



# Experimental and numerical studies of biodiesel combustion mechanisms using a laminar counterflow spray premixed flame



D. Alviso <sup>a,\*</sup>, J.C. Rolon <sup>a</sup>, P. Scoufflaire <sup>b,c</sup>, N. Darabiha <sup>b,c</sup>

<sup>a</sup>Laboratorio de Mecánica y Energía, Facultad de Ingeniería, Universidad Nacional de Asunción, Campus Universitario, San Lorenzo, Paraguay

<sup>b</sup>CNRS, UPR 288, Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion (EM2C), Grande Voie des Vignes, 92290 Châtenay-Malabry, France

<sup>c</sup>Ecole Centrale Paris, Grande Voie des Vignes, F-92290 Châtenay-Malabry, France

## HIGHLIGHTS

- We have done experimental and numerical studies of biodiesel and methyl decanoate (MD) spray premixed flames.
- OH PLIF as well as emission spectroscopy and visualization of CH<sup>\*</sup> and OH<sup>\*</sup> are employed experimentally.
- Numerically, a new biodiesel kinetic scheme was developed by combining two existing kinetic schemes.
- CH<sup>\*</sup> and OH<sup>\*</sup> submechanisms were added to both biodiesel and MD kinetic schemes.
- The schemes were validated, as well as CH<sup>\*</sup> and OH<sup>\*</sup> submechanisms for both biodiesel and MD.

## ARTICLE INFO

### Article history:

Received 30 July 2014

Received in revised form 10 October 2014

Accepted 19 February 2015

Available online 10 March 2015

### Keywords:

Biodiesel

Methyl decanoate

Emission spectroscopy

OH PLIF

Kinetic modeling

## ABSTRACT

Biodiesel is a mixture of long chain fatty acids such as methyl esters and is mainly used in diesel engines. Its fundamental properties and combustion pathways still need to be analyzed and validated. The present study concerns the creation and development of new data for the combustion of rapeseed methyl ester biodiesel (RME) and methyl decanoate as a surrogate fuel (MD). Experimental and numerical studies are conducted on a laminar counterflow premixed flame configuration where spray biodiesel/air (or MD/air) is injected against methane/air mixture at atmospheric pressure for different strain rates and equivalence ratio conditions. As chemical schemes for methane/air reactions are enough well known, this configuration is suitable to perform validations of chemical schemes for biodiesel/air (or MD/air) combustion, by taking methane/air flame as a reference. Planar Laser-Induced Fluorescence (PLIF) of OH as well as visible and UV chemiluminescence measurements of the excited radicals CH<sup>\*</sup>(A<sup>2</sup>Δ) and OH<sup>\*</sup>(A<sup>2</sup>Σ<sup>+</sup>) are employed to experimentally analyze the biodiesel and MD flame structure. The counterflow spray MD flame is simulated by choosing a skeletal reaction mechanism to which we add CH<sup>\*</sup> and OH<sup>\*</sup> reactions. In the case of biodiesel flame simulations, a new surrogate kinetics is developed by combining two existing skeletal kinetics schemes. The new scheme guarantees not only a good prediction of measured radicals but also a good methane/air flame speed which is necessary to well predict the flame front position in the counterflow configuration. CH<sup>\*</sup> and OH<sup>\*</sup> sub-mechanisms are also added to this kinetic scheme. The numerical predictions of the CH<sup>\*</sup> concentration are very close to the experimental profiles along the central axis, for both biodiesel and MD kinetic schemes. However the numerical and experimental results show differences in the OH<sup>\*</sup> production routes between MD and methane flames.

© 2015 Elsevier Ltd. All rights reserved.

## 1. Introduction

Biodiesel is a complex mixtures of several methyl esters with different chain lengths and degrees of unsaturation. Due to their long chain composition, the number of possible reaction pathways

in a chemical reaction scheme increases drastically. The development of such schemes is therefore very challenging and the simulation of biodiesel combustion becomes extremely time-consuming as it requires enormous computing resources even in simple configurations such as homogenous reactors. In practice, analysis are done on surrogates or synthetic fuels with shorter chain lengths. These surrogates are structurally very similar to actual biodiesel methyl esters. Thanks to the development of computer resources over last decade, the studied surrogate chain

\* Corresponding author.

E-mail address: [dalviso@ing.una.py](mailto:dalviso@ing.una.py) (D. Alviso).

length and the degree of unsaturation have been increased continuously.

In this sense, Seshadri et al. [1] have used the directed relation graph (DRG) method developed by Lu and Law [2,3] to reduce detailed combustion mechanism of methyl decanoate (MD)  $C_{11}H_{22}O_2$  [4] to a skeletal mechanism including 125 species and 713 elementary reactions. The model has been validated with experiments studying the limits of ignition and extinction of a counterflow MD/air diffusion flame.

More recently, Luo et al. [5] have developed a skeletal mechanism including 115 species and 460 elementary reactions to study a tri-component surrogate consisting of methyl decanoate  $C_{11}H_{22}O_2$  (MD), methyl 9-decanoate (MD9D)  $C_{11}H_{20}O_2$  and n-heptane  $C_7H_{16}$ . Validations have been performed against 0-D simulations using the detailed mechanism and experimental data for spatially homogeneous systems, 1-D flames and 3-D turbulent combustion.

Most of biodiesel surrogate chemical schemes have been validated employing either homogeneous reactors or diffusion flames [1–3]. Although spray counterflow flames have been studied [6–8], to our knowledge no spray biodiesel surrogate combustion has yet been conducted. The main objectives of the present work are first to develop a counterflow flame of spray biodiesel/air (or MD/air) against methane/air mixture in order to carry experiments, and then to use experimental results to validate biodiesel chemical schemes by performing detailed numerical simulations. We have chosen this configuration in order to have an additional requirement on the performances of the chemical schemes studied. This latter should be able to correctly predict both biodiesel and methane flame front structures simultaneously. This constraint is particularly interesting because it makes possible to validate relative radical peaks in both flame fronts. In fact, chemical schemes for methane/air reactions are enough well known. Therefore we first measure experimentally the relative profiles of the radicals in the biodiesel front with respect to those of the methane flame front. These relative experimental values are then used to validate the relative radical profiles obtained numerically.

A convenient way to experimentally study the flame behavior is to analyze space and time-resolved emissions of  $CH^*$  and  $OH^*$ . Indeed, these two radicals are naturally present in the reaction zone and permit to determine important macroscopic properties such as flame location, flame speed, and heat release rate evolution. However, these radicals are generally considered as tracers because they have no significant effect on combustion reaction mechanisms. For this reason,  $CH^*$  and  $OH^*$  are very often not taken into account in reduced chemical schemes, and comparison with experimental data are consequently not done [9,10].

In this work we perform measurements of  $CH^*$  and  $OH^*$  natural emissions as well as planar laser induced fluorescence (PLIF) of  $OH$ . We have also measured temperature profiles. Experiments have been conducted for several spray biodiesel and MD flames in the counterflow configuration for different values of equivalence ratio and strain rate. By these measurements we seek to obtain data to validate simulated flame structures and also the production and consumption reactions of  $CH^*$  and  $OH^*$  for both biodiesel and MD flames.

Simulations are performed using a one-dimensional axis-symmetric formulation as developed by Franzelli et al. [8]. MD/methane opposed configuration is simulated employing the skeletal kinetic scheme proposed by Seshadri et al. [1]. To carry biodiesel flames simulations this latter scheme could not be used because it does not contain all the chemical components structures contained in the rapeseed biodiesel. We therefore employed the scheme proposed by Luo et al. [5]. Although this scheme contains all pathways for all components of the biodiesel, it could not give a good methane/air flame speed. The consequence of this was that

the flame front locations and the stagnation point were not well predicted. We therefore have developed and validated a new chemical scheme by carefully combining the schemes proposed by Seshadri et al. [1] and Luo et al. [5]. We have also completed all mechanisms with  $CH^*$  and  $OH^*$  formation, chemiluminescence and quenching sub mechanisms. The available literature data were recently summarized by Panoutsos et al. [11]. Most  $CH^*$  and  $OH^*$  reactions and rate constants found in literature [9,11–14] are validated with experiments involving light hydrocarbon flames such as methane, but no validation has yet been made for biodiesel surrogate. Therefore another objective of this work is to validate these sub-mechanisms.

## 2. Experimental setup

### 2.1. Counterflow burner device

The experiments were carried out using a counterflow burner (Fig. 1). The setup will be briefly described below, further information can be found in [15,16]. The burner consists of two opposed axisymmetric convergent nozzles of 20 mm inner diameter. The distance between the two nozzle exits is kept constant to 40 mm in all experiments. A premixed gaseous flow of methane and air is injected at ambient pressure and temperature through the lower side of the burner, while a spray flow of methyl decanoate (MD) or rapeseed methyl ester (RME) conveyed by air is injected at 400 K from the upper side. Each nozzle is surrounded by a coaxial nozzle which is fed by nitrogen in order to protect the reaction zones from ambient perturbations that could disturb the measurements.

The fuel spray is obtained by a classical liquid atomizer same as the one used in [16] by injecting an air flow above a vertical pipe plunged in the reservoir with the liquid. The liquid is pushed up due to pressure difference and is pulverized by air. The advantage of this system is that the size distribution of the spray is particularly narrow [17]. The inconvenience is that we were restricted to work with small air flow rates and consequently with lean biodiesel and MD flames.

An electrically heated pipe is used to maintain the spray flow heated between the atomizer and the burner. The upper burner as well as surrounding nitrogen are heated electrically at the same temperature as the spray fuel flow. The whole line and the whole upper burner are kept at 400 K. The two opposed flows form a

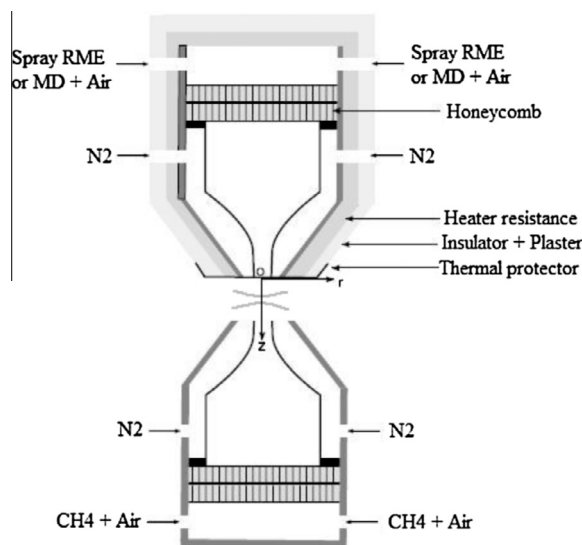


Fig. 1. Schematic of the counterflow burner.

Download English Version:

<https://daneshyari.com/en/article/6635564>

Download Persian Version:

<https://daneshyari.com/article/6635564>

[Daneshyari.com](https://daneshyari.com)