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The influences of pressure and temperature on laminar flame propagations of n-butanol, iso-octane and their blends

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ABSTRACT

On one hand, n-butanol as a potential alternative bio-fuel is accepted more and more attention presently in the fields of both scientific research and commercial market; on the other hand, some n-butanol's (or its mixtures blended with conventional fossil fuels) combustion properties, especially the flame propagation characteristic, are still unknown widely or profoundly, especially under the ICE (internal combustion engine) operating conditions. Within these conditions, pressure and temperature are two critical factors affecting the flame's propagation characteristic. Driven by these facts, in this study, we investigated the laminar flame characteristics of n-butanol, iso-octane and their blends by simulations. First, the experimental data on n-butanol's laminar burning velocity were collected, and the development of n-butanol's chemical kinetic mechanisms was reviewed. Then, the mechanisms used in this study can be chosen, and the numerical results can be validated by experimental data. Based on this, we extended the condition range, which is limited in experimental measurements, to that of realistic applications by numerical method; besides, correlations including the influences of pressure and temperature are developed and extended to consider the mixture fuel blended between n-butanol and iso-octane (which represents the gasoline in S_L, laminar burning velocity), this is useful to use the alcohol fuels for SI (spark-ignition) engines in an even better fashion; furthermore, their correlated parameters were resolved carefully through a wide range of data. From results, our correlations are sufficient in accuracy to describe the effects mentioned above. Within each effect, for better understanding the apparent influence on S_L, the effects of thermal, density ratio and chemical kinetic are discussed respectively. In addition, our correlations were compared to those in literature widely; these comparisons suggested that the inherent law of laminar flames of fuels still deserves more attentions and investigations. Our investigation is expected to make a step on the understanding of this field.

1. Introduction

Biofuels are receiving increasing public and scientific attentions [1–8], driven by factors such as the shortage of fossil oil supplying, the continued global environmental pollution, and the need for increased energy security and diversity. The governments of more than 35 countries, including the United States, Brazil and members of the European Union, have established policies promoting the production and use of biofuels [9]. Biofuels include a wide range of varieties which are in some way derived from biomasses. Although ethanol is currently the dominated biofuel, followed by biodiesel [10], bio-butanol has been proposed as a next-generation biofuel for vehicles to substitute or supplement gasoline due to its superior physical and chemical properties in terms of the energy per unit weight, volatility, causticity and its compatibility to the existing fuel storage and distribution infrastructures, as summarized in Ref. [11]. The comparison of properties between iso-octane and n-butanol is reported in Table 1.

In the aspect of butanol application used as the ICE (internal combustion engine) fuel, a series of investigations have been conducted by several research groups [12–39]. Among these studies, butanol exhibited its advantages that bring positive effects to ICEs. For example, in SI (spark-ignition) engines applications, butanol/gasoline blends produce lower CO and HC emissions but higher NOx emissions due to more complete combustion of butanol [14,15]. Of course, the higher combustion efficiency of butanol/gasoline blends is partially attributed to more advanced ignition timing relative to pure gasoline operation [16], but this is exactly caused by butanol's superiority since it has higher knocking resistance. Furthermore, butanol produces faster combustion relative to

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Table 1
Typical properties of iso-octane and n-butanol.

	iso-Octane	n-Butanol
Chemical formula	i-C_8H_{18}	n-C_4H_9OH
Composition (C,H,O) (mass%)	84,16,0	65,13.5, 21.5
Lower heating value (MJ/kg)	44.34	33.0
Density (kg/m^3)	691.9	810
Octane number (R + M)/2	95–96	89
Boiling temperature (°C)	99.3	118
Latent heat of vaporization (kJ/kg)	307.7	716
Self-ignition temperature (°C)	410	343
Stoichiometric air/fuel ratio	15.1	11.2
Calorific value of stoichiometric mixture (MJ/kg)	2.75	2.70
Adiabatic flame temperature (K)	2325	2315
Solubility in water at 20 °C (ml/100 ml H_2O)	<0.1	7.7

gasoline [17,19–21]. In addition, butanol can decrease the PM (particle matter) emissions and their size [19–22]. However, butanol also exhibited some disadvantages, such as the lower heat value relative to gasoline, and poorer evaporation and atomization [19,21], which may deteriorate the engine's performances [12,13]. Even more worrying is that, as illustrated by Aleiferis et al. [21], the injection butanol or its blend fuel would be more likely to impinge chamber wall due to its poorer atomization in the latest direct-injection SI combustion system application.

From above analysis, it seems that we need to redesign or adjust the existing engines to match the alternative fuels' properties, since the effects brought by butanol are very dependent on a specific engine and its operating strategies. These factors will affect the combustion environment represented by parameters such as pressure, temperature, fuel-air composition and dilute level surrounding the fuels. Obviously, the pressure and temperature are two critical parameters since they will interact with other parameters, and they are determined by engine design (such as the engine compression ratio) at a certain extent. Therefore, understanding completely the flame properties of fuels linked to those parameters is no doubt an important way to make better use of an alternative fuel. Regarding this issue, several experiments have been performed on butanol's premixed flame characteristic, see next section for details.

As a consecutive study on the n-butanol application in conventional engines, we provided insight into the laminar burning velocity, S_L, of n-butanol, iso-octane and their blends by numerical method in the present work. Iso-octane is chosen as basis conventional fuel species because it is commonly considered as a main component of gasoline surrogate, also because its value of S_L is very similar to that of PRF (primary reference fuel) or gasoline [40]. The main objectives of the present endeavor are listed as follows: a): to collect the experimental data on the butanol S_L from literature; b): to extend the existing experimental condition range to the realistic-used SI engine operating conditions (pressure and temperature) by numerical method. Sorting out the reaction kinetic mechanisms of n-butanol, as a result, is also within this objective; and c): to extend the existing correlations, or develop new correlation items, of S_L to n-butanol and its blends mixing with iso-octane. Also, the pressure and temperature's power rules developed by other groups in literature are collected for comparing. To the best of the authors' knowledge, this is the first time to present such a wide set of data for S_L of n-butanol and its iso-octane blends. Therefore, this systemic work is not only presented for understanding fundamentally the combustion characteristics of n-butanol and its iso-octane blends, but also useful, as a start point, to further study the turbulent flames of them, such that the effects brought by n-butanol in conventional gasoline engines can be more clearly understood.

2. Collection of measurements of butanol's laminar burning velocity

It is no doubt that S_L is a key property of fuels as it embodies the physicochemical properties of combustible mixtures such as reactivity, diffusivity and exothermicity. Additionally, S_L is the basic parameter in the turbulent flame modeling into which the local fluid turbulent parameters must be coupled. Furthermore, S_L has been constantly used to validate the chemical kinetic mechanism. In view of this, some studies about butanol's S_L, although not so extensive as conventional fuels or ethanol, have been published, as summarized in Table 2. A brief description about the experiment of butanol's laminar premixed flame is presented here. Firstly, from the view point of the isomers of butanol, the same trend for the S_L of the four butanols: n-butanol > s-butanol ≈ i-butanol > t-butanol is observed by several groups [53,55,61]. In fact, from the previous publications and the surveys by Sarathy's group [41,66], the n-butanol is almost the only one isomer among the four isomers used in conventional engines. Secondly, concerning the alcohol-based serial fuels (C_1–C_4 alcohols), methanol burns significantly faster than the other alcohols for equivalence ratios greater than one; ethanol has the lowest maximum S_L of all four alcohols at an equivalence ratio of 1.1; for equivalence ratios between 0.8 and 1.1, ethanol, n-propanol, and n-butanol are burning with nearly the same S_L within a range of 5% difference; the maximum difference between methanol and the other alcohols is around 15% for rich mixtures [42,52,62]. Finally, n-butanol has larger S_L when compared to fossil-based gasoline [50] or iso-octane [55,58,59], and

Table 2
Overview of the butanol and its blend fuels burning velocity measurements.

Year	Author	Ref.	Technique	Fuel/isomer	T (K)	P (atm)	ø	f (v%)
2009	Sarathy et al.	[48]	Combustion bomb	n-Butanol	350	0.89	0.8–1.4	0
2009	Gu et al.	[49]	Combustion bomb	n-Butanol	413–473	1–2.5	0.8–1.7	0
2009	Beeckmann et al.	[50]	Combustion bomb	iso-Octane, Ethanol, n-Butanol	373	10	0.8–1.3	0
2010	Beeckmann et al.	[51]	Combustion bomb	iso-Octane, gasoline, and their ethanol- or n-butanol- blends	373	10	0.7–1.3	0
2010	Veloo et al.	[52]	Counterflow burner	Methanol, Ethanol, n-Butanol	343	1	0.7–1.5	0
2010	Gu et al.	[53]	Combustion bomb	Four isomers of butanol	428	1–7.5	0.7–1.5	0
2011	Gu et al.	[54]	Combustion bomb	tert-Butanol	428–488	1–5	0.8–1.5	0
2011	Veloo et al.	[55]	Counterflow burner	Four isomers of butanol	343	1	0.8–1.5	0
2011	Broustail et al.	[56]	Combustion bomb	n-Butanol- and ethanol-iso-octane blends	400	1	0.8–1.4	0
2011	Gu et al.	[57]	Combustion bomb	n-Butanol	428	1	0.8–1.5	15
2011	Liu et al.	[58]	Combustion vessel	n-, iso-Butanol	353	1, 2	0.7–1.6	0
2012	Broustail et al.	[59]	Combustion bomb	n-Butanol- and ethanol-iso-octane blends	423	1–10	0.7–1.4	0
2013	Zhang et al.	[60]	Combustion bomb	n-Butanol-iso-octane blends	353–433	1	0.8–1.5	0
2013	Wu and Law	[61]	Dual-chamber vessel	Four isomers of butanol	353, 373	1, 2, 5	0.7–1.4	0
2014	Beeckmann et al.	[62]	Combustion vessel	Methanol, ethanol, n-propanol, and n-Butanol	373	10	0.7–1.2	0

Note: T represents unburnt temperature in K, P represents unburnt pressure in atm, ø is equivalence ratio, and f is the diluent volume fraction.