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Review on the production methods and fundamental combustion characteristics of furan derivatives

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ABSTRACT

Furan derivatives (DMF (2,5-dimethylfuran), MF (2-methylfuran), and furan) are the attractive oxygenated fuels to reduce the consumption of fossil fuel and engine emissions due to their comparable combustion properties to those of commercial gasoline and the productivities from lignocellulosic raw materials. Many experimental studies have been focused on these promising fuel characteristics including laminar burning velocities, laminar flame structures, ignition delay times, and pyrolysis species. Various kinetic mechanisms have been developed in detail as well based on up to date experimental data in accordance with the quantum chemical calculations. In the present study, the vast amount of experimental data have been collected, consolidated, and reviewed along with the kinetic model validations in order to envision a future fuel research on furan derivatives for minimizing the experimental uncertainties, improving the data fidelity, and developing accurate kinetic models.

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1. Introduction

Depletion of fossil fuels and the corresponding environmental effects lead to a wide investigation on alternative fuels. Biofuels, such as methanol and ethanol, have been blended with gasoline as transportation fuels in many countries [1–3]. Bioethanol could greatly reduce engine emissions while the lower heating value increases the transportation costs and the solubility in water poses a threat to water security. These intrinsic disadvantages hinder the practical utilization of bioethanol. Furan derivatives (DMF (2,5-dimethylfuran), MF (2-methylfuran), and furan) are representatives of the second generation biofuels [4], as well as bioethanol. Compared with bioethanol, furan derivatives have higher heating values which are closer to that of gasoline, as shown in Table 1.

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Table 1
Properties of furan derivatives, ethanol, gasoline, and diesel.

Fuel	DMF	MF	Furan	Ethanol	Gasoline	Diesel
Molecular formula	C_6H_8O	C_5H_6O	C_4H_4O	C_2H_5OH	C_4–C_{12}	C_{12}–C_{25}
Oxygen content (wt%)	16.7	19.5	23.5	34.8	0	0
Boiling point (K)	366.5[a]	336.0[b]	305.2[c]	351.6[d]	303–473[d]	443–633[d]
Lower heating value (MJ/kg)	33.7[b]	30.4[e]	29.5[f]	26.8[d]	42.7[d]	43[d]
Research octane number	119[b]	131[b]	–	120[d]	95[d]	–

[a] Collected from Weast et al. [5].
[b] Collected from Leshkov et al. [6].
[c] Collected from Tran et al. [7].
[d] Collected from Ballerini et al. [8].
[e] Collected from Thewes et al. [9].
[f] Calculated by the present work.

Moreover, the insolubility of furan derivatives in water avoids aqueous insecurity. Recently, several improved production methods of DMF were proposed by Zhao et al. [10], Leshkov et al. [6], and Mascal et al. [11]. These replenish the production processes of furan derivatives and greatly accelerate the research on DMF. The subsequent comparative studies of DMF based on the structural similarity favor the investigation of MF and furan. As oxygenated unsaturated cyclic esters, furan derivatives are expecting to exhibit different characteristics from hydrocarbon fuels. The previous engine tests showed that the trade-off between NO_x and soot in diesel engines with more than 40% fraction of DMF is greatly alleviated [12] while the combustion and emission behaviors of pure DMF in spark ignition engines are similar to those of gasoline [13]. To better understand these phenomena and improve the in-cylinder simulation, a series of investigations were conducted on the combustion characteristics of furan derivatives, including laminar burning velocities, laminar flame structures, ignition delay times, and kinetic studies, as shown in Table 2.

The potential harmfulness of the fuel should be fully understood before the practical implementation. For furan derivatives, some studies have been carried out on their biological accumulation and toxicity. Perbellini et al. [45] investigated the biological concentrations of DMF. The authors found that the concentration levels of DMF are below the limit of detection in alveolar air and blood, but always detectable in urine. Moreover, the levels of DMF in biological media of smokers are higher than those of non-smokers. Alonso et al. [46] pointed out that DMF is a major source of environmental tobacco smoke and is detectable from the passive smokers. Phuong et al. [47] predicted persistence, bio-accumulation, and aquatic toxicity of DMF and its derivatives using computational toxicology methods. Results showed that DMF has moderate-level aquatic toxicity, but no bioaccumulation concerns,

Table 2
Sources of research conducted on furan derivatives.

Fuel	Author/ year	Research
Laminar burning velocities		
DMF	Wu et al. [14], 2009	Laminar burning velocities in constant volume bomb (P=1 bar, T=393 K, ϕ=0.9–1.5), N_2 and CO_2 dilution (0–15%)
	Tian et al. [15], 2010	Laminar burning velocities in constant volume bomb (P=1 bar, T=323, 348, and 373 K, ϕ=0.6–2.0, DMF, ethanol, and gasoline)
	Wu et al. [16,17], 2010	Laminar burning velocities in constant volume bomb (P=1, 2.5, 5, and 7.5 bar, T=393 K, ϕ=0.8–1.5) Laminar burning velocities in constant volume bomb (P=1 bar, T=393, 433, and 473 K, ϕ=0.9–1.5)
	Qianqian Li et al. [18], 2011	Laminar burning velocities in constant volume bomb (P=1 bar, T=393 K, ϕ=0.9–1.5), N_2 and CO_2 dilution, DMF and *iso*-octane blends: D00 (0%DMF in *iso*-octane by volume), D10, D20, and D30
	Wu et al. [19], 2011	Laminar burning velocities in constant volume bomb (P=1, 2.5, and 5 bar, T=393, 433, and 473 K, ϕ =0.9–1.5), D00 and D20
MF	Ma et al. [20], 2013	Laminar burning velocities in constant volume bomb (P=1 bar, T=333, 363, and 393 K, ϕ=0.8–0.9). MF and *iso*-octane blends: MF, MF20 (20% MF in *iso*-octane by volume), MF50, and *iso*-octane.
Kinetic studies		
DMF	Lifshitz et al. [21], 1998	Shock tube (T=1070–1370 K, 0.5% DMF in argon)
	Simmie et al. [22], 2009	Quantum calculation of formation enthalpies and bond dissociation energies using CBS-QB3, CBS-APNO, and G3
	Wu et al. [23], 2009	Premixed laminar flame (P=4.0 kPa, ϕ=2.0)
	Simmie et al. [24], 2011	Quantum calculation of thermal decomposition using CBS-QB3, CBS-APNO, G3, and G3MP2G3.
	Djokic et al. [25], 2012	Flow reactor (T=873–1098 K, P=1.7 bar, residence time: 300–400 ms)
	Friese et al. [26], 2012	Shock tube (T=970–1240 K, P=1.6 and 4.8 bar)
	Sirjean et al. [27], 2013	Quantum calculation of DMF+H using CBS-QB3
	Sirjean et al. [28], 2013	Shock tube (T=1300–1831 K, P=1 and 4 bar, ϕ=0.5, 1.0, and 1.5)
	Sirjean et al. [29], 2013	Quantum calculation of unimolecular decomposition using CBS-QB3
	Somers et al. [30], 2013	Shock tube (T=1200–1350 K, P=2–2.5 bar, 3% DMF in argon) Shock tube (P=1 bar, T=1350–1800 K, ϕ=0.5, 1.0, and 2.0) Shock tube (T=820–1210 K, P=20 and 80 bar, ϕ=1.0) Laminar burning velocities using heat flux method (T=298 and 358 K, ϕ=0.6–1.6) Jet stirred reactor (T=770–1220 K, P=10 bar, ϕ=0.5, 1.0, and 2.0)
	Casimir Togbe et al. [31], 2014	Premixed laminar flame (P=20 and 40 bar, ϕ=1.0 and 1.7)
	Zhanjun Cheng et al. [32], 2014	Flow reactor (T=780–1470 K, P=30, 150, and 760 Torr)
	Eldeeb et al. [33], 2014	Shock tube (T=977–1570 K, P=2, 5, 10, and 12 bar, DMF, MF, and furan)
	Eldeeb et al. [34], 2015	Shock tube (T=1009–1392 K, P=5 and 12 bar, DMF, *iso*-octane, and DMF-*iso*-octane blends (1:1 by volume)
MF	Wei et al. [35], 2012	Premixed laminar flame (P=4.0 KPa, ϕ=0.8 and 1.5)
	Somers et al. [36], 2013	Shock tube (T=1200–1800 K, P=1 bar, ϕ=0.5, 1.0, and 2.0)
	Davis and Sarathy [37], 2013	Quantum calculation of decomposition using G4 and CBS-QB3
	Wei et al. [38], 2013	Shock tube (T=1120–1700 K, P=1.25–10.65 bar, ϕ =0.25–2.0)
	Somers et al. [39], 2014	Quantum chemical calculations of pyrolysis of MF using CBS-QB3, CBS-APNO, and G3
	Tran et al. [40], 2014	Premixed laminar flame (P=20 and 40 bar, ϕ=1.0 and 1.7)
	Uygun et al. [41], 2014	Shock tube (T=820–1215 K, P=40 bar, ϕ=1.0, undiluted; T=871–1098 K, P=10 bar, ϕ=1.0, 0.5% fuel in argon)
Furan	Tian et al. [42], 2011	Premixed laminar flame (P=35 Torr, ϕ=1.4, 1.8, and 2.2)
	Wei et al. [43], 2012	Shock tube (T=1320–1880 K, P=1.2–10.4 bar, ϕ=0.5–2.0)
	Liu et al. [44], 2014	Premixed laminar flame (P=20 and 40 bar, ϕ=1.0 and 1.7)