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# Influence of substituted furans on the formation of Polycyclic Aromatic Hydrocarbons in flames

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## Abstract

The structure of low-pressure (40 kPa) rich laminar premixed flames of two potential new biofuels, 2,5-dimethylfuran (DMF) and 2-methylfuran (MF), has been investigated using gas chromatography after sampling by a sonic probe. This work follows a study of the same flames made using electron-ionization molecular-beam mass spectrometry (EI-MBMS). Temperature profiles have been measured using a thermocouple with and without the probe and compared with those obtained during EI-MBMS experiments, showing the important influence of the probe geometry. The mole fraction profiles above the burner of numerous products and intermediates (31 for MF, 40 for DMF) have been quantified, including all the isomers which were globalized during EI-MBMS experiments, as well as some heavier aromatic products such as ethylbenzene and styrene. The profiles of these aromatics confirmed their significantly enhanced formation in the case of DMF compared to MF, which was already shown in the previous study. The model of the oxidation of these two substituted furans have been up-dated to include new reactions for the formation of C<sub>8</sub> aromatics, as well as reactions proposed in literature for large Polycyclic Aromatic Hydrocarbons (PAH) formation. Simulations show a significant enhancement effect on the formation of PAH, such as pyrene or phenanthrene: their maximum mole fractions are increased by a factor of more than 400 in the DMF flame compared to that of MF, while it is only a factor 3 in the case of benzene. Simulations show that PAH mole fractions are also slightly larger in the DMF flame than in a flame of a gasoline surrogate containing toluene as an octane improver under the same conditions. However the PAH mole fractions in the DMF flame are significantly lower than in a flame of pure toluene, showing that this biofuel could be an interesting octane improver in replacement of aromatics.

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**Keywords:** 2,5-Dimethylfuran; 2-Methylfuran; Toluene; Laminar premixed flames; PAH

## 1. Introduction

Furan family fuels are being proposed as new promising biofuels which can be produced from non-edible cellulosic biomass [1]. Substituted

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furans, 2,5-dimethylfuran (DMF) and 2-methylfuran (MF), have a high research octane number (RON of 131 for MF and 119 for DMF [2]), which could make them of interest as octane improvers in gasoline. Among these two compounds, DMF has the higher heating value (33.7 MJ/kg for DMF), the closest to that of gasoline (42.7) and diesel fuel (43.0) [2]. Although MF and DMF are oxygenated biofuels, recent work has shown that their ability to form small soot precursors during their combustion is close to that of hydrocarbon fuels [3–5]. Moreover, this potential is much higher in DMF combustion [5]. This unexpected tendency could limit the practical use of substituted furans in engines due to concerns about air quality improvement; it should thus be more thoroughly investigated.

The combustion of substituted furans has been the subject of a large interest in the recent years, with studies performed in flames [4–9], engines [10–12], shock tubes [13–17], and a jet-stirred reactor [17]. The modeling effort has been more limited [13–17].

In the present work, as part of a continuing effort to improve the knowledge on the combustion chemistry of substituted furans, we have reinvestigated the rich ( $\varphi = 1.7$ ) flames of MF and DMF studied by [4,5]. In this previous work, species profiles were fully obtained using electron-ionization molecular-beam mass spectrometry (EIMBMS) in Bielefeld, gas chromatography being only used in Nancy to differentiate between different isomers. In the present work, species profiles were fully obtained using gas chromatography, with the possibility to quantify isomers and products up to  $C_8$  aromatics. As an interesting side result, the temperature profiles obtained using the same flames in the two different set-ups were compared. Our previous model [4,5,16] has been completed with new reactions for  $C_8$  aromatics, as well as with channels accounting for the formation of PAH up to  $C_{16}$  using the mechanism proposed by Slavinskaya and Frank [18]. This updated model has been used to investigate if the enhanced formation of small aromatic compounds in the presence of DMF has an effect on the formation of actual soot precursor molecules, such as pyrene, used as a starting point in soot particle formation models [19,20]. Simulations have also been performed, under the same conditions, for a flame of a ternary n-heptane/iso-octane/toluene blend gasoline surrogate, as well as for flames of the pure compounds included in this blend.

## 2. Method

### 2.1. Experimental methodology

The experimental facilities of low-pressure laminar premixed flat flames used in this study

have been already described in detail in recent work [21]. Chemical species were measured by on-line gas chromatography (GC). In the present study, all the mole fraction profiles in premixed low-pressure (40 mbar) argon-diluted (50%) flat flames of the two substituted furans (MF, DMF) have been measured for the fuel-rich conditions ( $\varphi = 1.7$ ).

Flame temperature was measured with and without sampling probe, using a PtRh (6%)-PtRh (30%) type B thermocouple diameter 100  $\mu\text{m}$ . The thermocouple wire was supported by an arm and crossed the flame horizontally to avoid conduction heat losses. As described in [21], the thermocouple was coated with an inert layer of  $\text{BeO}-\text{Y}_2\text{O}_3$  to prevent catalytic effects when placed in a flame. The ceramic layer was obtained by dipping the thermocouple in a hot solution of  $\text{Y}_2(\text{CO}_3)_3$  (93% mass) and  $\text{BeO}$  (7% mass) followed by drying in a Meker burner flame. Radiative heat losses were corrected using the electrical compensation method.

Analyses were made by GC using a heated (at 423 K) on-line connection to a quartz probe. Two gas chromatographs were used. A first apparatus was equipped with two types of columns (HP-Plot Q, and HP-Molsieve) and two types of detectors, a flame ionization detector (FID) coupled with a methanizer and a thermal conductivity detector (TCD), to analyze argon, water, carbon oxides, and  $C_1-C_8$  organic compounds. A second gas chromatograph was equipped with a Carbosphere column with a TCD to analyze molecular hydrogen and oxygen using argon as carrier gas. In our previous work [21], CO and  $\text{CO}_2$  could only be detected by TCD, and formaldehyde could not be detected. Here, thanks to the methanizer, CO and  $\text{CO}_2$ , as well as formaldehyde, were converted to methane, and could then be detected by FID which is more sensitive (by a factor of 100) than TCD. Stable species were identified by the determination of their individual retention times and by mass spectrometry (GC/MS). Calibrations were made directly using cold-gas mixtures when available. For species for which a direct calibration procedure is not applicable, the calibration factors were estimated, thanks to hydrogenation by the methanizer, to be the same as that of the alkane involving the same number of carbon atoms. The calculated uncertainties of the mole fraction measurements of the quantified species were  $\sim 5\%$  for the major compounds and  $\sim 10\%$  for minor products ( $< 100$  ppm). The FID detection threshold was about 1 ppm, while the TCD detection limit was about 50 ppm for  $\text{H}_2\text{O}$ ,  $\text{H}_2$  and  $\text{O}_2$ . Oxygen and argon were supplied by Messer with a purity of 99.995% and 99.999%, respectively. Liquid MF and DMF were provided by Sigma-Aldrich with a purity better than 99%. The impurities present in the fuel reactants were analyzed by

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