Progress in Energy and Combustion Science 44 (2014) 40–102

Contents lists available at ScienceDirect

Progress in Energy and Combustion Science

journal homepage: www.elsevier.com/locate/pecs

Review

Alcohol combustion chemistry

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ARTICLE INFO

Article history:
Received 22 December 2013
Accepted 14 April 2014
Available online 14 June 2014

Keywords:
Biofuel
Combustion chemistry
Alcohols
Kinetic modeling
Pollutant emissions
Internal combustion engines
Flame speed
Ignition delay

ABSTRACT

Alternative transportation fuels, preferably from renewable sources, include alcohols with up to five or even more carbon atoms. They are considered promising because they can be derived from biological matter via established and new processes. In addition, many of their physical-chemical properties are compatible with the requirements of modern engines, which make them attractive either as replacements for fossil fuels or as fuel additives. Indeed, alcohol fuels have been used since the early years of automobile production, particularly in Brazil, where ethanol has a long history of use as an automobile fuel. Recently, increasing attention has been paid to the use of non-petroleum-based fuels made from biological sources, including alcohols (predominantly ethanol), as important liquid biofuels. Today, the ethanol fuel that is offered in the market is mainly made from sugar cane or corn. Its production as a first-generation biofuel, especially in North America, has been associated with publicly discussed drawbacks, such as reduction in the food supply, need for fertilization, extensive water usage, and other ecological concerns. More environmentally friendly processes are being considered to produce alcohols from inedible plants or plant parts on wasteland. While biofuel production and its use (especially ethanol and biodiesel) in internal combustion engines have been the focus of several recent reviews, a dedicated overview and summary of research on alcohol combustion chemistry is still lacking. Besides ethanol, many linear and branched members of the alcohol family, from methanol to hexanols, have been studied, with a particular emphasis on butanols. These fuels and their combustion properties, including their ignition, flame propagation, and extinction characteristics, their pyrolysis and oxidation reactions, and their potential to produce pollutant emissions have been intensively investigated in dedicated experiments on the laboratory and the engine scale, also emphasizing advanced engine concepts. Research results addressing combustion reaction mechanisms have been reported based on results from pyrolysis and oxidation reactors, shock tubes, rapid compression machines, and research engines. This work is complemented by the development of detailed combustion models with the support of chemical kinetics and quantum chemistry. This paper seeks to provide an introduction to and overview of recent results on alcohol combustion by highlighting pertinent aspects of this rich and rapidly increasing body of information. As such, this paper provides an initial source of references and guidance regarding the present status of combustion experiments on alcohols and models of alcohol combustion.

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http://dx.doi.org/10.1016/j.pecs.2014.04.003
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List of abbreviations

ARAS	atomic resonance absorption spectrometry
BDE	bond dissociation energy
CCD	charge-coupled device
CI	compression ignition
CMOS	complementary metal oxide semiconductor
CN	cetane number
CRDS	cavity ring down spectroscopy
CRV	constrained reaction volume
DI	direct injection
EAD	electronic absorption detection
EI	electron ionization
EPR	electron paramagnetic resonance
EVC	exhaust valve closing
FID	flame ionization detector
FTIR	Fourier transform infrared spectroscopy
GC	gas chromatography
HC	hydrocarbon
HCCI	homogenous charge compression ignition
HPLC	high-pressure liquid chromatography
IR	infrared
JSR	jet-stirred reactor
LDV	laser Doppler velocimetry
LHV	lower heating value
LIF	laser-induced fluorescence
LS	laser schlieren
LTC	low-temperature combustion
mb/d	million barrels of oil per day
MBMS	molecular beam mass spectrometry
mboe/d	million barrels of oil equivalent per day
MON	motor octane number
MP-VTST	multi-path variational transition state theory
MS	mass spectrometry
MS-VTST	multi-structure variational transition state theory
NDIR	non-dispersive infrared
NMR	nuclear magnetic resonance
NO_x	nitrogen oxides
NTC	negative temperature coefficient
NUIG	National University of Ireland Galway
PAH	polycyclic aromatic hydrocarbon
PDPA	phase Doppler particle anemometry
PEPICO	photoelectron photoion coincidence spectrometer
PES	potential energy surface
PI	photon ionization
PIV	particle image velocimetry
PM	particulate matter
RA	resonance absorption
RCM	rapid compression machine
REMPI	resonance enhanced multiphoton ionization
RF	resonance fluorescence
RON	research octane number
RRKM	Rice–Ramsperger–Kassel–Marcus
SAR	structure–activity relationship
SMPS	scanning mobility particle sizer
SI	spark-ignition
ST	shock tube
TCD	thermal conductivity detector
UV	ultraviolet
VUV	vacuum ultraviolet
YSI	yield sooting idex

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1. Introduction

Energy is among the most important factors influencing economic and industrial development. Today, combustion of fossil fuels accounts for more than two-thirds of the world's primary energy utilization [1]. The growing global population, the increasing mobility of that population, the increasing production and consumption of goods, and the transportation of those goods are considerable concerns in future energy strategies. The need for clean, efficient, and affordable energy sources is often seen in contrast to the environmental and health issues connected with fossil fuel use. Projections for the next two decades assume the

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