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Laminar burning characteristics of 2,5-dimethylfuran and *iso*-octane blend at elevated temperatures and pressures

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ABSTRACT

2,5-Dimethylfuran, known as DMF, is a promising second-generation biofuel candidate. The potential of 2,5-dimethylfuran as an additive in *iso*-octane (used as gasoline fuel substitute in this study) was studied. Using outwardly spherical flame method and high speed schlieren photography, laminar burning characteristics of 2,5-dimethylfuran/*iso*-octane (20%/80% vol., designated as D20)/air mixtures were experimentally investigated. Laminar flame speeds and Markstein lengths of D20–air mixtures were empirically organized as a function of initial pressures and temperatures. Onset of cellular structures at the flame front was observed at relatively higher initial pressures due to the combined effect of diffusional-thermal and hydrodynamic instabilities. Laminar flame speeds of D20–air mixtures are higher than those of *iso*-octane–air mixtures when the equivalence ratio is greater than 1.2.

1. Introduction

2,5-Dimethylfuran (DMF), which can be massively produced from non-food biomass [1–3], has been regarded as a promising second-generation biofuel candidate. Compared to ethanol (the favored gasoline-alternative biofuel), DMF has a higher energy density, a higher boiling point and a higher research octane number (RON) [1,4]. It is insoluble in water, thus will not contaminate underground water during production or storage. It has the potential to become an alternative to fossil fuels and octane improver.

Most of previous work focused on the fundamental combustion characteristics [5–7] of DMF. Possible reaction pathways of DMF were proposed by Wu et al. [8] using the experimentally measured flame structure of the low-pressure premixed laminar DMF–O_2–Ar flame with tunable vacuum ultraviolet synchrotron radiation photoionization and molecular-beam mass spectrometry. Practically, Zhong et al. [9] studied the engine performance and emissions of DMF at fixed spark timing regardless of load in a direct-injection spark-ignition single cylinder research engine. Daniel et al. [10] compared the engine performance and emissions of DMF, gasoline and ethanol under gasoline MBT ignition timing and fuel-specific ignition timing in the same engine. These engine studies suggest that the resistance of DMF to knock is not as high as expected and lower than that of ethanol. Wu et al. [11] studied the flexible, bi-fuel concept – dual-injection strategy on a spark-ignition engines fueled with various gasoline, DMF and ethanol blends and they proposed that dual-injection strategy is a promising engine concept.

Laminar flame speed is an important fundamental physico-chemical property of a fuel–air mixture, which can be used to validate the chemical reaction mechanisms and to gain a better understanding of the combustion process, such as the turbulence combustion in SI engines and power generation systems [12]. Wu et al. [13–15] studied the laminar flame speeds, Markstein lengths and flame instabilities of DMF–air premixed mixtures at elevated temperatures and pressures over a wide range of equivalence ratios. Tian et al. [16] studied the flame propagation characteristics of DMF using the schlieren optical method. They found that the laminar flame speed of DMF was very similar to gasoline and the difference was within 10% in the equivalence ratio range 0.9–1.1.

Practical options of using DMF as engine fuel should consider it as an additive to primary fuel so as to avoid large modifications of the combustion devices. *Iso*-octane is widely used as gasoline alternate in fundamental combustion study. Thus, it is necessary to study the laminar combustion characteristics of DMF and *iso*-octane blend, which are important for assessing the possibility of DMF as an alternative for fossil fuels or octane improver. Laminar flame speed is useful for the analysis and performance predictions of various spark ignition engines. The objective of the present work is to provide fundamental laminar flame data of DMF and *iso*-octane

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Nomenclature

DMF	2,5-dimethylfuran
D20	20% by volume of 2,5-dimethylfuran in *iso*-octane
E20	20% by volume of ethanol in gasoline
f	laminar burning flux
L_b	Markstein length of the burned gas
M15	15% by volume of methanol in gasoline
M30	30% by volume of methanol in gasoline
MTBE	methyl *t*-butyl ether
P	initial pressure
RON	research octane number
r_u	instantaneous flame radius
SD	*standard deviation*
S_l	unstretched flame propagation speed
S_n	stretched flame propagation speed
T	initial temperature
T_a	adiabatic flame temperature
u_l	laminar flame speed
α	stretch rate
α_T	temperature exponent
β_p	pressure exponent
δ_l	flame thickness
ρ_u	density of unburned gases
ρ_b	density of burned gases
σ	density ratio
ν	kinematic viscosity of the unburned mixture
φ	equivalence ratio

blend at elevated temperatures and pressures over a wide range of equivalence ratios using the spherical flame method and high speed schlieren photography. The fuel blend investigated here contains 20% DMF and 80% iso-octane in volume (designated as D20).

2. Experimental setup and procedures

The details of the experimental setup are reported in previous literatures [15,17,18]. Briefly, the experimental setup consists of a combustion chamber with the heating system, a high-speed schlieren photography system, a mixture preparation system, an ignition system and a data acquisition system. The cylindrical chamber (Inner diameter: 180 mm; Volume: 5.5 l) has two quartz windows of 80 mm diameter. A Redlake HG-100 K digital camera record the flame images with a frame speed of 10,000 frames/s during the combustion.

The chamber was first heated to the required equilibrium temperature and the pre-blended liquid fuel (purity levels: DMF-99.0%, *iso*-octane-99.5%) was injected into the chamber by the micro-syringe. The required gases (purity levels: O_2-99.99%, N_2-99.99%) were introduced into the chamber according to their corresponding partial pressures. The mixtures of nitrogen and oxygen with a molar ratio of 3.76 were used to simulate air in this study. After filling, the chamber was left undisturbed for at least 5 min to ensure attainment of an approximate quiescent condition. The mixtures were ignited by the centrally located electrodes and the flame propagation was recorded by the high-speed digital camera. The chamber was then vacuumed and flushed with fresh air at least three times before next run.

The test matrix and major results (adiabatic flame temperature, density of unburned mixture, density ratio, laminar flame speed and Markstein length) of this study are summarized in Table 1. The initial pressures and temperatures were set at 0.10 MPa, 0.25 MPa, 0.50 MPa and 393 K, 433 K, 473 K, respectively, while the equivalence ratios varied from 0.9 to 1.5 in 0.1 intervals. A minimum initial temperature of 393 K was selected to ensure that D20 can be completely vaporized before the ignition (boiling points of DMF and *iso*-octane are 365 K and 372 K, respectively). The experiments were repeated twice at each condition and the average data is used in the analysis.

Table 1
Test matrix and results.

φ		0.9	1.0	1.1	1.2	1.3	1.4	1.5
P_u = 0.10 MPa, T_u = 393 K	T_a (K)	2256	2332	2344	2298	2229	2156	2083
	ρ_u(kg/m^3)	0.92	0.93	0.93	0.94	0.94	0.95	0.95
	σ	6.05	6.33	6.47	6.47	6.42	6.35	6.26
	L_b (mm)	3.92	2.36	1.98	1.54	1.03	0.57	0.02
	u_l (m/s)	0.44	0.47	0.50	0.51	0.47	0.40	0.33
P_u = 0.10 MPa, T_u = 433 K	T_a (K)	2280	2353	2367	2328	2263	2191	2119
	ρ_u(kg/m^3)	0.84	0.84	0.85	0.85	0.85	0.86	0.86
	σ	5.55	5.80	5.94	5.96	5.92	5.86	5.79
	L_b (mm)	5.38	3.31	2.2	1.82	1.79	0.74	0.1
	u_l (m/s)	0.52	0.55	0.57	0.59	0.60	0.51	0.42
P_u = 0.10 MPa, T_u = 473 K	T_a (K)	2305	2374	2391	2357	2296	2227	2157
	ρ_u(kg/m^3)	0.77	0.77	0.78	0.78	0.78	0.79	0.79
	σ	5.14	5.36	5.49	5.52	5.50	5.45	5.39
	L_b (mm)	6.1	3.46	2.2	1.92	1.8	1.02	0.59
	u_l (m/s)	0.59	0.61	0.65	0.67	0.67	0.63	0.54
P_u = 0.25 MPa, T_u = 393 K	T_a (K)	2274	2360	2365	2308	2234	2159	2085
	ρ_u(kg/m^3)	2.31	2.32	2.33	2.34	2.35	2.37	2.38
	σ	6.09	6.39	6.52	6.50	6.43	6.35	6.27
	L_b (mm)	1.13	1.08	0.76	0.75	0.28	−0.35	−0.32
	u_l (m/s)	0.31	0.35	0.42	0.44	0.40	0.32	0.31
P_u = 0.50 MPa, T_u = 393 K	T_a (K)	2286	2379	2378	2314	2237	2160	2086
	ρ_u(kg/m^3)	4.62	4.64	4.66	4.69	4.71	4.73	4.75
	σ	6.12	6.43	6.55	6.51	6.44	6.36	6.27
	L_b (mm)	0.8	0.36	0.3	0.22	−0.44	−0.49	−0.93
	u_l (m/s)	0.28	0.32	0.38	0.37	0.34	0.31	0.23