



# Ethanol flame structure investigated by molecular beam mass spectrometry

T.S. Kasper, P. Oßwald, M. Kamphus<sup>1</sup>, K. Kohse-Höinghaus\*

*Physikalische Chemie I, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany*

Received 5 September 2005; received in revised form 25 September 2006; accepted 6 December 2006

Available online 21 June 2007

---

## Abstract

The oxidation of ethanol was studied in low-pressure, premixed flat flames using molecular beam mass spectrometry (MBMS) in combination with electron impact ionization (EI) and resonance-enhanced multiphoton ionization (REMPI). Flame temperature profiles were measured by laser-induced fluorescence (LIF) of seeded NO. Two ethanol/oxygen/argon flames with stoichiometries of  $\phi = 1.00$  and  $\phi = 2.57$  were investigated at 50 mbar by EI-MBMS. Profiles of a variety of stable and radical species were measured as a function of height above the burner. The benzene profile in the fuel-rich ethanol flame was obtained by REMPI-MBMS. The same technique was used to determine the dependence of the benzene concentration on the ethanol/propene ratio in low-pressure flames with blended fuels (propene/ethanol/oxygen/argon). The C/O ratio of all blends was kept constant at C/O = 0.773 or C/O = 0.600. Ethanol addition ranged from 0 to 15% for flames with C/O = 0.773, and from 0 to 100% for flames with C/O = 0.600. In both data sets, a decrease of the benzene concentration with increasing ethanol percentage was observed. Qualitative information on some other aromatic species with higher mass was also obtained.

© 2007 Published by Elsevier Inc. on behalf of The Combustion Institute.

**Keywords:** Molecular beam mass spectrometry; Electron impact ionization; Resonance-enhanced multiphoton ionization; Laser-induced fluorescence; Thermometry; Ethanol; Propene; Doped flames; Combustion; Oxidation

---

## 1. Introduction

In recent years, tightened regulations for emissions of environmental and health concern from internal combustion engines have stimulated a pronounced interest in nonconventional oxygenated fuels and fuel additives. Ethanol can be used as a fuel extender for

petroleum-derived fuels, an oxygenate, an octane enhancer, and a pure fuel [1]. In a number of recent studies on practical engines, reduction of NO<sub>x</sub> and particulate emissions has been observed when ethanol is added to diesel and gasoline fuels [2–7]. These studies also suggest an increase in acetaldehyde emissions, while other regulated emissions (CO, smoke) are not adversely affected. Furthermore, the production of ethanol from renewable sources such as biomass can balance the emission of carbon dioxide, a major greenhouse gas, from the combustion process. As renewable energy programs in several countries promote the use of oxygenated, biomass-derived fu-

---

\* Corresponding author.

E-mail address: [kkh@pc1.uni-bielefeld.de](mailto:kkh@pc1.uni-bielefeld.de)

(K. Kohse-Höinghaus).

<sup>1</sup> Current address: Institut für Physik der Atmosphäre, Johannes Gutenberg-Universität, 55099 Mainz, Germany.

els, the amount of ethanol combustion could increase and demand a critical evaluation of its performance in combustion applications and of its emission characteristics. Both tasks require a more detailed understanding of the reaction pathways of ethanol oxidation and pollutant formation.

Several previous studies have used ethanol diffusion flames to determine the flame structure [8–10] or to investigate soot formation [11]. Product profiles from ethanol pyrolysis and oxidation studies in static reactors [12–19], flow reactors [20–22], and jet-stirred reactors [23] add to the experimental data base. Several shock tube experiments [24–27] have measured ignition delay times, while other detailed studies of ethanol combustion have included the determination of laminar flame speeds [28,29] and of the sooting behavior [30]. The experimental data cover an extensive temperature, pressure, and stoichiometry range and have led to the development of several chemical kinetic models of ethanol combustion [18, 22,23,25,27,29,31–33].

While many aspects of ethanol combustion have been investigated, nonflame situations, such as reactors and shock tubes, are not necessarily representative of the entire species mix and temperature range encountered under combustion conditions, especially because previous studies have highlighted the temperature sensitivity of the initial decomposition and oxidation reactions of ethanol [21,22,32]. Premixed low-pressure flames are suitable model systems for studying the combustion chemistry by mass spectrometry and have been employed for a number of fuels, e.g., [34–37]. Premixed flame data on ethanol, however, have been limited to one study of a stoichiometric ethanol flame [38] and have thus not been included in the validation of reaction mechanisms. Here, we present flame structure data of a stoichiometric and a fuel-rich ethanol/oxygen/argon flame obtained by EI-MBMS as well as the associated flame temperatures measured by NO-LIF thermometry. All experiments were carried out under conditions similar to those for previous studies by this group, which have included fuels such as propene [39–41], acetylene [41], cyclopentene [42], pent-1-ene [43], and penta-1,3-diene [44].

The use of ethanol as a fuel extender or an oxygenated additive and its ability to suppress the formation of soot in practical applications have been reported [2–7]. However, only a limited number of experimental studies on the effect of ethanol additives on soot formation in simpler combustion situations such as shock tubes [45,46] and flames [47–49] exist and have in part served as a basis for modeling studies [50,51]. The formation of small aromatic structures from linear unsaturated compounds is a major step in the mechanism toward polyaromatic hydrocar-

bon (PAH) and soot production at high temperatures. A key role is attributed to benzene, and several pathways of benzene formation have been identified. Recent reviews [52,53] summarize the present status of the development of reaction mechanisms for the formation of PAH and soot and their validation against experimental data. Since this work was submitted, two further studies have been performed on ethanol addition to a premixed fuel-rich propene flame in our own laboratory [54] and to a nonpremixed fuel-rich ethene flame by McEnally and Pfefferle [55], which indicates the increasing interest in this subject.

In the present paper, concentration profiles of benzene and higher aromatic structures were measured by REMPI-MBMS in a fuel-rich ethanol flame and a propene/ethanol/oxygen/argon flames with varying ethanol fractions. Ethanol flames (this work) and propene flames [39,41] of corresponding stoichiometries have been characterized by EI-MBMS. Trends in the benzene concentration profiles of the mixtures can thus be compared to those in the unblended fuels. The concentration profiles of the higher aromatics extend the data set to a mass and species range that is of significant importance to modeling efforts of PAH production in flames. Temperature effects can be assessed from the respective temperature profiles obtained by NO-LIF.

## 2. Experiment

### 2.1. Flames and sampling systems

All flames are stabilized on the 62.8-mm-diameter, water-cooled, sintered bronze plate of a flat-flame burner. The cooling water has a constant temperature of 80 °C and is also used to temper the burner head and the gas lines. Calibrated mass flow controllers adjust the gas flows. The ethanol flux is set in the REMPI experiment by metering the liquid via a syringe pump (ISCO, 1000D), which generates a highly precise and stable liquid flow, and where a heated vaporizer (125 °C) ensures complete evaporation. For the EI measurements, the ethanol vapor was metered directly by a calibrated valve. Flame conditions are summarized in Table 1. The cold gas velocity (298 K) is 50 cm/s for all flames.

The burner is transferable between the flame chambers of the EI-MBMS system and the REMPI-MBMS system. The flame chamber of the EI-MBMS setup has a smaller diameter than the REMPI-MBMS system, which leads to decreased flame stability due to recirculation of burnt gases. In this case, a quartz tube is mounted on the burner head; it shields and

Download English Version:

<https://daneshyari.com/en/article/169668>

Download Persian Version:

<https://daneshyari.com/article/169668>

[Daneshyari.com](https://daneshyari.com)