InfiTOF™
Direct Analysis of a Methanol Flame by Using a Compact High-Resolution Multi-Turn Mass Spectrometer

Introduction

The InfiTOF™ is a compact high resolution time-of-flight mass spectrometer (TOF-MS) that has a unique multi-turn ion optics system capable of providing a variable-length ion-flight path (up to 200m) in a very compact analyzer (20cm x 20cm). As a result of this, the InfiTOF allows the user to choose a resolving power based on path length in order to separate similar mass gas components like carbon monoxide and nitrogen as CO^+ (*m/z* 27.9949) and N_2^+ (*m/z* 28.0062).

With this in mind, the InfiTOF can be used for "In-situ" high-resolution monitoring of real-time gas phase reactions like combustion. In this work, we show the real-time monitoring of combustion products in a diffuse methanol flame by using this compact high resolution TOF-MS system.

Experimental

A commercial alcohol lamp was used to make a diffusion flame of vaporized methanol. The InfiTOF was set to a resolving power of approximately 5,000 at *m/z* 28, and the ionization energy was set to 70eV. A deactivated fused silica capillary tube (Length 50cm, inner diameter 0.1 mm) was used as the gas inlet into the MS. The other end of this capillary tube was directly inserted into the methanol flame as shown in Figure 1.

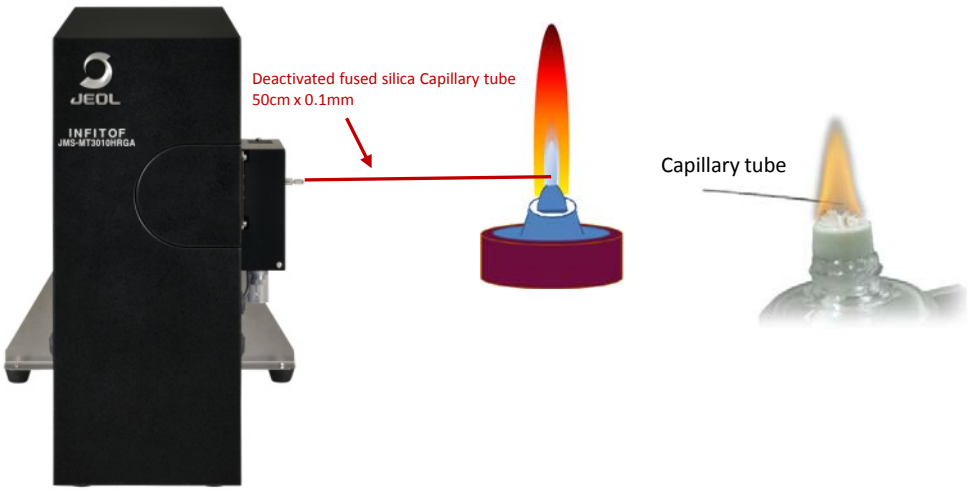

Figure 1. Experimental scheme showing configuration of InfiTOF and alcohol lamp.

Table 1 Measurement Conditions

Sample	Alcohol Lamp with Methanol
MS	JMS-MT3010HRGA InfiTOF™
Resolving Power	≥ 5000 (m/z 28)
Ionization Voltage	70 eV
Recording Interval	500 msec/spectrum
Column	Deactivated fused silica capillary tube (50cm x 0.1mm)

Results

The mass spectra for the region very close to the cotton core, before and after ignition, are shown in Figure 2. The mass spectrum before ignition showed methanol, N_2, O_2 and Ar. As it turns out, O_2 and CH_3OH have the same nominal mass of 32, but the InfiTOF was able to completely separate and detect each peak (O_2^+, 31.9898 and CH_3OH^+, 32.0262). After ignition, the intensities of O_2 and CH_3OH were reduced, and the H_2O and CO_2 peak intensities increased.

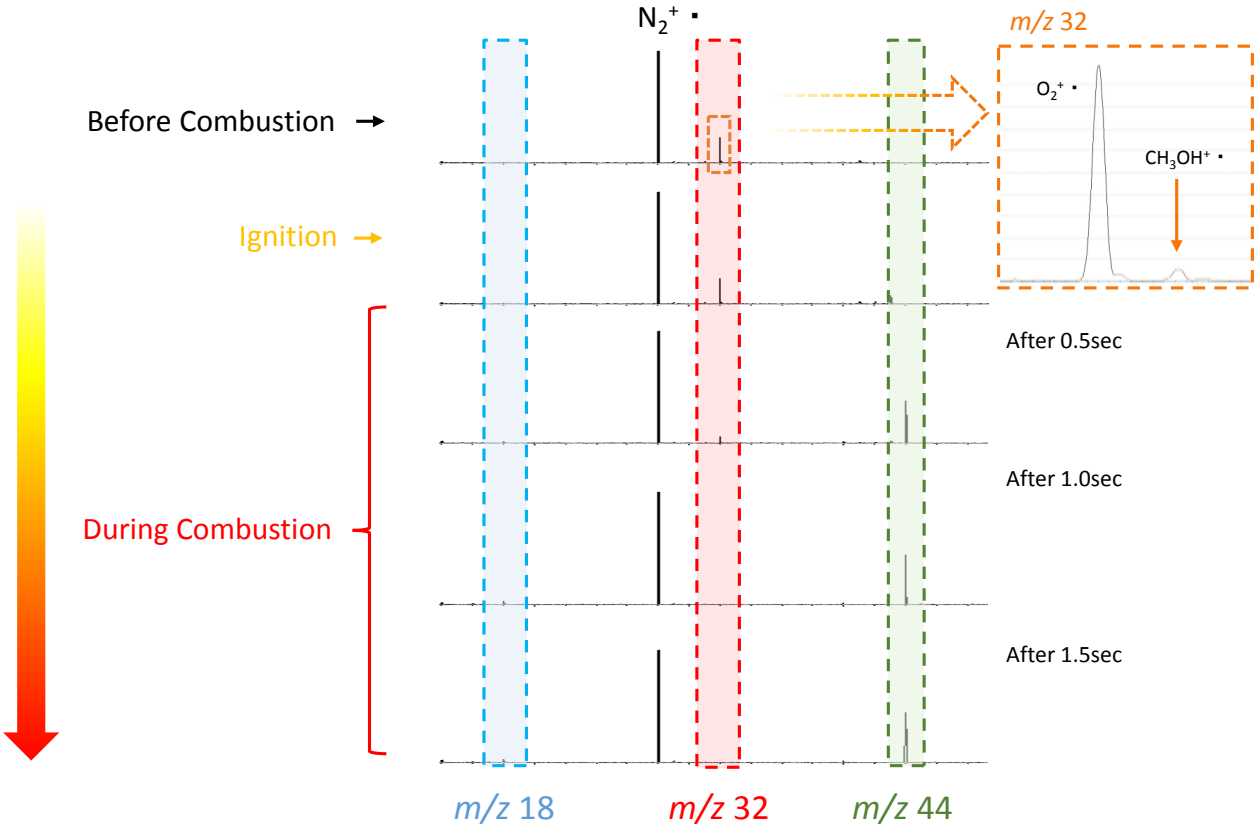

Figure 2. Behavior of H_2O (*m/z* 18), O_2 (*m/z* 32) and CO_2 (*m/z* 44) during the combustion process.

Figure 3 shows an expanded view of two mass spectra from Figure 2. All peak labels show the elemental compositions calculated from each m/z shown in these spectra. H_2O, CO_2, H_2, CO, and NO were all detected during the combustion of methanol. Additionally, these compounds were combustion products, as indicated by the fact that they were not detected prior to flame ignition. Also, the drop in O_2 peak intensity within the flame was expected given that oxygen is required for the combustion of methanol to occur. Additionally, N_2^+ and CO^+ were observed as separate peaks in the flame spectra as a result of the high resolving power setting of the InfiTOF.

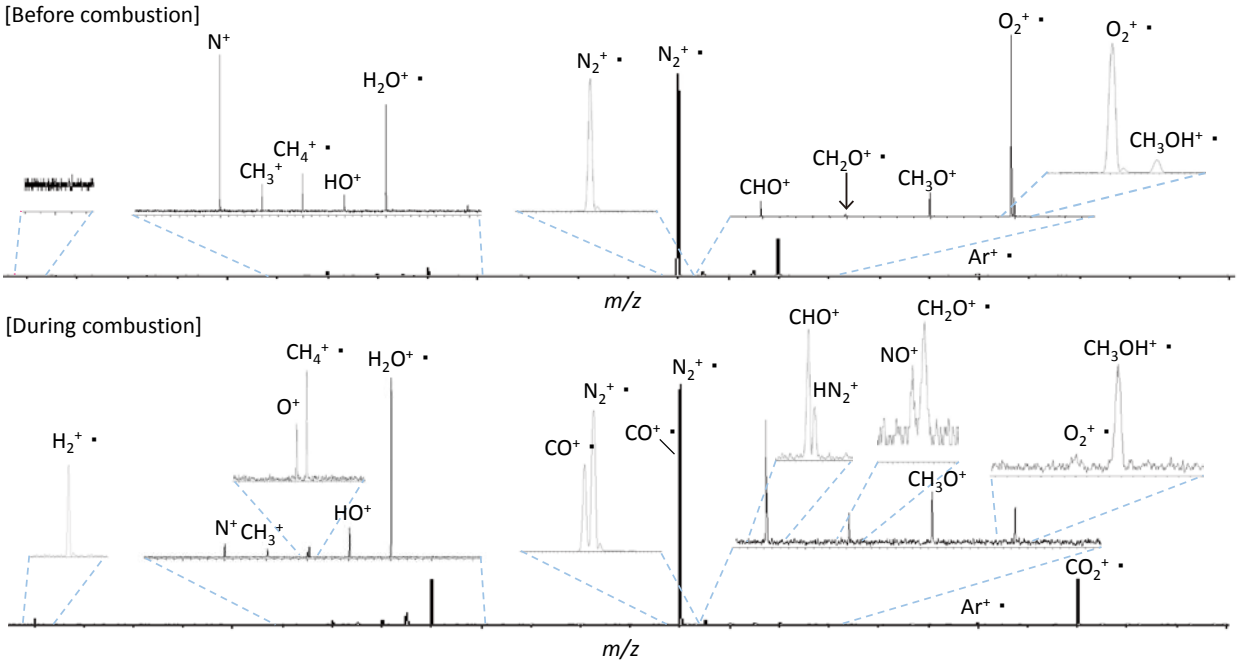

Figure 3. Mass spectra of out gases in before or during combustion.

Figure 4 shows the mass spectra observed for positioning the capillary column in different locations within the flame. A small amount of H_2 was detected near the cotton core. And intensities of H_2 and CO_2 decreased as the distance increased from the cotton core. In contrast, intensities of H_2O and O_2 increased as the distance increased from the cotton core.

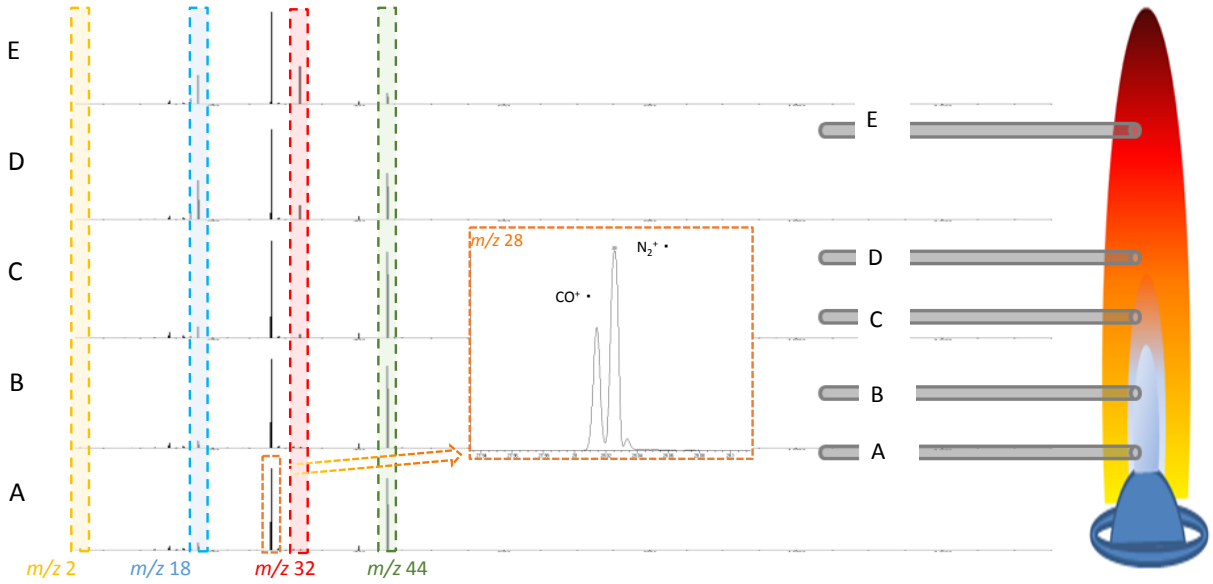

Figure 4. Mass spectra in different flame position.

Conclusion

This report showed that the InfiTOF is suitable for high-resolution, real-time monitoring combustion reactions. The system was able to separate compounds with similar exact masses like CO and N_2 from each other as well as detect low mass peaks like H_2 under high resolving power conditions. Although these results were done using a simple fuel like methanol, the infiTOF's high resolving power is expected to be suitable for combustion applications involving more complicated fuel such as petroleum fuels or biofuels.

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