



ELSEVIER

Available online at www.sciencedirect.com

Proceedings of the Combustion Institute xxx (2010) xxx–xxx

**Proceedings
of the
Combustion
Institute**

www.elsevier.com/locate/proci

Ignition delay of fatty acid methyl ester fuel droplets: Microgravity experiments and detailed numerical modeling[☆]

Anthony J. Marchese^{a,*}, Timothy L. Vaughn^a, Kenneth Kroenlein^b,
Frederick L. Dryer^c

^a Colorado State University, Fort Collins, CO 80523, USA^b National Institute of Standards and Technology, Boulder, CO 80305, USA^c Princeton University, Princeton, NJ 08544, USA

Abstract

Recent optical engine studies have linked increases in NO_x emissions from fatty acid methyl ester combustion to differences in the premixed autoignition zone of the diesel fuel jet. In this study, ignition of single, isolated liquid droplets in quiescent, high temperature air was considered as a means of gaining insight into the transient, partially premixed ignition conditions that exist in the autoignition zone of a fatty acid methyl ester fuel jet. Normal gravity and microgravity (10^{−4} m/s²) droplet ignition delay experiments were conducted by use of a variety of neat methyl esters and commercial soy methyl ester. Droplet ignition experiments were chosen because spherically symmetric droplet combustion represents the simplest two-phase, time-dependent chemically reacting flow system permitting a numerical solution with complex physical submodels. To create spherically symmetric conditions for direct comparison with a detailed numerical model, experiments were conducted in microgravity by use of a 1.1 s drop tower. In the experiments, droplets were grown and deployed onto 14 μm silicon carbide fibers and injected into a tube furnace containing atmospheric pressure air at temperatures up to 1300 K. The ignition event was characterized by measurement of UV emission from hydroxyl radical (OH*) chemiluminescence. The experimental results were compared against predictions from a time-dependent, spherically symmetric droplet combustion simulation with detailed gas phase chemical kinetics, spectrally resolved radiative heat transfer and multi-component transport. By use of a skeletal chemical kinetic mechanism (125 species, 713 reactions), the computed ignition delay period for methyl decanoate (C₁₁H₂₂O₂) showed excellent agreement with experimental results at furnace temperatures greater than 1200 K.

© 2010 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Keywords: Droplet combustion; Laminar flames; Methyl esters; Microgravity combustion

[☆] Contribution of the National Institute of Standards and Technology, not subject to copyright in the US.

* Corresponding author. Address: Department of Mechanical Engineering, Colorado State University, 1374 Campus Delivery, Fort Collins, CO 80523-1374, USA. Fax: +1 970 491 3827.

E-mail address: marchese@colostate.edu (A.J. Marchese).

1. Introduction

Biodiesel is a renewable alternative fuel produced from vegetable oil or animal fat via a chemical reaction with an alcohol (typically methanol). This reaction results in a mixture of fatty acid methyl esters (FAME) of varying carbon chain

length, and this FAME mixture is what is known as biodiesel [1]. Biodiesel is considered a renewable fuel because the majority of the carbon present in the raw feedstocks originates from carbon dioxide already present in the air as opposed to petroleum diesel where the carbon in the fuel is liberated from beneath the surface of the earth and released into the atmosphere.

The chemical constituents of FAME biodiesel consist of mixtures of saturated and unsaturated methyl esters containing carbon chains of 12–24 atoms in length [1,2]. The length and the degree of unsaturation of the carbon chain are highly dependent on the feedstock. For example, soybean FAME contains 27% mono-unsaturated and 61% doubly unsaturated methyl esters (weight per cent) with an average carbon chain length of 18. Coconut FAME, on the other hand, contains 90% fully saturated methyl esters with an average carbon chain length of 12. Many algae strains currently under consideration for future production of FAME contain up to 30% highly unsaturated fatty acids that have five or more double bonds [3]. The carbon chain length and degree of unsaturation have been shown to impact both the NO_x and particulate matter (PM) emissions from biodiesel combustion in compression ignition engines [3–5].

Biodiesel combustion reduces carbon monoxide (CO), unburned hydrocarbons (HC), and PM mass emissions in comparison to those from petroleum combustion in diesel engines [6]. However, many studies have reported that biodiesel FAME combustion results in increased emissions of NO_x . A US Environmental Protection Agency (EPA) report that compiled the results of numerous diesel engine emission studies suggests that 100% biodiesel will generally produce a 10% increase in NO_x emissions [6]. Subsequent studies strongly suggest that biodiesel NO_x emissions are highly dependent on the engine type, duty cycle and biodiesel feedstock [7].

A verified explanation for the increased NO_x emissions from FAME has yet to be fully established and research continues with regard to the importance of differences in physical and chemical kinetic properties between FAME and petroleum diesel. Numerous mechanisms have been hypothesized including effects related to differences in viscosity [8], bulk modulus [9], boiling point [10], adiabatic flame temperature [11], radiative heat loss [12] and their effects on thermal NO_x and/or prompt NO_x production. Recent studies [3,12] have strongly suggested that biodiesel NO_x increases are a consequence of increased fraction of the heat release occurring in the premixed autoignition zone near the lift-off length of the biodiesel fuel spray. The mechanism by which increased premixed burn fraction produces increased NO_x emissions has yet to be explained but theories include higher local and average in-cylinder temperature, less radiative heat loss,

higher O-atom concentrations and/or increased prompt NO_x production.

Several researchers have theorized that methyl ester combustion chemistry might promote the formation of prompt NO_x within the premixed autoignition zone of the diesel spray [4,13]. The increased formation of prompt NO_x might be related to the number of C=C bonds in the methyl ester hydrocarbon chain and their effect on CH production [14] based on evidence that NO_x emissions from biodiesel often increase with increasing levels of unsaturation [4]. Alternatively, the increased formation of prompt NO_x might be related to increased levels of C_2O radical, which has recently received attention as a possible prompt NO_x precursor [15,16] via the reaction $\text{C}_2\text{O} + \text{N}_2 \rightarrow \text{NCN} + \text{CO}$. Marchese and coworkers [13] have suggested that methyl esters may produce higher levels of the C_2O radical in comparison to petroleum-based hydrocarbons via fuel decomposition pathways [17] that form stable oxygenated species such as CH_2CO and CH_2CCO .

Marchese and coworkers [18] have suggested studying the ignition of isolated liquid FAME droplets in quiescent, high-temperature, oxidizing environments as a means to gain further insight into the transient, partially premixed autoignition zone of a FAME fuel jet sheath and its possible role in prompt NO_x production. Droplet ignition experiments were suggested because spherically symmetric droplet combustion represents the simplest two-phase, time-dependent chemically reacting flow system, allowing for numerical treatments with detailed chemical kinetics and transport. Moreover, the experimental configuration is conducive to quantitative temporal and spatial measurements of various gas phase species such as NO and prompt NO_x precursors by use of optical diagnostics.

This paper presents the results of microgravity FAME droplet experiments conducted in a 1.1 s drop tower, along with comparisons against a detailed numerical model. A previous paper presented initial normal gravity FAME droplet ignition experiments [18]. A falling droplet apparatus is currently under development along with a laser diagnostic system to measure NO, CH, OH, NCN and C_2O by use of Planar Laser Induced Fluorescence in the vicinity of an igniting FAME droplet [13].

2. Experimental setup

In a droplet ignition delay experiment, a liquid droplet is injected into a hot ambient environment and the period between injection and the initial observation of a flame is measured. The first examples of this experimental configuration are the ignition delay experiments of Faeth and Olsen [19].

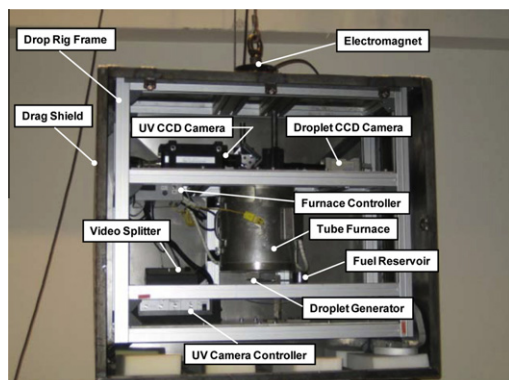


Fig. 1. Droplet ignition delay apparatus in microgravity configuration [18].

Fig. 1 shows a photograph of the droplet ignition apparatus that was utilized in the experiments reported herein and described previously by Vaughn et al. [18]. A tube furnace is used to generate the hot ambient air into which the liquid droplets are inserted. The tube furnace can reach temperatures of up to 1300 K and is regulated by an Omega CN-132 temperature controller.¹ To enable optical access, each end of the furnace is covered by a 50.8 mm sapphire window manufactured by CVI Optics. Furnace temperature data are measured at three separate locations using type K thermocouples and acquired using an Agilent 34970A data logger.

In addition to furnace temperature, the two main measurements required for these experiments are initial droplet diameter and ignition delay period, which are accomplished by use of video data from two separate video cameras. A Hitachi KP-D50 CCD camera is used along with an Infinity KC IF-2 zoom lens to record back-lit droplet images which are used to measure droplet diameter to within an accuracy of $\pm 23 \mu\text{m}$ based on a measured calibration factor of 44 pixels/mm. Ultraviolet emission from gas phase hydroxyl radical chemiluminescence is acquired using a Xybion ISG-250 intensified-array CCD video camera fitted with a Hamamatsu A4869 UV transmissive lens and an Andover 310FS10-50 narrow band interference filter centered at 310 nm. The video data are synchronized and merged into a split screen by use of a video splitter and digitized at 30 frames per second along with

the output of a Horita time code generator by use of a Dazzle Digital Video Creator 150 frame grabber and NASA Spotlight software [20].

For the experiments reported herein (both normal and microgravity), the droplets were supported on silicon carbide fibers 14 μm in diameter. A previous microgravity study described a piezoelectric droplet generator that injected freely floating droplets into the furnace [18]. For the present study, droplets of 1.0–1.2 mm were generated by use of a syringe pump fitted with a 10 μl hypodermic syringe, which deposited the droplets on the suspension fiber. The silicon carbide suspension fibers were equipped with small epoxy beads upon which the droplets were tethered. The epoxy beads were necessary to keep the droplet from migrating along the fiber. The suspension fibers were stretched across a fork that could be rapidly translated into the furnace environment by use of a linear stepper motor. To perform experiments in microgravity, the droplet ignition delay experiment was installed into an experimental test rig for use in a 1.1 s microgravity drop tower as described in [18] and shown in Fig. 1.

3. Experimental results

By use of the apparatus described above, FAME droplet experiments were conducted in normal gravity and microgravity. For all of the experiments, after the tube furnace achieved the prescribed steady temperature, an automated computer control system initiated a sequence that grew and deposited a liquid droplet on the suspension fiber, released the rig into freefall (for the microgravity experiments), and inserted the droplet into the furnace. Fig. 2 shows representative video data for a 0.95 mm methyl dodecanoate droplet ignition delay experiment conducted in normal gravity with a furnace temperature of 1079 K. The left image shows the backlit droplet

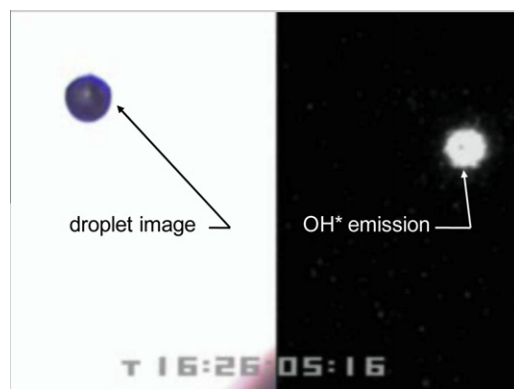


Fig. 2. Droplet ignition video images for a 0.95 mm methyl dodecanoate droplet ignition delay experiment with a furnace temperature of 1079 K.

¹ Certain commercial equipment, instruments, or materials are identified in this paper only to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

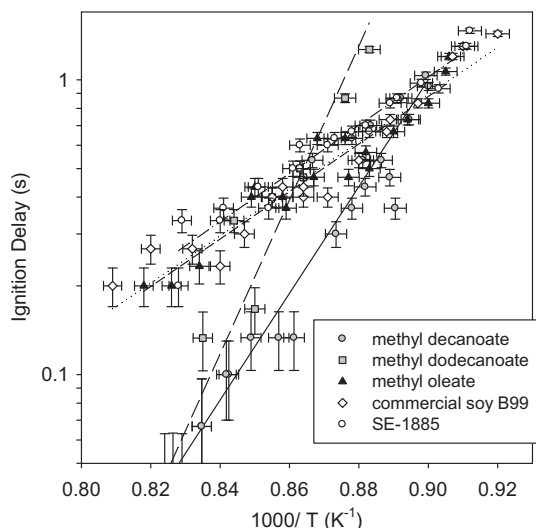


Fig. 3. Normal gravity ignition delay vs. furnace temperature for 1.2 mm ($\pm 100 \mu\text{m}$) droplets of methyl decanoate, methyl dodecanoate, methyl oleate, SE-1885 soy methyl ester and commercial B99 soy methyl ester.

image, while the right image shows the ignition event as measured in the ultraviolet images. The images indicate that both the droplet and the flame exhibit a high degree of spherical symmetry even for the experiments conducted in normal gravity.

3.1. Normal gravity results

Normal gravity droplet ignition delay experiments were performed with methyl decanoate (C10:0), methyl dodecanoate (C12:0), methyl oleate (C18:1), SE-1885 soy methyl ester and commercial soy methyl ester biodiesel (B99). The nomenclature Cx:y denotes the carbon chain length (x) and number of double bonds (y). The SE-1885 soy methyl ester is a blend of approximately 11% (by volume) methyl palmitate (C16:0), 4% methyl stearate (C18:0), 25% methyl oleate (C18:1), 52% methyl linoleate (C18:2) and 7% methyl linolenate (C18:3) produced by Proctor and Gamble.

Fig. 3 shows the results of normal gravity experiments comparing the droplet ignition delay of methyl decanoate, methyl dodecanoate and methyl oleate with that of the SE-1885 soy methyl ester and commercial soy B99. All of the experimental results plotted in Fig. 3 were for initial droplet diameters of 1.2 mm ($\pm 100 \mu\text{m}$) and atmospheric pressure. The error bars in Figs. 3–5 represent the uncertainty in ignition delay due to the finite frame rate of the video cameras (30 Hz) and the accuracy of the furnace temperature measurements ($\pm 2^\circ\text{C}$). The results show that the SE-1885 had ignition delay characteristics similar to those of the commercial B99 biodiesel, with the latter exhibiting slightly shorter ignition delay times for the entire tempera-

ture range. The results also show that the methyl decanoate exhibited shorter ignition delay periods than the soy methyl esters at the higher temperatures but comparable ignition delay periods at lower temperatures. Methyl dodecanoate exhibited shorter ignition delay periods than the soy methyl esters at higher temperatures, but much longer ignition delay periods at lower temperatures. Conversely, methyl oleate exhibited similar ignition delay periods to both soy methyl esters for the entire temperature range. These results suggest that methyl oleate might be an ideal single component surrogate fuel for soy biodiesel studies. Indeed, the overall activation energy for methyl oleate ignition delay as derived from a linear regression analysis was calculated to be $67 \pm 12 \text{ kJ/mol}$, which is quite comparable to that for the SE-1885 and commercial B99 soy methyl esters for which overall activation energies of $68 \pm 13 \text{ kJ/mol}$ and $67 \pm 10 \text{ kJ/mol}$ were measured, respectively.² Conversely, the overall activation energies for methyl decanoate and methyl dodecanoate were measured to be $151 \pm 22 \text{ kJ/mol}$ and $193 \pm 37 \text{ kJ/mol}$, respectively.

The fact that methyl dodecanoate (C12:0) had an overall activation energy that was larger than methyl decanoate (C10:0) underscores the importance of liquid phase transport, vapor/liquid equilibrium and gas-phase transport (along with gas-phase chemical kinetics and thermal radiation) in the droplet ignition configuration. Specifically,

² Uncertainties in overall activation energy are based on 95% confidence intervals for the linear regression analysis.

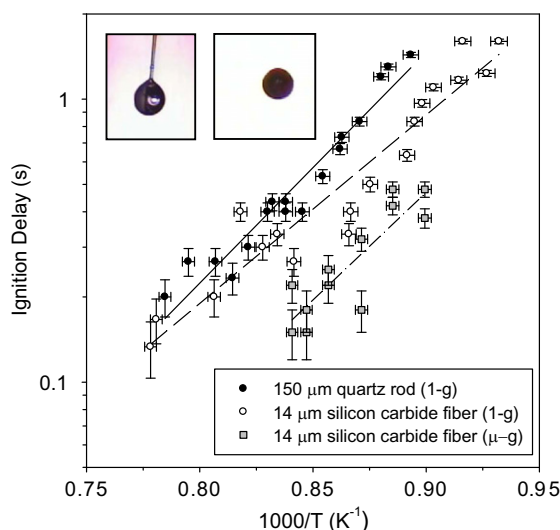


Fig. 4. Measured normal gravity ignition delay of suspended 1 mm soy methyl ester droplets on a 150 μm quartz rod (left inset) and 14 μm silicon carbide fiber (right inset) along with microgravity results for 1 mm soy methyl ester droplets on a 14 μm silicon carbide fiber.

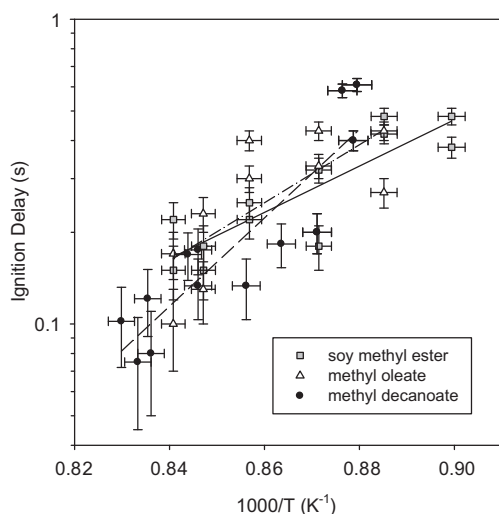


Fig. 5. Experimentally measured microgravity droplet ignition delay as a function of furnace temperature for 1 mm ($\pm 100 \mu\text{m}$) methyl decanoate, methyl oleate and soy methyl ester droplets. (—) denotes linear regression for soy methyl ester, (---) denotes linear regression for methyl decanoate and (- · -) denotes linear regression for methyl oleate.

the total measured ignition delay is a consequence of time intervals associated with heating of the liquid droplet, evaporation at the droplet surface, diffusion of the gaseous fuel into the oxidizing atmosphere and the chemical kinetic ignition delay. FAME ignition delay in a premixed homogeneous gaseous system will not necessarily show the

same trends as those shown in Fig. 3. For example, based solely on gas phase chemical kinetic considerations, it would be expected that the longer chain methyl esters would exhibit shorter ignition delay periods because of their higher reactivity at low temperatures. However, the longer chain methyl esters are also less volatile, so their liquid surface needs to be heated to a higher temperature in order to create an ignitable mixture surrounding the liquid droplet. The gas phase mass diffusivity is also a function of the molecular weight and carbon chain length so the longer chain methyl esters have longer diffusive transport time scales as well.

3.2. Effect of droplet suspension technique

One complication of performing experiments with the silicon carbide fibers is that the epoxy bead can ignite once the liquid fuel is completely consumed. For the normal gravity experiments, it was possible to rapidly remove the suspension fork from the furnace after ignition of the droplet, but prior to complete consumption of the liquid fuel. For the microgravity experiments, this technique was not possible. Accordingly, prior to conducting the experiments in microgravity, experiments were performed to evaluate the possibility of utilizing a 150 μm quartz rod for the droplet suspension medium. Fig. 4 shows the effect of the suspension fiber on the measured ignition delay of SE-1885 soy methyl ester droplets of 1 mm ($\pm 100 \mu\text{m}$) diameter suspended on 14 μm silicon carbide fibers and 150 μm quartz rods, respectively. The effect of the suspension fiber diameter on the measured ignition delay is significant. At 1100 K, for example, the

measured ignition delay with the 150 μm quartz rod is nearly double of that measured with the silicon carbide fiber. This result is consistent with recent work by Farouk and Dryer [21] that has numerically investigated the effects of fiber diameter and material properties on droplet combustion observations. Suspension fibers can affect the burning rate by as much as 50% in space-based droplet combustion experiments. Fig. 4 also presents backlit images of the droplets prior to ignition. The figure shows that the quartz- suspended droplets exhibit substantial asymmetry in comparison with those suspended on the silicon carbide fiber.

3.3. Microgravity results

Based on the results of §3.2, the use of freely floating droplets in experiments would be preferred, but were impractical in the present work. The freely floating technique proved to be significantly more challenging due to the inherent difficulty of injecting a single droplet in an upward trajectory into the furnace and deploying the drop rig into free fall at the precise moment when the droplet reaches the trajectory apex. We therefore chose to conduct microgravity experiments principally using a 14 μm silicon carbide fiber [18]. Fig. 4 shows microgravity ignition delay results for SE-1885 methyl ester droplets suspended on 14 μm silicon carbide fibers. The results show that, although the normal gravity silicon carbide supported droplets appear to exhibit a high degree of spherical symmetry, the measured ignition delay for the microgravity experiments was much shorter than the normal gravity results. It should be noted, however, that the overall activation energy of the microgravity experiments was comparable to that of the normal gravity experiments, suggesting that the differences in ignition delay between normal and microgravity are caused primarily by flow field and not chemical kinetic effects.

Fig. 5 shows the results of all of the microgravity droplet ignition experiments, which were conducted with 1 mm ($\pm 100 \mu\text{m}$) methyl decanoate, methyl oleate and SE-1885 methyl ester droplets. The data exhibit significantly more scatter than the normal gravity experiments and it is difficult to clearly delineate the differences in ignition delay behavior between the three different methyl esters in microgravity. Despite the increased scatter, a linear regression analysis of the methyl oleate and SE-1885 methyl ester once again reveals that these fuels exhibit comparable overall activation energies of $79 \pm 32 \text{ kJ/mol}$ and $63 \pm 27 \text{ kJ/mol}$, respectively. As was observed in normal gravity, the methyl decanoate exhibits a higher overall activation energy ($121 \pm 41 \text{ kJ/mol}$) than that of the methyl oleate or SE-1885 methyl ester. Because the experiments were limited to conditions wherein ignition delay was less than 1 s, experiments with

furnace temperature less than 1000 K could not be conducted in microgravity. Therefore, two-stage ignition due to the onset of low-temperature chemistry was not observed in the experiments.

4. Numerical modeling

To supplement the above experimental studies, observations were compared against predictions from an independently developed numerical model that has been described in detail elsewhere [22,23]. This time-dependent, spherically symmetric droplet combustion model features detailed gas phase chemical kinetics, spectrally resolved radiative heat transfer and multi-component transport. Liquid property correlations were chosen based upon experimental data regression as performed by the NIST ThermoData Engine software package [24]. For the simulations presented herein, a skeletal methyl decanoate mechanism of Seshadri and coworkers [25] was employed. This skeletal mechanism was developed for extinction and ignition conditions in non-premixed laminar flows by reducing the detailed 3036-species mechanism of Herbinet and coworkers [26] to 125 species and 714 reactions using the directed relation graph method.

The major motivation for conducting experiments in microgravity is to create spherically symmetric conditions for direct comparison against numerical models with detailed chemical kinetics and transport. Indeed, in all cases the droplet and flame image data strongly suggest that both the liquid droplets and the surrounding gas phase ignition event do indeed exhibit a high degree of spherical symmetry. It should be noted however, that the experimental initial conditions deviate from spherical symmetry due to forced convection from the droplet insertion process and natural convection within the furnace prior to release of the experiment into free fall.

Fig. 6 shows the modeling results of a representative transient ignition calculation for a 1 mm methyl decanoate droplet with an initial liquid temperature of 298 K injected into a hot ambient air environment at 1200 K. The figure contains plots of the mass fractions of the major gas-phase species along with the temperature as a function of normalized radius at 0.070, 0.081 and 0.100 s after insertion. At 0.070 s, significant thermal transport into the liquid droplet has resulted in the formation of a fuel boundary layer surrounding the droplet, but gas-phase chemical reaction has not yet resulted in fuel consumption or heat release. At 0.081 s, an ignition event has occurred as signified by the temperature rise and oxygen depletion in the vicinity of 1.5 radii from the droplet surface. By 0.100 s, the flame has transitioned into a quasi-steady diffusion flame with a normalized flame radius of approximately 4.

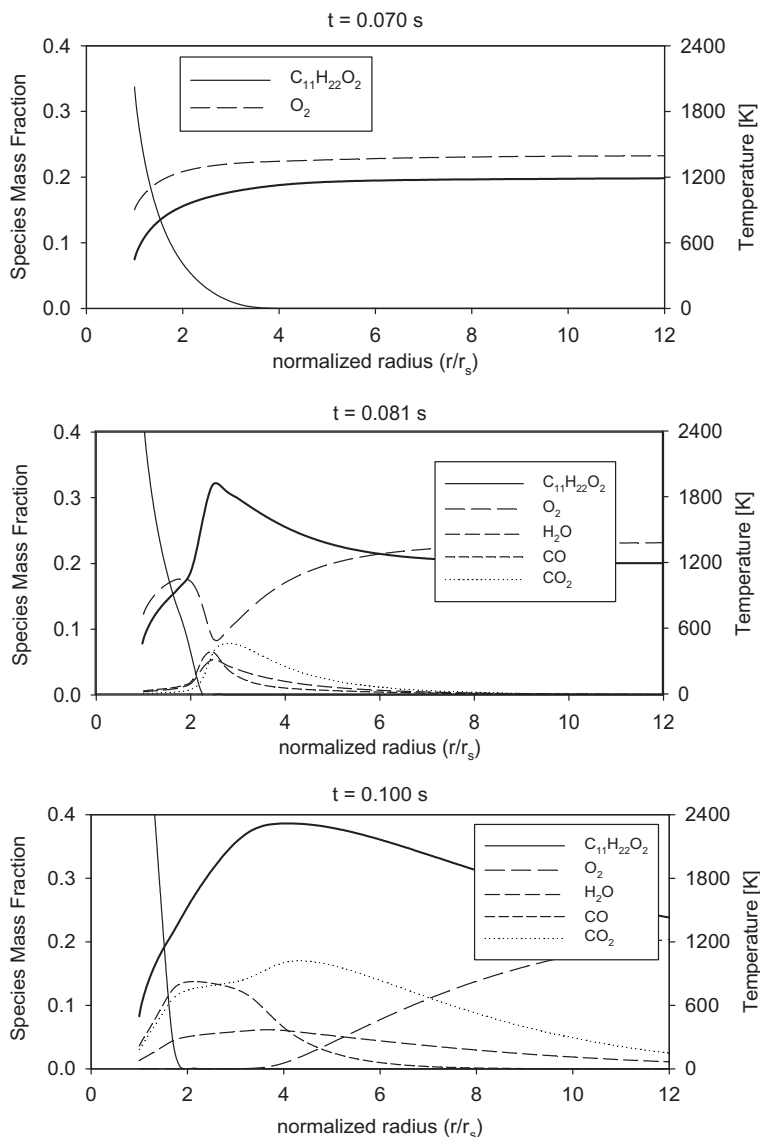


Fig. 6. Calculated major gas phase species mass fractions and temperature (solid bold line) surrounding a 1 mm methyl decanoate droplet at 0.070, 0.081 and 0.100 s after injection into 1200 K air at 101.3 kPa.

Fig. 7 shows the calculated instantaneous gasification rate for 1 mm droplets with an initial liquid temperature of 298 K inserted into high-temperature air for a range of air temperatures. The gasification rate is defined as $-\frac{d}{dt}[d_s^2]$ and the classical d^2 -law predicts this value to be a constant for both vaporization and combustion. As shown in Fig. 7, at an ambient air temperature of 850 K, the droplet evaporative lifetime exceeds the chemical/transport ignition delay, and ignition was not observed. This result is consistent with the normal gravity results for methyl decanoate reported by Vaughn and coworkers [18]. For ambient air tem-

peratures greater than 900 K, the gas phase surrounding the methyl decanoate droplets ignites, as signified by the rapid increase in gasification rate. Of particular note, a significant fraction of all time histories show negative instantaneous gasification rates due to droplet thermal expansion overwhelming volume loss due to vaporization. The extent of this period is an indicator of the sensitivity of ignition delay and droplet lifetime in this system to transport effects prior to vigorous chemical reaction.

Fig. 8 is a plot of the calculated ignition delay as a function of furnace temperature for 1 mm methyl

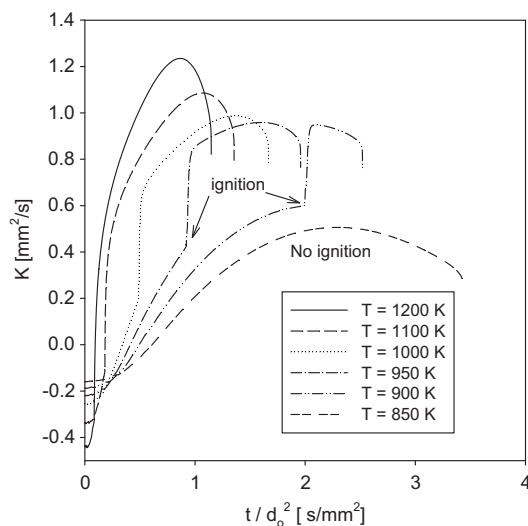


Fig. 7. Calculated instantaneous gasification rate for 1 mm methyl decanoate droplets inserted into high temperature air ($850 < T < 1200$ K) at 101.3 kPa.

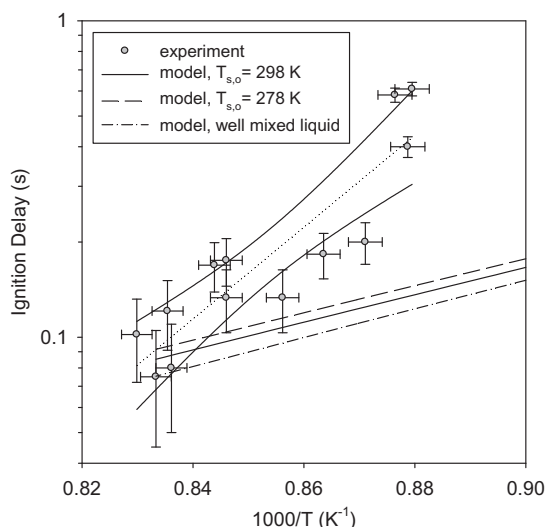


Fig. 8. Experimental (symbols) and numerical (thick lines) microgravity droplet ignition delay as a function of furnace temperature for 1 mm methyl decanoate droplets. For the experimental data, a linear regression is plotted along with 95% confidence interval (thin lines).

decanoate droplets, along with the experimental results. The calculated and measured ignition delay show good agreement at higher temperatures. For decreased air temperatures, however, the model predicts shorter ignition delay than that observed experimentally. This result appears to be one due predominantly to the behavior of the skeletal chemical kinetic model. Specifically, the skeletal chemical kinetic mechanism [25] employed in this study was previously shown to under-predict ignition delay (in comparison to the detailed Herbinet

[26] mechanism) in transient homogenous constant pressure calculations at initial temperatures less than 1100 K. Seshadri and coworkers [25] attributed the discrepancy to the lack of detail in the low-temperature reaction pathways in the skeletal mechanism. It is notable that at 1200 K, Seshadri and coworkers found that the skeletal and detailed mechanisms yielded identical constant-pressure ignition delay, which is consistent with the droplet ignition calculations presented in Fig. 8, which show excellent agreement at 1200 K.

Additional calculations were performed to examine the effects of initial droplet temperature and internal liquid mixing. To explore the effect of decreased initial droplet temperature caused by evaporative cooling, calculations were performed at an initial droplet temperature of 278.16 K, which is the triple point temperature for methyl decanoate. As shown in Fig. 8, decreasing the initial droplet temperature increases the calculated ignition delay, but this effect is minor. To explore the effect of enhanced liquid-phase circulation (as caused by the presence of the suspension fiber and/or atmospheric drag on the droplet during rapid insertion), calculations were performed with increased liquid phase thermal diffusivity to simulate a well mixed droplet interior. As shown in Fig. 8, the effect of increasing the rate of heat transfer into the liquid interior has only a minimal effect on the calculated ignition delay. In addition to its effect on internal circulation, the suspension fiber provides an additional conductive path from the hot gas environment to the liquid droplet. A recent study by Farouk and coworkers [27] showed that the addition of a suspension fiber submodel to the spherically symmetric model employed herein shortens the predicted ignition delay period by up to 8%.

5. Conclusions

Droplet ignition delay experiments were conducted with neat long chain saturated and unsaturated fame fuels and compared against experiments with two different soy methyl esters. Methyl decanoate exhibited shorter ignition delays than commercial biodiesel at the higher temperatures and similar ignition delays at lower temperatures. Methyl dodecanoate exhibited shorter ignition delays than commercial biodiesel at higher temperatures, but much longer ignition delays at lower temperatures. Methyl oleate exhibited ignition delays similar to the commercial biodiesel for the entire temperature range. Based on these results, methyl oleate is suggested as a single-component surrogate fuel for soy biodiesel studies.

The microgravity methyl decanoate experiments were compared against predictions from an independently developed numerical model with a skeletal chemical kinetic mechanism. At initial furnace temperatures of 1200 K, the model shows agrees very well with experiments. At lower furnace temperatures, the disagreement between the model and the experiments is attributed to the limitations in the skeletal chemical kinetic mechanism.

Acknowledgments

The experimental component of this research was supported by Grants CTS-042080 and CBET-0854134 from National Science Founda-

tion. Development of the droplet combustion model used in this work was supported under NASA Cooperative Agreements NCC3-375 and NNCO4AA66A at Princeton University.

References

- [1] J. Van Gerpen, *Fuel Process. Technol.* 86 (2005) 1097–1107.
- [2] G. Knothe, *Fuel Process. Technol.* 86 (2005) 1059–1070.
- [3] B.C. Fisher, A.J. Marchese, J. Volckens, T. Lee, J.L. Collett, *SAE* 2010-01-1523, 2009.
- [4] R.L. McCormick, M.S. Graboski, T.L. Alleman, A.M. Herring, K.S. Tyson, *Environ. Sci. Technol.* 35 (2001).
- [5] A. Schonborn, N. Ladommatos, R. Allan, J. Williams, J. Rogerson, *SAE* 2008-01-1578, 2008.
- [6] A Comprehensive Analysis of Biodiesel Impact on Exhaust Emissions. EPA420-P-02-001, 2002.
- [7] W. Clark, B. McCormick, Recent Research to Address Technical Barriers to Increased Use of Biodiesel. in: *Diesel Engine Emission Reduction Conference*, Chicago, IL, August 2005.
- [8] J. Patterson, M.G. Hassan, A. Clarke, G. Shama, K. Hellgardt, R. Chen, *SAE* 2006-01-0234, 2006.
- [9] J. Szybist, A. Boehman, J. Taylor, R. McCormick, *Fuel Process. Technol.* 86 (2005) 1109.
- [10] C. Choi, G. Bower, R. Reitz, *SAE* 970218, 1997.
- [11] G.A. Ban-Weiss, J.Y. Chen, B.A. Buchholz, R.W. Dibble, *Fuel Process. Technol.* 88 (2007) 659–667.
- [12] C.J. Mueller, A.L. Boehman, G.C. Martin, *SAE* 2009-01-1792, 2009.
- [13] A.J. Marchese, T.L. Vaughn, T. Grumstrup, Examination of the Role of C₂O Radical in Methyl Ester NO_x Formation. 2010 Spring Technical Meeting of the Western States Section of the Combustion Institute, Boulder, CO, March 21–23, 2010.
- [14] S. Garner, R. Sivaramakrishnan, K. Brezinsky, *Proc. Combust. Inst.* 32 (2009) 461–467.
- [15] B.A. Williams, J.W. Fleming, *Proc. Combust. Inst.* 31 (2007) 1109–1117.
- [16] A.A. Konnov, *Combust. Flame*. 156 (2009) 2093–2105.
- [17] L.K. Huynh, A.J. Violi, *Org. Chem.* 73 (2008) 94–101.
- [18] T. Vaughn, M. Hammill, M. Harris, M. Wessel, A.J. Marchese, *AIAA* 2007-0741, 2007.
- [19] G.M. Faeth, D.R. Olsen, *The Ignition of Hydrocarbon Fuel Droplets in Air*. *SAE Trans.* 77 (1968) 1793.
- [20] B. Klimek, T. Wright, *NASA/TM*-2006-214084, 2006.
- [21] T. Farouk, F.L. Dryer, *Effect of Supporting Fibers on Tethered Droplet Combustion in Reduced Gravity Environments: A Numerical Study and Comparison with Experiment* (submitted to Combustion Theory and Modeling, 2010).
- [22] K. Kroenlein, A. Kazakov, F.L. Dryer, *AIAA*-2008-1416, 2008.
- [23] K. Kroenlein, *Numerical Simulation of Isolated Droplet Combustion under Microgravity Conditions*, Ph.D. thesis, Princeton University, Princeton, NJ, 2007.

- [24] M. Frenkel, R.D. Chirico, V. Diky, X. Yan, Q. Dong, C. Muzny, *J. Chem. Inf. Model.* 45 (4) (2005) 816–838.
- [25] K. Seshadri, T. Lu, O. Herbinet, S. Humer, U. Niemann, W.J. Pitz, R. Seiser, C.K. Law, *Proc. Combust. Inst.* 32 (2009) 1067–1074.
- [26] O. Herbinet, W.J. Pitz, C.K. Westbrook, *Combust. Flame.* 154 (2008) 507–528.
- [27] T. Farouk, F.L. Dryer, A.J. Marchese, T.L. Vaughn, K. Kroenlein, *A Numerical Study on the Impact of Supporting Fibers on Tethered Droplet Ignition under Microgravity Conditions*. 2010 Spring Technical Meeting of the Western States Section of the Combustion Institute, Boulder, CO, March 21–23, 2010.