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Virtual Special Issue of Recent Advances in Fundamentals of Biomass and Biofuel Combustion

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Virtual Special Issue of Recent Advances in Fundamentals of Biomass & Biofuel

Combustion

In the context of the urging depletion of fossil fuels and of the increased concerns about the climate impact induced by anthropogenic CO₂ emissions, biomass has become a more and more welcome feedstock for power and chemical industries. In the context of heating and power generation, biomass can be burnt directly; in the context of transportation, it can be pyrolyzed or gasified, with the goal of producing a synthesis gas (CO/H₂) to be later transformed to hydrocarbons or directly used to catalytically synthesize oxygenated biofuels. In that case, numerous pathways are proposed to produce a wide range of molecules to be used as a drop-in fuel in combustion engines¹.

The combustion of biomass and derived molecules has consequently become a hot topic in recent years, making the publication of a dedicated Virtual Special Issue (VSI) very timely. This VSI (Recent Advances in Fundamentals of Biomass & Biofuel Combustion) aims to report the latest advances in fundamental research on the combustion of biomass and derived biofuels, which can find various energy applications including their use in internal combustion engines. The common point in all of the considered studies is to investigate combustibles containing not only C and H-atoms but also heteroatoms, naturally abundant in biomass and consequently biofuels. The included papers are related to (1) the combustion of alcohols and esters, so the first types of liquid biofuel historically proposed and currently used to fuel vehicles; here, the studies focused primarily on determining the kinetics of the involved multi-step reactions, (2) the combustion of new biofuels, such as hydrocarbons with a carbonyl group, or ammonia; again, primarily discussing the new chemical mechanisms, and (3) the conversion of solid biomass, with particular focus on fundamentals of combustion, char oxidation and the creation of pollutants.

Because the VSI focuses both on biomass and biofuels, we received a large number of submissions, describing new and exciting research ideas and perspective studies. Following the journal's usual rigorous peer-review process, a total of 30 papers (including 9 review articles) were accepted for publication in this VSI, as listed in **Table 1**.

Table 1. Papers published in the Virtual Special Issue of Recent Advances in Fundamentals of Biomass & Biofuel Combustion

Topic	First author and corresponding author	Corresponding author's institution	Title (DOI)	Article type
Review	Yang & Hansen ¹	Sandia National Laboratories (USA)	Review of the influence of oxygenated additives on the combustion chemistry of hydrocarbons (10.1021/acs.energyfuels.1c01841)	Review
	Westbrook ³	Lawrence Livermore National Laboratory, (USA)	Key chemical kinetic steps in reaction mechanisms for fuels from biomass: A perspective (10.1021/acs.energyfuels.1c02210)	Review
	Fenard & Vanhove ⁴	PC2A-CNRS, Lille (France)	A mini-review on the advances in the kinetic understanding of the combustion of linear and cyclic oxymethylene ethers (10.1021/acs.energyfuels.1c01924)	Review
	Sabia & De Joannon ⁵	STEMS-CNR, Napoli (Italy)	MILD combustion and biofuels: A minireview. (10.1021/acs.energyfuels.0c02973)	Review
	Liu & li ⁶	Shanghai Jiao Tong University (China)	Mini review of current combustion research progress of biodiesel and model compounds for gas turbine application (10.1021/acs.energyfuels.1c01841)	Review
	Singh & Kumar ⁷	IIT Bombay (India)	Effect of engine parameters on the performance of dual-Fuel CI engines with producer gas - a review (10.1021/acs.energyfuels.0c02279)	Review
	Tomlin ⁸	University of Leeds (United Kingdom)	Air quality and climate impacts of biomass use as an energy source: A review (10.1021/acs.energyfuels.0c01523)	Review
	Kwong & Marek ⁹	University of Cambridge (United Kingdom)	Combustion of biomass in fluidized beds: a review of key phenomena and future perspectives (10.1021/acs.energyfuels.0c01947)	Review
	Coppola & Scala ¹⁰	Università degli Studi di Napoli "Federico II" (Italy)	Chemical looping for combustion of solid biomass: A review (10.1021/acs.energyfuels.0c2600)	Review
Combustion of alcohols and esters	Drost & Maas ¹¹	University of Duisburg-Essen (Germany)	Experimental investigation of ethanol oxidation and development of a reduced reaction mechanism for a wide temperature range (10.1021/acs.energyfuels.1c01993)	Original article
	Michelbach & Tomlin ¹²	University of Leeds (United Kingdom)	The Influence of iso-butanol blending with a reference gasoline and its surrogate on spark-ignition engine performance	Original article
	Comandini & Chaumeix ¹³	ICARE-CNRS, Orléans (France)	Laminar flame speeds and ignition delay times of gasoline/air and gasoline/alcohol/air mixtures: the effects of heavy alcohol compared to light alcohol (10.1021/acs.energyfuels.0c01454)	Original article
	Lokachari & Wagnon ¹⁴	Lawrence Livermore National Laboratory (USA)	Experimental and kinetic modeling study of 3-methyl-2-butenol (prenol) oxidation (10.1021/acs.energyfuels.1c01530)	Original article
	Tran & Carstensen ¹⁵	PC2A-CNRS, Lille (France)	Exploring the flame chemistry of C ₅ tetrahydrofuranic biofuels: tetrahydrofurfuryl alcohol and 2-methyltetrahydrofuran (10.1021/acs.energyfuels.0c01949)	Original article

	Xiaoyuan & Sarathy ¹⁶	KAUST, Thuwal (Saudi Arabia)	High-temperature pyrolysis and combustion of C ₅ -C ₁₉ fatty acid methyl esters (FAMES): A lumped kinetic modeling study (10.1021/acs.energyfuels.0c02973)	Original article
	Singh & Masri ¹⁷	The University of Sydney (Australia)	Spray atomization and links to flame stability over a range of weber numbers and pressure ratios (10.1021/acs.energyfuels.0c02273)	Original article
Combustion of other biofuels	Belmekki & Farooq ¹⁸	KAUST, Thuwal (Saudi Arabia)	Symmetric ethers as bioderived fuels: Reactivity with OH radicals (10.1021/acs.energyfuels.1c01408)	Original article
	Mulvihill & Klippenstein ¹⁹	Argonne National Laboratory (USA)	Non-Boltzmann effects in chain branching and pathway branching for diethyl ether oxidation (10.1021/acs.energyfuels.1c02196)	Original article
	Fan & Yang ²⁰	Tsinghua University, Beijing (China)	Pyrolysis of lignocellulosic biofuel di-n-butyl ether (DBE): flow reactor experiments and kinetic modeling (10.1021/acs.energyfuels.1c01939)	Original article
	Jacobs & Heufer ²¹	RWTH Aachen University (Germany)	A comprehensive experimental and kinetic modeling study of the combustion chemistry of diethoxymethane (10.1021/acs.energyfuels.1c016100)	Original article
	Li & Li ²²	Shanghai Jiao Tong University (China)	Exploration on thermal decomposition of cyclopentanone: a flow reactor pyrolysis and kinetic modeling study (10.1021/acs.energyfuels.0c01672)	Original article
	Shrestha & Mauss ²³	Brandenburg University of Technology, Cottbus (Germany)	Detailed chemical kinetic study of acetaldehyde oxidation and its interaction with NO _x (10.1021/acs.energyfuels.0c01948)	Original article
	Cornell & Burke ²⁴	Columbia University, New York (USA)	Toward a more comprehensive understanding of the kinetics of a common biomass-derived impurity: NH ₃ oxidation by N ₂ O in a jet-stirred reactor (10.1021/acs.energyfuels.0c01544)	Original article
Conversion of solid biomass	Locapsi & Faravelli ²⁵	Politecnico di Milano (Italy)	A predictive physico-chemical model of biochar oxidation (10.1021/acs.energyfuels.0c01559)	Original article
	Branca & Di Blasi ²⁶	Università degli Studi di Napoli "Federico II" (Italy)	Burning dynamics of straw chars under the conditions of thermal analysis (10.1021/acs.energyfuels.0c01441)	Original article
	Fradet & Braun-Unkoff ²⁷	German Aerospace Center, DLR, Stuttgart (Germany)	Parametrization of a sectional approach for the entrained-flow gasification of biomass char (10.1021/acs.energyfuels.0c01946)	Original article
	Darido & Battin-Leclerc ²⁸	LRGP-CNRS, Nancy (France)	Emissions from a domestic wood heating appliance: experimental measurements and numerical study using an equivalent reactor network (ERN) approach coupled with a detailed chemical mechanism (10.1021/acs.energyfuels.0c01927)	Original article
	Li & Van Geem ²⁹	Ghent University (Belgium)	Primary thermal decomposition pathways of hydroxycinnamaldehydes (10.1021/acs.energyfuels.0c01662)	Original article
	Ulusoy & Wu ³⁰	Technical University of Denmark Lyngby (Denmark)	Multifunctional additives for NO _x abatement in fluidized bed biomass combustion (10.1021/acs.energyfuels.0c01186)	Original article
	Cardoso & Silva ³¹	Universidade de Lisboa, Lisbon, (Portugal)	Small-scale biomass gasification for green ammonia production in Portugal: a techno-economic study (10.1021/acs.energyfuels.0c01928)	Original article

■ Review papers

The VSI includes nine review papers. Three review papers describe the progress in the research on the chemical kinetics of biofuel combustion. Yang *et al.*¹ reviewed recent experimental studies to understand how adding oxygenated additives, such as dimethyl ether, ethanol, or dimethyl carbonate, influences the formation of oxidation intermediates and the ignition behavior for hydrocarbons. Westbrook *et al.*³ provided an overview of detailed kinetic models, explaining how does the combustion chemistry of biofuels (alcohols, aromatic oxygenates, alkyl esters, cyclic ethers) differ from that of alkanes. Fenard and Vanhove's⁴ review focused on a newly considered class of biofuels, oxymethylene ethers. Three more review papers discuss the use of biofuels in applied combustion processes. Sabia *et al.*⁵ presented a comprehensive review of the utilization of MILD combustion of a wide range of gases and liquids produced from biomass. It is worth mentioning, that this excellent review on MILD combustion was selected by ACS Editors to be featured in the ACS Editors' Choice. Liu *et al.*⁶ reported on the recent progress in using blends of fatty acid methyl esters and hydrocarbon fuels in gas turbines. Singh *et al.*⁷ discussed dual-fuel combustion engines, which can run on bio-diesel and gas from biomass gasification, the latter also called producer gas. The last three review articles focus on the combustion of solid biomass. Tomlin⁸ offered a comprehensive analysis of the emission of particulate matter from biomass combustion, looking at the variability of emissions connected to the scale of combustion installations, and later, on the resulting air quality. Prof. Tomlin's work was also noticed by the Editors, being selected for the cover of Issue 18 of *Energy&Fuels*.³² Kwong and Marek⁹ analyzed combustion of biomass in fluidized beds, looking at all fundamental phenomena, and later identifying research gaps and describing new research perspectives. Coppola and Scala¹⁰ reviewed technological challenges currently facing the chemical looping (CLC) processes that need to be addressed before implementing CLC for large scale biomass utilization with CCS, as in bioenergy with carbon capture and storage (BECCS).

■ Combustion of alcohols and esters

The VSI provides seven papers on the combustion of alcohols and esters. Of those, five papers focused on chemical kinetics related to alcohols. Drost *et al.*¹¹ reported a comprehensive range of measurements for the combustion of ethanol performed using a large set of experimental set-ups. They further developed a reduced reaction mechanism applicable in a large temperature range. Michelbach and Tomlin¹² analyzed the influence of branching in alcohol fuels, specifically, looking at iso-butanol and its knocking behavior in a spark-ignition engine, comparing it further to gasoline and a gasoline surrogate. Comandini *et al.*¹³ looked into two bio-derived components, ethanol and iso-pentanol, and their performance when used as gasoline additives. Specifically, they compared how laminar flame speeds and ignition delay times vary with the content of both alcohols. Lokachari *et al.*¹⁴ reported results from ignition and combustion experiments with an unsaturated

alcohol species, 3-methyl-2-butenol (prenol), performed in a shock tube and a rapid compression machine. They obtained ignition delay times as well as a new detailed kinetic model for the oxidation of this alcohol. Tran *et al.*¹⁵ investigated the structure of laminar flames of methane co-fueled with tetrahydrofurfuryl alcohol, quantifying more than 40 produced intermediates and showing that the flames doped by this cyclic alcohol produce more aldehydes, alcohols, and ethers than similar flames doped with 2-methyltetrahydrofuran. Another paper focused on the chemical kinetics of methyl esters, the type of components frequently found in biodiesel. Xiaoyuan and Sarathy proposed a lumped kinetic model for combustion of 52 saturated, mono-unsaturated and poly-unsaturated C₅-C₁₉ fatty acid methyl esters.¹⁶ The last paper in this group described spray vaporization characteristics of alcohols and esters. Specifically, Singh *et al.*¹⁷ investigated acetone, ethanol and biodiesel spray flames to link the spray characteristics and flame stability.

■ Combustion of other biofuels

Seven papers concerned biofuels other than alcohols and esters. Of those, five papers focused on a recently proposed class of biofuels, linear ethers heavier than dimethyl ether. Belmekki *et al.*¹⁸ used a shock tube to investigate reaction kinetics of hydroxyl radicals with dimethyl ether, diethyl ether, di-*n*-propyl ether, and di-*n*-butyl ether. Mulvihill *et al.*¹⁹ proposed a high-level theoretical study of non-Boltzmann effects on the formation of ketohydroperoxides during the low-temperature oxidation of diethyl ether. Fan *et al.*²⁰ investigated the pyrolysis of di-*n*-butyl ether with experiments in a flow reactor with photoionization molecular-beam mass spectrometry and detailed kinetic modelling. Jacobs *et al.*²¹ investigated the combustion chemistry of diethoxymethane in a shock tube and a flow reactor, obtaining experimental results to validate a newly developed detailed kinetic model. Two papers discussed the combustion of hydrocarbons containing a carbonyl group. Li *et al.*²² reported their experimental and modelling study of the thermal decomposition of cyclopentanone in a flow reactor. Shrestha *et al.*²³ explored the effect of NO_x on the oxidation of acetaldehyde in a shock tube, proposing a comprehensive kinetic model to explain the obtained experimental results. The last paper in the group discussed the oxidation of ammonia. Here, Cornell *et al.*²⁴ performed experiments in a jet-stirred reactor, providing kinetics results for the ammonia reaction with N₂O, being used as the oxidizer instead of O₂. They further pointed out the importance of $\text{N}_2\text{O} + \text{NH}_2 = \text{N}_2\text{H}_2 + \text{NO}$ reaction.

■ Conversion of solid biomass

Six papers focused on the combustion of solid biomass. Three papers were interested in the reactivity of biochars. Locapsi *et al.*²⁵ modelled combustion of biochar using a detailed multi-step reaction mechanism to describe the heterogeneous reactions. They thoroughly described the physical evolution of the particle upon conversion, which, in combination with the reaction model, provided a new, comprehensive framework for

future modelling of char combustion. Branca and Di Blasi²⁶ investigated the burning of straw chars produced from pyrolysis in packed beds. For combustion, they used thermogravimetry, which allowed them to investigate the dominating mechanisms at various operating temperatures. Fradet *et al.*²⁷ numerically simulated entrained-flow gasification of biofuels, bio-slurries, and secondary biochars. Three papers described the combustion of biomass and other solid derivatives. Using an equivalent reactor network approach coupled with a detailed description of chemical mechanisms, Darido *et al.*²⁸ modelled the creation and emission of harmful chemical components from small domestic combustion appliances, such as stoves or fireplaces. Li *et al.*²⁹ experimentally and numerically explored the primary pathways of fast pyrolysis of hydroxycinnamaldehyde monomers, which are important intermediates in the lignin biosynthesis. Ulusoy *et al.*³⁰ used various additives to the combustion of biomass in fluidized beds. They focused mainly on mineral additives, introduced to simultaneously reduce NO_x emissions and prevent bed agglomeration when burning straw-type biomass. In the final paper of this VSI, Cardoso *et al.*³¹ described results from their techno-economic study of an ammonia plant, where gasification of biomass is used to produce the required H₂ feedstock.

This VSI is part of the series of VSIs on Recent Advances in Selected Energy Research Areas, launched by *Energy & Fuels* in January 2021. Further information on this series of VSIs can be found in a dedicated editorial (10.1021/acs.energyfuels.0c04048).³²³

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