



Flammability limits of iso-butanol/iso-octane/n-heptane blends



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ABSTRACT

A set of experiments was carried out to determine the flammability limits (FL) of blends of *iso*-butanol and a surrogate fuel for gasoline at 154 ± 11 °C and ≈ 91.4 kPa. The surrogate gasoline was a binary PRF mixture of 87% *iso*-octane and 13% *n*-heptane (PRF 87). The volumetric fraction of *iso*-butanol in the liquid fuel was varied from 0 to 0.25 at a step of 0.05. Flammability tests with pure fuels were also performed to confirm the reliability of the applied experimental procedure. The homogeneous air/fuel mixtures were defined as flammable when formed a self-sustained flame able to travel upward a 0.3 m long open combustion tube. The lower FL of the blends of *iso*-butanol and PRF 87 (0.80–0.98%) were estimated correctly with the mixing rule of Le Chatelier, but the same simplified model failed to reproduce the measured upper flammability limits (5.10–5.61%).

1. Introduction

The use of fuels from renewable sources has been encouraged around the world mainly because of the difficulty of exploration of the still enormous amounts of fossil reserves in a way that does not increase the already serious concerns regarding the global warming [1,2]. In spite of the many well-known disadvantages of bioethanol when compared to higher chain alcohols as a transportation biofuel [3,4], it has been extensively used as a potential additive [5], or substitute to gasoline. The primary reason for it was the difficulties to produce higher chain alcohols via fermentation with native microorganisms, a drawback that has now been partially solved because of recent advances in the anaerobic fermentation (via the well-known ABE process) and in non-fermentative pathways, mainly for biosynthesis of biobutanol isomers [6–8,3].

Among biobutanol isomers that emerge as next-generation biofuels, particular attention has been paid to *iso*-butanol [8,9]. It has all the properties that make the other butanol isomers specially attractive for combustion in vehicles summarized in the literature [10,8,3,4]. Moreover, it presents the benefit of having a higher octane rating (RON 94) when compared to *n*-butanol (RON 78), *sec*-butanol (RON 32) and *tert*-butanol (RON 89) [10]. It is also less toxic than renewable *n*-butanol now obtained industrially from ABE fermentation [7], and it may be produced from modified ethanol plants that involve grains, cellulose or sugarcanes as raw materials [8].

As far as the authors know, at least two important chemical companies are at advanced stages to produce commercially *iso*-butanol

(Gevco Inc., BP-Dupont joint venture) [7,8]. Because one of the most expected large-scale applications of *iso*-biobutanol is as a gasoline blendstock [11,7,8,9], flammability limits of mixtures of *iso*-butanol and gasoline, unavailable in the literature, will be necessary to mitigate risks of fires and explosions mainly when such blends will be piped and stored at refineries [8]. FL are in general one of the most important safety parameters for risk assessment in plants that operate with flammable substances [12,15,14,13]. It basically explains the main aim of the current study, that is, to determine experimentally FL of *iso*-butanol/surrogate gasoline blends in air.

The main reason for using a surrogate fuel instead of a real gasoline was to have data of flammability limits that could be more easily reproduced in future studies by predictive methods, such as those based on chemical equilibrium or detailed kinetic models (ignition codes able to describe the ignition of a mixture of fuels) (e.g.; [16]). It is important to remember that gasoline is a complex mixture of different kinds of hydrocarbons that presents significant variation in composition depending on the origin. Such a factor and the hard task of accommodating all their species in a computational code make it difficult to compute FL of an actual gasoline. However, it does not mean that the chosen surrogate fuel is a reliable model for gasoline in terms of flammability limits. Blends of *iso*-octane/*n*-heptane were basically used as a gasoline surrogate because they are simple binary mixtures that have been extensively studied to emulate target properties of real gasoline, such as; ignition delay time, laminar burning velocities [17].

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Nomenclature

ABE	acetone-butanol-ethanol
FL	flammability limits
LFL	lower flammability limit (%)
LFL_{calc}	lower flammability limit calculated with the rule of Le Chatelier (%)
P	pressure of unreacted gases in the combustion tube (91.4 kPa)
Q_a	volumetric flow rate of air at T and 91.4 kPa ($\text{m}^3 \text{s}^{-1}$)
$Q_{a,25}$	volumetric flow rate of air at 25 °C and 91.4 kPa ($\text{m}^3 \text{s}^{-1}$)
Q_{lf}	volumetric flow rate of liquid fuel ($\text{m}^3 \text{s}^{-1}$)
Q_{vf}	volumetric flow rate of vapor fuel at T and 91.4 kPa ($\text{m}^3 \text{s}^{-1}$)
R	universal gas constant (8.314 $\text{m}^3 \text{kPa K}^{-1} \text{kmol}^{-1}$)
R^2	coefficient of determination for Eqs. (1) and (2).
ρ_{lf}	density of pure liquid fuels (kg m^{-3})
T	temperature of unreacted gases in the combustion tube (°C)

UFL	upper flammability limit (%)
UFL_{calc}	upper flammability limit calculated with the rule of Le Chatelier (%)
W	molar mass of pure fuels (kg kmol^{-1})
x_i	molar fraction of the i th pure fuel in the fuel blend ($\text{m}^3 \text{m}^{-3}$)
x_{iso}	molar fraction of the <i>iso</i> -butanol in the fuel blend ($\text{m}^3 \text{m}^{-3}$)
y	fuel volumetric fraction in the vapor fuel/air mixture ($\text{m}^3 \text{m}^{-3}$)
y_{iso}	volumetric fraction of <i>iso</i> -butanol in the vapor fuel/air mixture ($\text{m}^3 \text{m}^{-3}$)
y_{gas}	volumetric fraction of the gasoline surrogate in the vapor fuel/air mixture ($\text{m}^3 \text{m}^{-3}$)
z_i	volumetric fraction of the i th pure fuel in the liquid fuel blend ($\text{m}^3 \text{m}^{-3}$)
z_{iso}	volumetric fraction of <i>iso</i> -butanol in the liquid fuel blend ($\text{m}^3 \text{m}^{-3}$)

2. Materials and methods

The flammability tests were carried out in a cylinder whose dimensions were in accordance with the German DIN 51649 standard method for determination of explosion limits, that is, a glass open tube 0.06 m diameter and 0.3 m high [18]. At the base of the combustion tube, and in the vicinity of an electric arc igniter, there was a porous glass plate to promote the good mixing between the vapor fuel and air. To vaporize the liquid fuel, the fuel/air mixture was early passed through a copper serpentine (1.27×10^{-2} m internal diameter and 1.5 m long) placed inside an oven with a PID control of temperature (400–2ND, Ethik Technology, Vargem Grande Paulista, Brazil). The liquid fuel with a known flow rate was introduced into the serpentine by a calibrated peristaltic pump (1001, Milan, Colombo, Brazil). Air at approximately 25 °C and 91.4 kPa was also admitted at the entrance of the serpentine from a 746 W high-pressure blower (MSV 6/30, Schulz S.A., Joinville, Brazil). To perform the flammability tests in the combustion tube with different volumetric fractions of vapor fuel, a condition needed to determine the FL, the air flow rate at 25 °C was manually controlled with a needle valve and measured with a rotameter (0–5 L min^{-1} , RMA-26-SSV, Dwyer Instruments Inc., Michigan City, USA; or 0–15 L min^{-1} , Central Scientific Company, Chicago, USA).

As it has been conventionally done [19], the FL were estimated with Eqs. (1) and (2):

$$LFL = \frac{y_{h,n} + y_{l,f}}{2} \quad (1)$$

$$UFL = \frac{y_{h,f} + y_{l,n}}{2} \quad (2)$$

where $y_{h,n}$ and $y_{l,f}$ represent the highest and the lowest fuel volumetric fractions in a lean non-flammable and flammable mixture, respectively. $y_{h,f}$ and $y_{l,n}$ are instead the highest and the lowest fuel volumetric fractions in a rich flammable and non-flammable mixture, respectively. Direct observation of propagation of a self-sustained upward flame from the igniter up to the top of the open combustion tube (i.e.; 0.3 m) was the criterion that defined a tested fuel/air mixture as flammable.

The fuel volumetric fraction was basically assessed from the known volumetric flow rates of vapor fuel (Q_{vf}) and air (Q_a) at the temperature T and pressure P (always close to 91.4 kPa) at which the flammability test was conducted, as given by Eq. (3).

$$y = \frac{Q_{vf}}{Q_{vf} + Q_a} \quad (3)$$

Q_{vf} was computed with Eq. (4), based on the measured volumetric flow rate of liquid fuel (Q_{lf}), the known volumetric fractions of liquid fuel in the fuel blend (z_i), and the physical properties of the pure fuels presented in Table 1 (i.e.; W_i and $\rho_{lf,i}$). The air volumetric flow rate at the inlet temperature of the unreacted gases was calculated with Eq. (5) as a function of the measured air flow rate at 25 °C ($Q_{a,25}$).

$$Q_{vf} = \frac{R(T + 273.15)Q_{lf}}{P} \sum_{i=1}^n \frac{z_i \rho_{lf,i}}{W_i} \quad (4)$$

$$Q_a = Q_{a,25} \frac{T + 273.15}{298.15} \quad (5)$$

A set of 5 different available commercial solvents were used as fuels (acetone, ethanol, *iso*-butanol, *iso*-octane, *n*-heptane), but the first two were merely burned to validate the flammability tests. The companies that produced them, their purities, normal boiling points, densities at 25 °C, and molecular masses are summarized in Table 1.

The lower flammability limits (LFL) and upper flammability limits (UFL) of the pure fuels in air were individually determined at three different temperatures, always above their boiling points at the examined atmospheric pressure (≈ 91.4 kPa). Based on the well-known linear dependence of FL on temperature [21–23,34], a linear regression model with parameters tuned on the experimental data was suggested to estimate such a property at temperatures different from those considered experimentally (see Eqs. (6) and (7)). These calculated FL were compared with analogous results available in the literature to check the reliability of the flammability tests [25–27].

All the values of flammability limits from the literature reported in such a study were based on flammability experiments performed at atmospheric pressure by involving air as oxidant. However, except for the data from Zabetakis et al. [27], the references that present them are a compilation of results obtained by different authors that not necessarily used the same apparatus and the same procedure to obtain them. Anyway, it is well-accepted in the literature that minor differ-

Table 1
Fuels used in the flammability tests and some of their physical properties [20].

Fuel	Purity	Company	Boiling point (°C)	ρ_{lf} at 25 °C (kg m^{-3})	W (kg kmol^{-1})
Acetone	99.5	Biotec	56	791	58.1
Ethanol	99.5	Labsynth	78.4	789	46.1
<i>iso</i> -butanol	99.5	Neon	108	802	74.2
<i>iso</i> -octane	99.84	Neon	99.5	692	114.2
<i>n</i> -heptane	99.0	Vetec	98.4	690	100.2

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