



# Investigation of the effect of molecular structure on sooting tendency in laminar diffusion flames at elevated pressure



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## ABSTRACT

A specially designed High Pressure Vessel and Burner and fueling system (called “doped flame”) are presented in this paper. This setup allows for soot measurements in laminar diffusion flames of liquid fuel blends at elevated pressure. Fuels with two typical molecular structures, namely linear and saturated cyclic hydrocarbons, are examined in both non-oxygenated (n-hexane ( $C_6H_{14}$ ) and cyclohexane ( $C_6H_{12}$ )) and oxygenated form (1-hexanol ( $C_6H_{14}O$ ) and cyclohexanol ( $C_6H_{12}O$ )). All compounds are blended into n-heptane. Focus of the research is on soot volume fraction at elevated pressure in the range of 1.5–2.0 bar. Sooting tendency is evaluated by means of Laser Induced Incandescence (LII) with Line of Sight Attenuation calibration (LOSA), and the data suggests that soot is more prevalent for cyclic structures relative to their linear counterparts.

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## 1. Introduction

Soot emitted from combustion (e.g. from internal combustion engines) is a major pollutant, and it has been categorized as a known carcinogen for humans and recognized to contribute to environment pollutions. The research of reduction on soot emission is mostly carried out by engine researchers [1]. However, in order to reduce the soot emission from practical combustion devices further, it is requisite to clarify the fundamental mechanism of soot formation in combustion processes. Consequently, studies of soot formation have been published more and more on laminar diffusion flames.

It is well known that soot formation in laminar diffusion flames is strongly affected by system pressure [2,3]. Many studies have focused on soot formation in laminar flames of gaseous fuels at elevated pressure [4–12]. On liquid fuels, however, there is a clear scarcity of data [2,4,13–20], notably under for elevated pressure [14]. Spatial soot distributions in laminar diffusion flames of liquid fuel at elevated pressure have been reported only in our previous paper on n-heptane [18]. This earlier work has primarily focused on understanding the effect of fuel molecular structure on sooting propensity (e.g. [19]). This has resulted in various characteristic parameters to quantify sooting propensity, such as the Threshold Soot Index (TSI [21–25]), Yield Sooting Index (YSI [26,27]) and

Normalized Smoke Point (NSP [20]). In the present paper we will not attempt an exhaustive survey of different fuels, but rather try to separate the effect of fuel molecular structure on sooting propensity in elevated pressure laminar diffusion flames, by carefully selecting four liquid fuels as additive to the n-heptane base fuel. Spatial soot distributions are obtained by means of LII, which is quantified by LOSA [18].

Fuels with two typical molecular structures, linear and saturated cyclic, have been studied in this research. As shown in Fig. 1, fuels in question here are in the non-oxygenate fuels group: n-hexane ( $C_6H_{14}$ ) and cyclohexane ( $C_6H_{12}$ ), as well as the corresponding oxygenate fuels group: 1-hexanol ( $C_6H_{14}O$ ) and cyclohexanol ( $C_6H_{12}O$ ). Their properties are summarized in Table 1. In addition, as its general property is close to that of conventional diesel fuels, n-heptane is chosen as the base fuel, and it will be blended with these four kinds of fuels in certain volumetric percentages in this research.

In the non-oxygenate fuels group, cyclohexane plays a relevant role in practical fuel chemistry due to its significant presence in diesel fuel and jet fuel [28], and in oil-sand derived fuels [29]. However, there are no experimental data on sooting propensity of cyclohexane. n-Hexane has the same carbon number as benzene and has been used to represent paraffin fuels [30]. Therefore, measurements of soot formation in laminar diffusion flames of n-hexane blends and cyclohexane blends (blended in n-heptane), from atmospheric pressure up to 1.5 bar have been carried out in this work. Above 1.5 bar, flame instabilities were too severe to allow measurement.

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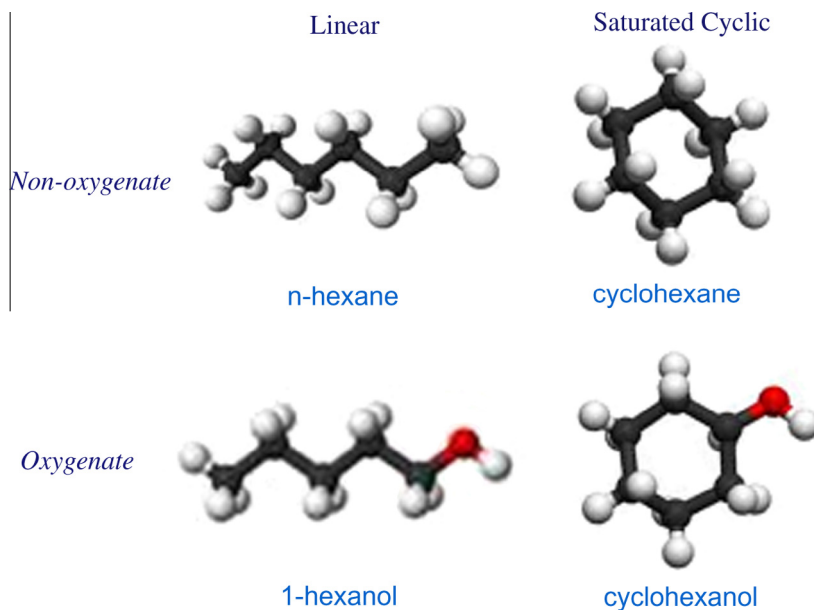


Fig. 1. Structures of studied fuels.

**Table 1**  
Properties of studied fuels.

Name of fuel	Density (kg/m <sup>3</sup> ) (at 15 °C)	Boiling point (°C)	Lower heat value (MJ/kg)	Molar mass (g/mol)
n-Heptane (base fuel)	680	99	45	100
n-Hexane	655	69	45	86
Cyclohexane	779	81	43	84
1-Hexanol	814	158	39	102
Cyclohexanol	962	161	37	100

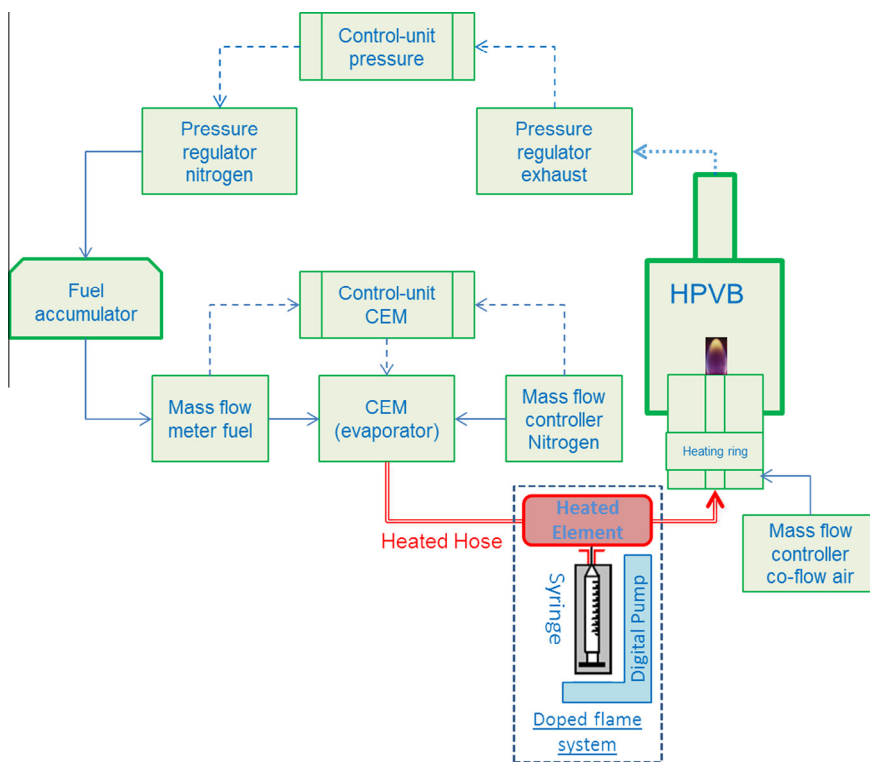


Fig. 2. Layout for liquid fuels setup with 'doped flame' system.

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