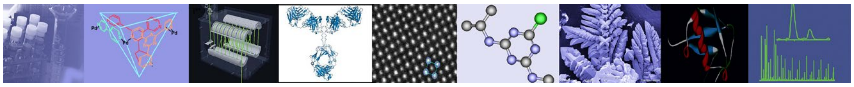


Direct analysis of a butane combustion flame by using a high-resolution multi-turn mass spectrometer

Introduction

Butane is known to be the main component of liquefied petroleum gas and is widely used as a fuel. The elementary mechanistic reactions that occur during premixed butane/air combustion have been investigated through computer simulations. However, there are relatively few experimental mass spectrometric studies that supplement these computer simulations due to the technical challenges of combustion product sampling from within the premixed butane/air flame.

The JMS-MT3010HRGA is a compact high-resolution multi-turn mass spectrometer the can be used to measure combustion products. In this report, we identified combustion products in the premixed butane/air flame by using the JMS-MT3010HRGA.

Experimental

The premixed butane/air flame was generated using a commercially butane micro touch. The diffusion flame was generated by introducing an excessive amount air into the touch. Figure 1 shows that JMS-MT3010HRGA connected on a simple sampling tube and combustion products generated in the flame were measured with the Table 1 conditions. The sampling positions of the premixed flames were 5 positions A to E, and the center of each position of the flame was measured (see Fig.2). The diffusion flame was measured in the center of flame position F (see Fig.3).

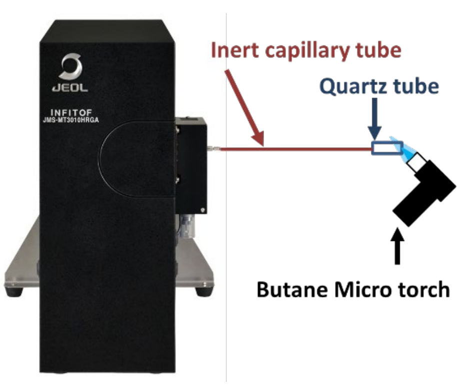


Fig. 1 Experimental scheme

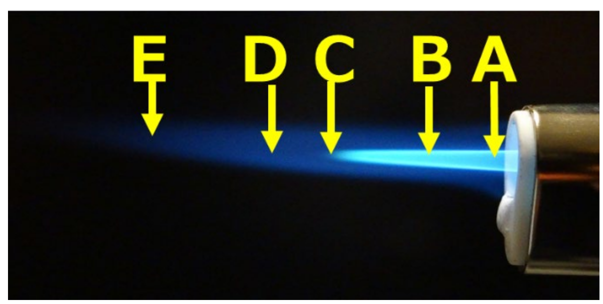


Fig. 2 sampling positions (Premixed flame)

Table 1. Measurement Conditions

Instrument	JMS-MT3010HRGA "INFITOF" (JEOL Ltd.)
Gas Introduction method Capillary Column	Introduction by vacuum Quartz tube (3.8cm x 0.4mm) + Inert capillary tube (30 cm x 0.1 mm)
MS conditions Ionization method Ion source chamber temp. Recording interval *m/z* Range Mass resolution (cycle)	 EI(+) ; 20 eV, 50 µA 100 ˚C 1sec / spectrum 0 to 100 R≈5,000 *m/z* 28 (16Turn)

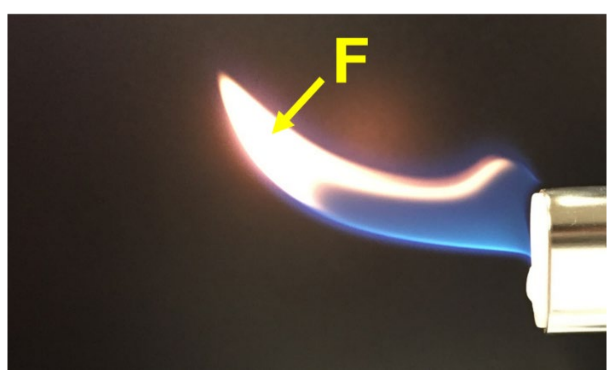


Fig. 3 Sampling position (Diffusion flame)

Results

【Identification of major components】

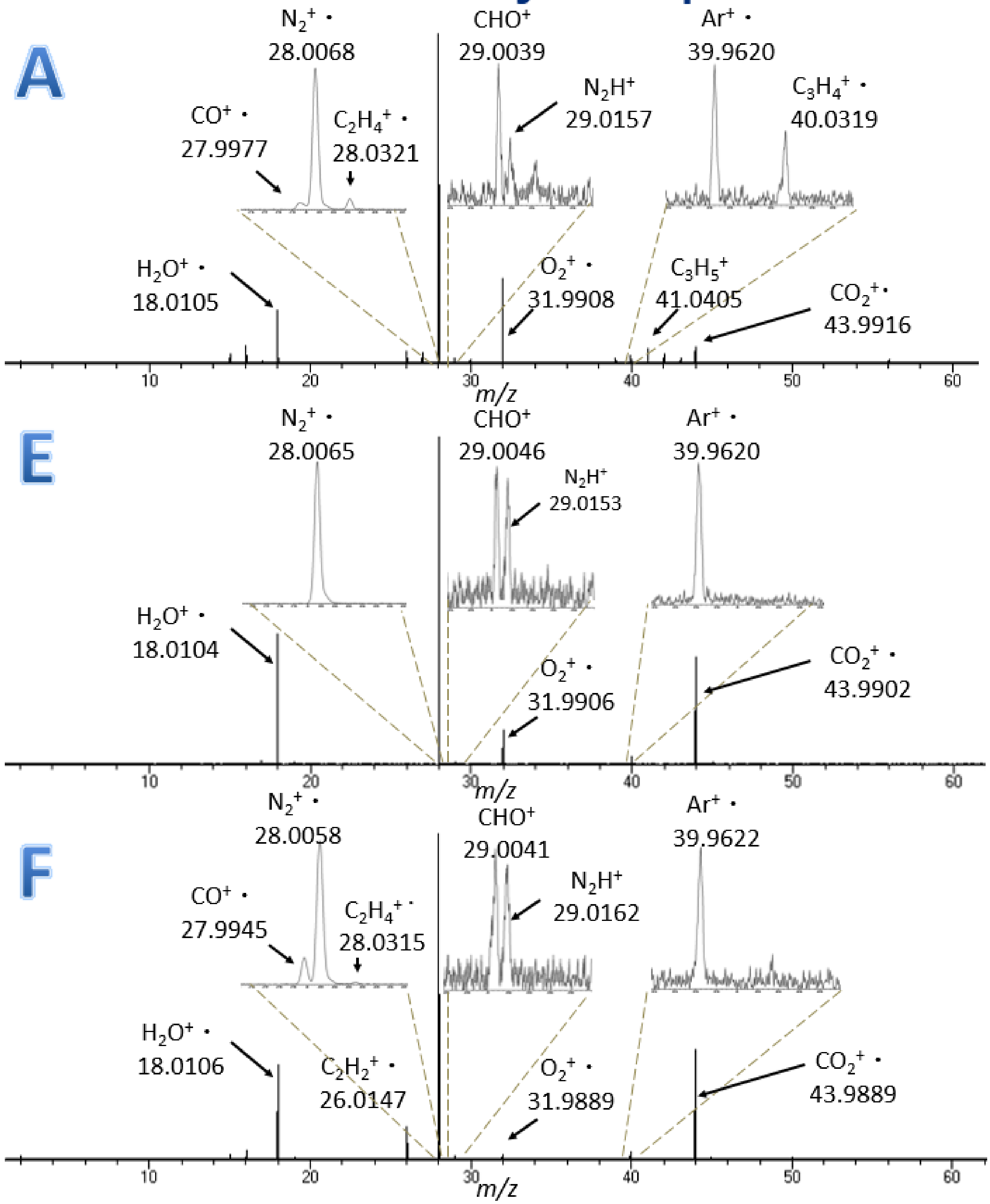
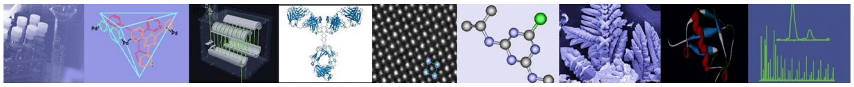


Fig. 4 Mass spectra (Detector voltage = 2,400V)



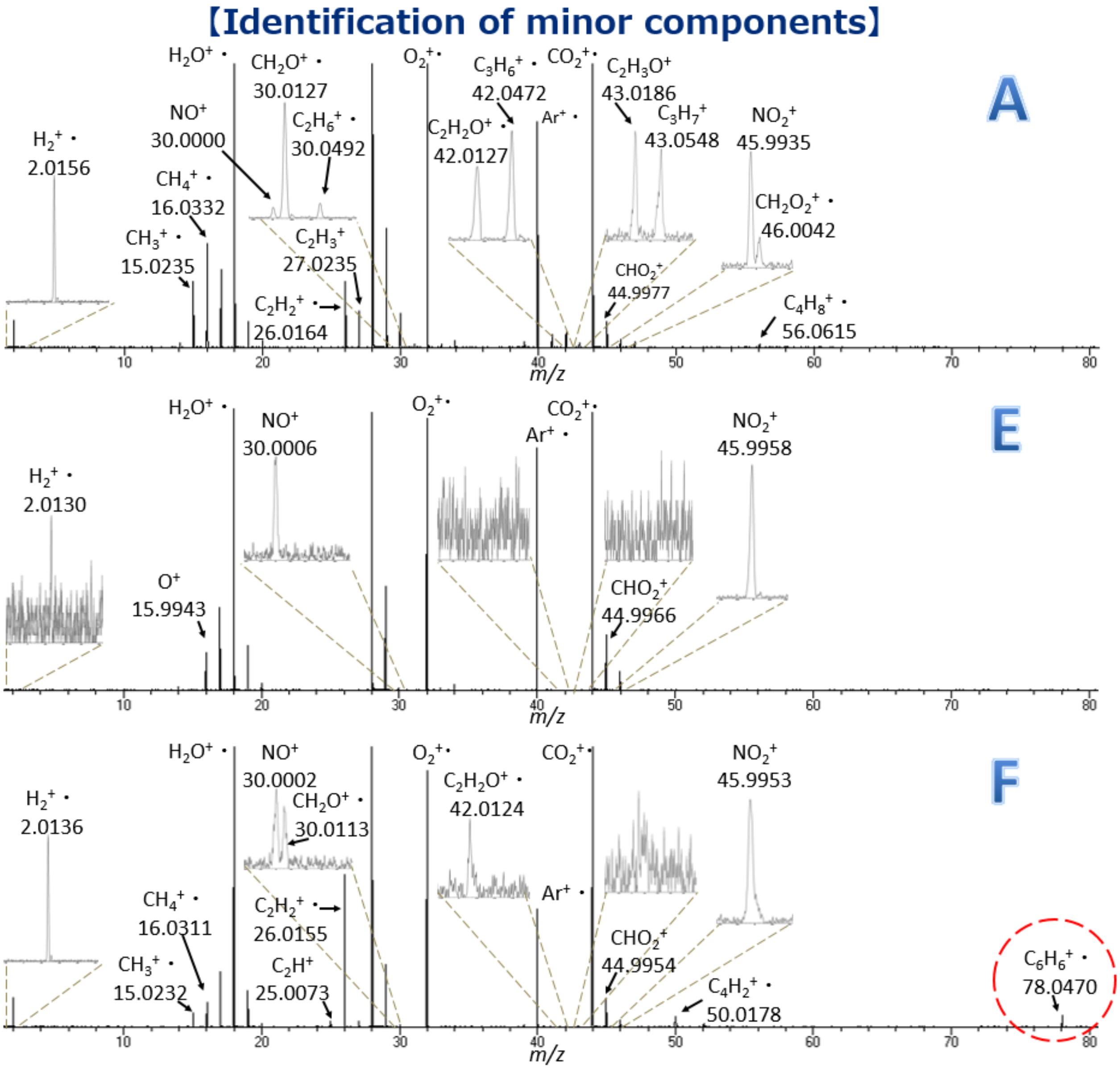
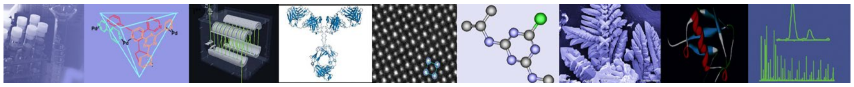


Fig. 5 Mass spectra (Detector voltage = 2,700V)

5-second averaged mass spectra obtained from position A, position E, and diffusion flame F are shown Fig. 4 and Fig. 5. The detector voltage was varied between spectra because concentration differences between main components and minor components are large. Position A contained air components such as $N_2^{+}\cdot$, $O_2^{+}\cdot$ and $Ar^{+}\cdot$ along with combusted and un-combusted components such as $H_2^{+}\cdot$, $CH_4^{+}\cdot$, $H_2O^{+}\cdot$, $C_2H_2^{+}\cdot$, NO^{+}, $C_3H_5^{+}$, $CO_2^{+}\cdot$, NO_2^{+} and $C_4H_8^{+}\cdot$. Some components such as $CO^{+}\cdot$/ $N_2^{+}\cdot$/ $C_2H_4^{+}\cdot$ and $Ar^{+}\cdot$/ $C_3H_4^{+}\cdot$ requiring high mass resolution were also detected. At position E, almost no hydrocarbon component was detected. $C_6H_6^{+}\cdot$ which is a larger mass than the butane fuel was detected at diffusion flame F.



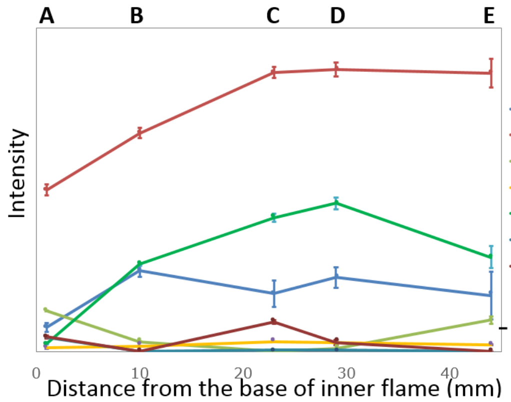


Fig.6 Intensity distribution of major components in premixed flame (Detector voltage = 2,400V)

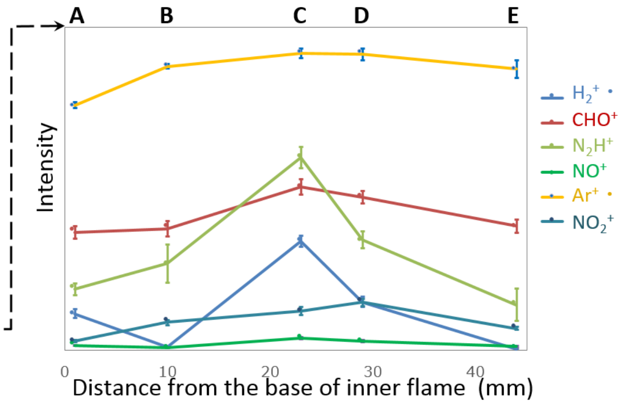


Fig.7 Intensity distribution of minor components in premixed flame (Detector voltage= 2,700V)

Figure 6 and Fig.7 show intensity distributions of components detected at all positions A to E of the premixed flame. The Intensity of atmospheric $N_2^{+}\cdot$ increased within the distance from the base of inner flame, and intensity of $Ar^{+}\cdot$ was almost constant each position. Moreover, intensities of $O_2^{+}\cdot$ and $C_2H_4^{+}\cdot$ decreased as the distance increased from the base of inner flame. Intensity of $H_2O^{+}\cdot$ showed lowest in position A, and other positions B to E were almost constant. $H_2^{+}\cdot$, $CO^{+}\cdot$, CHO^{+}, N_2H^{+} and NO^{+} showed maximum intensity at position C, which is near the boundary between inner and outer flame. $CO_2^{+}\cdot$ and NO_2^{+} showed the maximum intensity at position D.

Conclusion

JMS-MT3010HRGA system can

- detect Hydrogen molecules
- separate isobaric masses such as $CO^{+}\cdot$ / $N_2^{+}\cdot$ / $C_2H_4^{+}\cdot$
- detect minor components such as NO^{+} and NO_2^{+}
- identify elemental composition from exact mass
- measure intensity distribution of combustion products by flame position

Consequently, JMS-MT3010 HRGA is a useful tool for combustion studies.

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