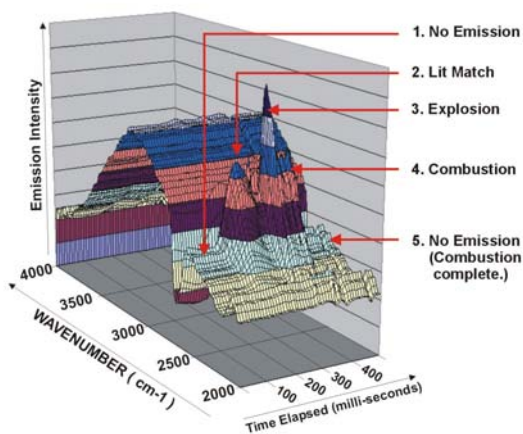


Figure 2: Emission spectra

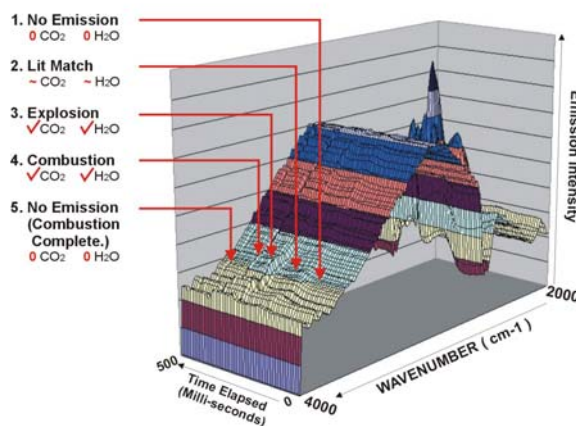


Figure 4: Emission spectra; focus on H<sub>2</sub>O<sub>(g)</sub> and CO<sub>2</sub> (g)

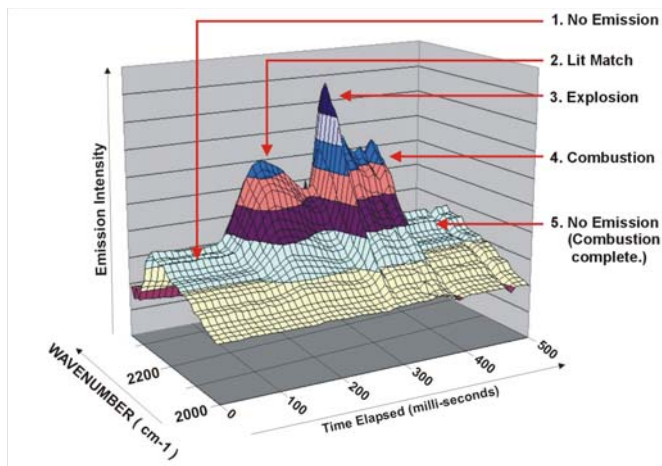


Figure 3: Emission spectra; 2000-2300 cm<sup>-1</sup> detail

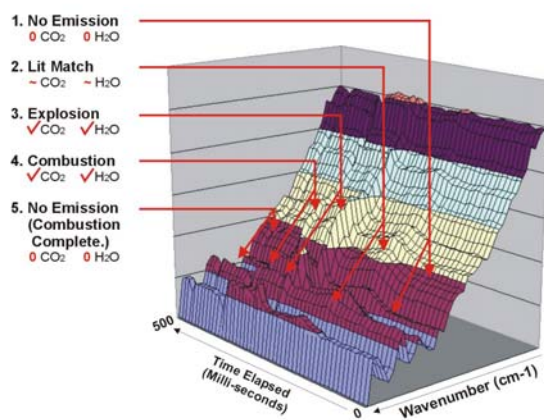


Figure 5: Emission spectra; focus on H<sub>2</sub>O<sub>(g)</sub> and CO<sub>2</sub> (g)- detail.

Copyright © 2005 By Aspectrics, Inc. All Rights Reserved Worldwide

Aspectrics, inc. (Headquarters & Manufacturing)  
6900 Koll Center Pkwy, # 401  
Pleasanton, CA 94566  
Tel. : 925.931.9270  
Fax : 925.931.9272

[www.aspectrics.com](http://www.aspectrics.com)

Aspectrics, Inc. (Applications Center)  
3510 Parmenter Street  
Middleton, WI 53562  
Tel. : 608.835.2057  
Fax : 847.235.3130