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Effect of furans on particle formation in diffusion flames: An experimental and modeling study

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Abstract

Furans have recently raised as possible transportation fuels which can be produced from biological sources and biotechnological methods. Their role on combustion-generated particle formation results quite unexplored. Few studies showed that dimethylfuran (DMF) among the other furanic hydrocarbons seems to have a great tendency to form soot precursors. This unexpected trend should be kept in mind before a further usage of furans, especially DMF, as transportation fuels.

The effect of furans as substituent to traditional fuels has been investigated both experimentally and numerically in a counter-flow diffusion flame. Furan, 2-methylfuran and 2,5-dimethylfuran have been chosen as standards for furanic fuels. Optical techniques, previously validated, namely laser induced fluorescence and incandescence, have been adopted to detect small nanoparticles and soot aggregates, respectively. On the modeling part, a sectional approach has been used to confirm the sooting tendency experimentally found for the investigated fuels. A gas phase kinetic mechanism available in literature for oxidation and decomposition of furans has been integrated in a recently developed detailed kinetic mechanism for particulate formation.

Experiments confirmed by model show that furanic fuels increase particle production. Furan has the lowest impact on the particle production whereas 2,5-dimethylfuran and 2-methylfuran show a higher propensity; in particular, 2-methylfuran has a greater tendency to produce particles with respect to 2,5-dimethylfuran.

Modeling analysis showed that 2-methylfuran produces large amounts of C₄-species and thus benzene and polycyclic aromatic hydrocarbons (PAHs). 2,5-dimethylfuran mainly forms phenol during its decomposition, which leads to cyclopentadiene and thus naphthalene formation. However, in the operating conditions analyzed in this study the overall PAHs and first particle production result less strong than in 2-methylfuran. However, different combustion conditions can change the effectiveness of these channels and might invert the particle production tendency of furanic fuels.

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1. Introduction

The increase of the contribution of transport systems to the total energy consumption and greenhouse gas emissions requires the formulation of more energetically efficient and environmentally friendly new fuels.

Biofuels from different origins have been identified as a viable alternative to traditional fossil fuels because when used mixed with traditional fuels, they do not require changes to existing internal combustion engines. Consequently, many Countries have announced measures to promote their use in road transportation.

The use of biofuels is mainly related to the mitigation of climate change to produce less net carbon dioxide emissions than conventional fuels. However there is general agreement also about their ability to reduce emissions at the exhaust of conventional motor vehicles [1].

Ethanol is one of the most used oxygenated fuels because it can be obtained from biomass at reasonable cost. Ethanol suffers from several limitations, including low energy density, high volatility, and contamination by the absorption of water from the atmosphere [2]. Recent experimental studies performed in engines and gas turbines using ethanol blends have shown that mixing ethanol with fossil fuels reduces the total emission of particulate matter because smaller size particles are produced with respect to hydrocarbon fuels. Although the reduction of the total mass of the emitted particles is beneficial to the environment [3,4], smaller particles could represent a risk for our health [5].

The search of alternatives to ethanol has focused the attention on furanic fuels as possible transportation fuels which can be produced from biological sources and biotechnological methods. Furanic fuels offer several advantages over current biofuels including their higher energy density close to that of gasoline [6–10].

The behaviors of fuels of the furan family, i.e., furan (F), 2-methylfuran (MF), and 2,5-dimethylfuran (DMF), have been studied in a wide range of experimental facilities including flames, shock-tubes, and engines, in order to investigate the relatively unexplored combustion chemistry of this interesting class of oxygenated hydrocarbons [8–14]. Measurements performed at the exhaust of a gasoline engines [13,14] have shown that furanic fuels, in particular DMF, exhibit very similar combustion and emissions characteristics to gasoline. This indicates that DMF may be suitable to use as an existing gasoline-type engine fuel and that no major modifications and adjustments would be needed to produce an equivalent engine performance and emission levels [13,14].

Different results have been obtained from studies performed in laboratory reactors, such as shock-tubes, jet-stirred reactors and flat-flame

burners which show that burning of furanic fuels produces a larger amount of soot precursors including acetylene, 1,3-butadiene, 1,3-cyclopentadiene, and benzene [8–12]. Experimental data show the surprising ability of DMF among the three furanic hydrocarbons to form soot precursors. This unexpected trend should be kept in mind before a further usage of furanic fuels, especially DMF, as transportation fuels.

We have developed a diagnostic tool to follow the formation of high-molecular mass aromatics and of large soot particles in flames based on laser induced emission [15,16]. A UV laser light source has been used to investigate flames and broadband fluorescence, incandescence and emission lifetimes have been measured. UV and visible fluorescence and incandescence have been associated to high-molecular mass compounds, i.e., nano-sized aromatic structures, and large soot particles, respectively. The technique has been used to study the effect of ethanol [17,18] and dimethyl-ether [19] – DME – addition to ethylene in a counter-flow diffusion flame. Although an increase of both nanoparticle and soot particle concentrations was found in the pyrolytic region of the flame for 10–20% of ethanol and DME used as substituents, a strong decrease of the particulate formation, both nanoparticles and soot, was observed for larger amounts of oxygenated fuels and in the oxidizer side of the flame. The results showed that the role of oxygenated hydrocarbons in the formation of nanoparticles and soot is not always in the sense of reduction, but it strongly depends on the combustion conditions [17–19].

In the present work, we have used the same *in situ* spectroscopic diagnostics to investigate the effect on particulate formation when furanic fuels are used as substituent to ethylene in a counter-flow diffusion flame. The study focuses the attention on the role of biofuels in the formation of fine and ultrafine particles. Furan, 2-methylfuran, and 2,5-dimethylfuran have been chosen as standards for furanic fuels. The amount of furans used as substituent is varied from 10% to 30% of total carbon fed, a range typical of the percentage of biofuels currently used in transport fuels.

2. Experimental methods

A counter-flow burner system was used to stabilize flames of ethylene/furanic fuel blends. The burner consists of two opposed jet nozzles (ID 2.54 cm) vertically positioned; the oxidizer stream is introduced from the upper nozzle while the fuel stream is introduced from the lower nozzle. Flames were stabilized by feeding 25% (volumetric percentage) ethylene-furanic mixtures and 75% Ar as fuel stream, and 22% O₂ and the remaining Ar as oxidizer stream. The oxidizer and fuel stream velocities were fixed at 16.1 and 13.2 cm/s at

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