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Low Temperature Autoignition of Jet A and Surrogate Jet Fuels

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Abstract

An experimental study of the low-temperature and low-pressure autoignition of Jet A and surrogate fuels was conducted using the ASTM-E659 standardized test method. Two surrogate fuels (Aachen and JI mixtures), their individual components and two batches (POSF-4658 and POSF-10325) of standardized Jet A were tested using the ASTM-E659 method for a range of fuel concentrations and temperatures. The ignition behaviors were categorized into four distinct ignition modes. The individual hydrocarbon components had a wide range of ignition behaviors and AIT values depending on the molecular structure. The two Jet A batches showed similar ignition behavior with measured AITs of 229°C ± 3°C and 225°C ± 3°C respectively. Both surrogates exhibited similar ignition behavior to Jet A with comparable AITs of 219°C ± 3.1°C (Aachen) and 228°C ± 3°C (JI) with the JI mixture proving to be a more suitable surrogate to Jet A in the low-temperature thermal ignition regime.

Keywords: *Thermal Ignition, Autoignition, Surrogate Fuel, Jet Fuel*

1 Introduction

1.1 Autoignition Background

The study of thermal ignition has been of interest to the combustion community for over a century with initial motivation arising from areas like process safety where the use, storage and shipment of combustible liquids was rapidly becoming commonplace in many areas of the world economy. This led to the development of standardized methods for determining minimum autoignition (AIT) or self ignition temperature (SIT) criteria for spontaneous thermal ignition of a given substance in air at atmospheric pressure.

A comprehensive summary of the early efforts to create an AIT test was given by Setchkin (1954). His studies led him to develop what would become the forerunner to the modern day ASTM-E659 standardization for determination of the AIT (ASTM, 2005). In this test, a small quantity of liquid fuel (0.05 to 0.5 mL) is injected into a preheated flask containing hot air with ignition determination made by visual observations and temperature measurements. Setchkin's study found that the minimum AIT is typically decreased as combustion chamber size is increased. Depending on the substance, this can have a large effect (50 – 100°C) on the measured AIT. From this and other details uncovered in these early studies it became clear that the AIT is not a fundamental property of a substance alone but is rather highly dependent on the method and apparatus used in its determination. More recent work at PTB has further illustrated this fact through studies on the influence of increased pressure, nitrogen dilution levels, and combustion vessel volume on AIT (Hirsch and Brandes, 2005, Brandes and Hirsch, 2017a,b).This makes it crucial to fully understand the methodology used in obtaining an AIT value if it is to be of any use in practical analysis and engineering design applications where conditions may differ significantly from the standard tests.

A similar test was also proposed by Zabetakis et al. (1954) in the same year as Setchkin (1954), with the major differences being the use of a 200 mL Erlenmeyer flask in place of the larger spherical flask and the use of the flask temperature instead of the gas temperature to report the test condition. This apparatus seems to also have been the forerunner of a separate AIT standardization, ASTM-D2155, which was discontinued in 1978 in favor of the E659 standard (ASTM, 1976), as well as the current international standard (ISO/IEC, 2017).

Although the ASTM-E659 is the now the widely accepted standard in North America for AIT determination, literature sources rarely specify this as the method used in obtaining their reported AIT's. Many safety data sheets (SDS) and chemical databases cite the origin of reported AIT numbers, but in almost all cases these sources are simply other chemical databases or property handbooks which do not claim to have performed any testing themselves or have cited a different test method for AIT determination, e.g., Sax (1957), Zabetakis (1965), CRC (1983), NFPA (1991), USCG (1999), Zakel et al. (2019). As a consequence, it is challenging to determine the origin of reported AIT numbers or the details of the testing method. This lack of consistency in the literature complicates the comparison of AIT values of different fuels or the same fuels tested by different research groups.

The nature of the data also hampers the development of models for the prediction of the AIT based on molecular properties alone. Affens et al. (1961) used the same apparatus as Setchkin (1954) in an effort to correlate ignition behavior to chemical structure for various classes of alkane and aromatic substances. They noted some correlations between a decrease in chain length, methyl groups, unsaturation, and chain branching with an increase in the minimum AIT for aliphatic hydrocarbons as well as a correlation between existing side chains and side chain length and increased AIT for alicyclic compounds and aromatics (Affens et al., 1961). More recently, a study by Tsai et al. (2012) attempted to fit a model to the AIT of 820 compounds reported in the DIPPR database based on a set of molecular descriptors. This approach was moderately successful (36°C mean absolute error) in reproducing experimental AIT values. Given the manual nature of the injection process and the wide range of fuel viscosity and vapor pressure examined in these studies, it is not surprising that there are significant discrepancies between test data and predictions based solely on molecular structure.

A significant issue in interpreting and modeling the ASTM-E659 test is the lack of characterization or control of the mixing processes between the fuel and hot air. The formation of droplets, vaporization and diffusion of the fuel into the air, convective motion and the potential impingement of the fuel on the hot flask surface make this a very challenging situation to measure and model. The fuel-air mixture is likely to be highly nonuniform as is the temperature distribution due to the cooling effects of fuel vaporization. Despite the widespread use of ASTM-E659 and related test methods, the inherent variability and complexity has inhibited scientific investigations and modeling efforts. A brief summary and discussion of some of these issues related modeling and theoretical treatment of AIT is presented in Hattwig and Steen (2004).

Although widely used in safety assessment and setting design criteria, it is apparent that the ASTM-E659 test is not always an appropriate method for evaluating industrial thermal ignition hazards. In the particular case of aircraft, most of the hot surfaces encountered are metals (steel, nickel and titanium alloys, and aluminum) rather than glass as in ASTM-E659 testing. Heating transients and ignition events can also occur over much longer times than the 10 minutes examined in ASTM-E659 testing. These are important considerations since the surface material can have a significant effect on the ignition thresholds for a given fuel ($>$ 100°C variation) and longer duration experiments can lead to significant fuel decomposition (Smyth, 1990) as well as unusual ignition transients (Boettcher et al., 2012) without any obvious rapid energy release. Even more important than surface material are the differences between the confined flow within the vessel used in ASTM-E659 testing and unconfined or partially confined external flows that occur in many industrial situations. The heated surface geometry and residence time in the thermal layer (Jones and Shepherd, 2020) can be significantly different in actual hazards than in ASTM-E659 testing. This is important because fuel decomposition and the formation of the ignition kernel has been observed to take place preferentially close to the heated surface (Coronel et al., 2019).

Studies of autoignition behavior of commodity fuels have been conducted using heated shock tubes and rapid compression machines (RCMs) to measure ignition delay times. In comparison to ASTM-E659 testing, these studies have well-controlled conditions and instrumentation that enables validation of chemical reaction models of ignition. However, the test gas temperatures are significantly higher than those relevant to low temperature thermal hazards and the minimum AIT conditions examined in ASTM-E659 testing. These ignition studies (Vasu et al., 2008, Wang and Oehlschlaeger, 2012, Liang et al., 2012, Zhukov et al., 2014, De Toni et al., 2017) have also mainly been conducted at elevated pressures (8-51 atm) which are uncharacteristic of thermal ignition hazards in aircraft and industrial hazards associated with accidental releases. These studies examined kerosene fuels (including Jet A) however with the typical wide variation in composition found in commodity supplies (Edwards, 2017). The variability in commodity fuels and the associated uncertainty in the experimental results has motivated the development of surrogate fuels as well as standardized batches of Jet A to facilitate comparison between experimental studies.

1.2 Surrogate Fuels

Commodity fuels like gasoline, diesel or Jet A typically consist of hundreds of different hydrocarbon species in imprecise and varying quantities, even between different batches of the same fuel. This complexity makes it difficult both to accurately reproduce experimental results across distinct fuel batches and to model the reaction mechanisms leading to ignition. As an alternative, suitably representative mixtures of hydrocarbons, called surrogate fuels, can be developed to mimic a few important commodity fuel characteristics such as laminar flame speed, ignition delay time, cetane number and distillation curve while consisting of only a handful of species in well controlled concentrations (Mueller et al., 2012, Chen et al., 2016, Kim and Violi, 2018). This makes surrogates much more amenable to experimental reproducibility as well as numerical modeling because the species and reaction pathways to consider are both far fewer in number and typically much better understood than they are for many components of the commodity fuel. Several surrogate fuels have been developed in the literature to mimic Jet A ignition behavior at high pressures and a range of temperatures similar to the studies previously mentioned (T=645-1750 K at 8.5-20 atm). These surrogate fuel studies have used the existing shock tube and RCM data from the previously mentioned studies as sources of validation of their proposed surrogate blends (Dean et al., 2007, Dooley et al., 2010, Chen et al., 2016). Few if any of these detailed surrogate studies have been performed in the very low-temperature (<600 K) and low pressure regime of autoignition likely due to the scarcity of data available in this regime for model validation. Some simple fuels like n-Hexane have been studied extensively at these conditions (Mével et al., 2019) but these studies have not yet been performed on larger hydrocarbon molecules that are more characteristic of Jet A. For this reason, it is unclear if the previously developed surrogates are relevant to autoignition of Jet A at low pressure and temperature conditions.

Two Jet A surrogates from the literature have been identified in this study for their relevance to matching ignition behavior as well as for their simplicity in composition. These surrogates are: (1) the Aachen surrogate (Honnet et al., 2009): n-Decane/1,2,4-Trimethylbenzene, (80/20 wt%), and (2) the JI surrogate (Chen et al., 2016): n-Dodecane/Isocetane/Trans-decalin/Toluene, (0.3/0.36/0.246/0.094 mol%). These surrogates were formulated in an effort to match high-temperature and high-pressure autoignition behavior of Jet A so it is crucial to determine if their usefulness can be extended to Jet A studies focused on the low temperature and low pressure regime of thermal ignition. This is indeed one of the main goals of the present study. To validate these surrogates' ignition behavior in the regime of interest, two well-controlled and extensively studied (Edwards, 2017) blends of Jet A were also examined: POSF-4658 and POSF-10325. These fuel blends also provide a quantifiable baseline for comparison with the surrogate samples on a chemical level which is shown in Table 1.

Table 1: Comparison between composition of Jet A blends and surrogate fuels

		% by Weight			
		POSF-4658	**POSF-10325**	**Aachen Surrogate**	**JI Surrogate**
Alkanes	n-Alkanes	19	19.98	80	29.17
	iso-Alkanes	31.34	29.69	-	46.53
	cyclo-Alkanes	28.42	31.79	-	-
	Total	78.76	81.46	80	75.7
Aromatics	Alkylbenzenes	13.69	12.9	20	4.94
	Alkylnapthalenes	1.76	2.34	-	-
	Cycloaromatics	5.79	3.29	-	19.41
	Total	21.24	18.53	20	24.35
Avg. Molecular Formula		$C_{11.69}H_{22.62}$	$C_{11.4}H_{22.1}$	$C_{9.77}H_{19.7}$	$C_{12.49}H_{25.22}$
H/C ratio		1.935	1.939	2.016	2.019

In studying multi-component liquid fuels like these surrogates and Jet A, there are several difficulties one must be aware of. The major challenge in performing experiments in particular is the discrepancy between the gas phase and liquid phase compositions owing to differences in vapor pressure of the individual species. This is especially important in this work as all ignition takes place in the vapor phase. Therefore in order to appropriately match the Jet A ignition behavior with a surrogate, it is the vapor phase composition that must be matched. This approach is taken in the literature with the computational formulation of the JI surrogate which was designed to match the distillation curve of Jet A in order to match both droplet evaporation and ignition behavior (Chen et al., 2016). Other surrogate studies like that of the Aachen surrogate instead simply attempted to reduce to as few representative components as possible and to roughly capture the properties of the alkanes and aromatics with one compound of each without a comprehensive analysis of the physical chemistry at play in the mixture (Honnet et al., 2009).

2 Experiments

The procedure and testing apparatus employed in this study was the same as that described in the ASTM-E659 standardized test specification for the determination of the AIT and so the test method is only briefly discussed. The test apparatus is shown in Fig. 1 along with a schematic representation of the combustion vessel contained within the furnace. A small liquid sample of the fuel to be tested was injected via syringe into a uniformly heated 500mL flask containing room air and left open to the atmosphere. The lights were turned out and the sample was observed via a mirror mounted above the flask opening using a Phantom VR3746 high speed camera which was manually triggered upon ignition of the sample. The gas temperature within the flask was also recorded and monitored during each test in order to determine the extent of self heating occurring in the sample and to provide a secondary indication of ignition via the presence of a sharp temperature spike. This was also used to obtain a measure of ignition delay time, τ_{ign} which was defined as the time between fuel injection and ignition. Typically these events were very easily distinguished in the temperature profile with the injection corresponding to a steep temperature drop by a few degrees and the ignition evidenced by a sharp temperature rise. However, as will be discussed in section 3.1, some temperature profiles did not exhibit such a sharp spike in temperature which led to the classification of multiple distinct ignition modes.

Each test was limited to no more than 10 minutes, at which point if ignition had not yet been observed then a non-ignition case was recorded. If instead a flame appeared or the temperature profile indicated some steep temperature increase then an ignition or cool flame event was recorded. However, in many cases it would become clear that the sample was not going to ignite long before the 10 minute limit as self heating typically only lasted for 4-5 minutes after injection for the substances studied here. After the gas temperature leveled off, it was usually evidence that a limit had been reached and the temperature would begin to decay. In these cases, the sample was observed for an extra 1-2 minutes after the level off and if the decay continued then the test was considered as a non-ignition case and preparation for the next test would begin. Preparation for the next test included the use of a hot air gun or blow dryer applied to the top of the apparatus for up to 30 seconds in order to purge the flask of any remaining ignition products or unburnt fuel. Following purging, temperature adjustments were made via a temperature controller and the furnace was allowed to return to equilibrium at the new set temperature.

2.1 Equipment

The furnace used was a Mellen CV12 crucible furnace with a 13.3 cm diameter by 20 cm deep cylindrical heated volume capable of achieving temperatures up to 1250°C. A PID controller (Love Controls series 16B) system was used to set the furnace at the desired temperature and was accurate to 1°C. A schematic cross section of the apparatus is shown in Fig. 1 which illustrates the location of the 500 mL round bottom borosilicate flask within the heated volume along with the four thermocouples used to monitor the temperature evolution during a test. The flask was suspended and secured in the furnace by means of an insulating ceramic holder fabricated using a fused silica casting compound.

The location of the four type K thermocouples are also shown in the schematic in Fig. 1 with the gas temperature being read from T_4 which was suspended approximately in the center of the flask volume. Preliminary tests to characterize the apparatus showed that the location of the gas phase thermocouple within the volume had little effect on the reading (±0.5°C) providing indication of temperature uniformity within the flask at elevated temperatures. The thermocouples were constructed from 36 gauge (0.127 mm diameter) wire and sheathed in stainless steel for protection. The temperatures at the bottom, side, and neck of the flask's outer wall were monitored via T_1,T_2,and T_3 respectively. The temperature of the flask wall was much less uniform than the gas, with typical variations of up to 5°C when set near 250°C or 10-15°C above 400°C.

Temperature profiles were recorded from the time of injection through any self heating or ignition event using an OMEGA HH520 four channel data logger calibrated to the nearest 0.1°C up to 600°C and 1°C for higher temperatures. All channels were sampled at 1 Hz as per the ASTM-E659 specification. Reported experimental errors were estimated based on both the standard error limits for type K thermocouple probes and the reported error of the HH520 datalogger itself.

2.2 Surrogate Fuel Preparation

An early attempt at mixing the surrogates was made using a Tree Model HRS3100 scale calibrated to the nearest 0.001 g to weigh out the individual compounds, but this method proved unreliable as shown by GC-FID (Gas Chromatography with Flame Ionization Detector) measurements (Sund, 2019). The first batch of surrogate used a mixture of Trans- and Cis-decalin (the AITs of these isomers are similar) and the mixture is much easier to obtain in larger quantities than either isomer individually. The second batch of the surrogate which was used for the AIT testing used only the Trans-decalin isomer. The mass fractions obtained in the GC-FID analysis as well as target values are shown in Table 2.

The results showed that for the JI surrogate, two of the four components had relatively large percent errors in their measured mass fractions (Toluene and Decalin). These two components also both happened to have the smallest target mass fractions and Toluene in particular had the highest vapor pressure by far at room temperature. As a result, it was determined that there were two possible factors at play in producing such larger errors, (1) inaccurate mixing and (2) poor sealing/storage of the fuel batch. To address these issues, two changes were made in mixing the second batch of JI, namely (1) the use of pipettes to measure out the components volumetrically, and (2) the

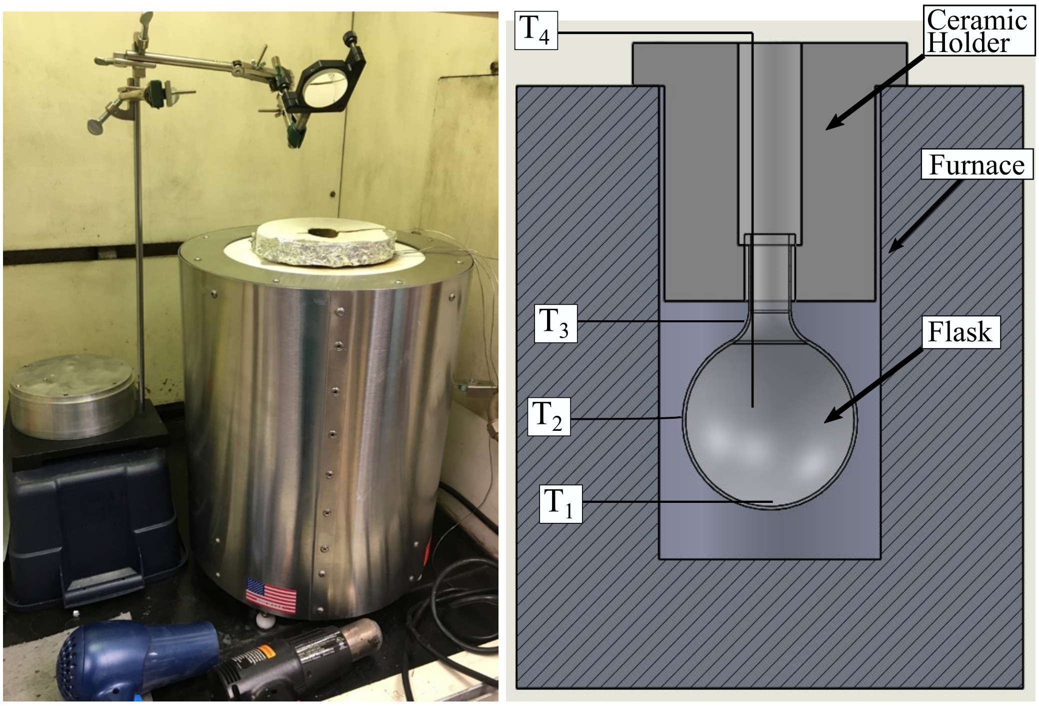

***Fig. 1**: (left) ASTM-E659 test apparatus (right) Cross section of internal heated region with thermocouple locations highlighted*

use of higher quality storage vessels (PTFE lined caps) and a chemical refrigerator to maintain the batch at a low temperature in order to lower the vapor pressure of the entire mixture and mitigate the preferential loss of lighter compounds over time. The second batch was mixed on a volumetric basis using graduated pipettes into a large 146 mL total batch in order to minimize volume measurement errors especially in the more dilute components. This batch was then stored in an ABS flammable storage refrigerator maintained at 3°C and smaller quantities were extracted for use in the autoignition experiments.

Table 2: JI surrogate (Batch 1) results from GC-FID analysis

	Mass fraction			**Vapor Pressure**[a] **(T=20°C) [kPa]**
Fuel	**Target**	**Measured**	**% Error**	-
n-Dodecane	0.2915	0.2980	2.24	0.012
Isocetane	0.4651	0.4643	0.15	0.004
Decalin	0.1940	0.2066	6.49	0.116
Toluene	0.0494	0.0310	37.2	2.903

[a] Sund (2019)

3 Results and discussion

3.1 *Classifications*

Throughout the range of ignition tests conducted here, there were 4 distinct ignition modes observed along with non-ignition cases. These ignition behaviors were classified as (I) Ignition, (II) Cool Flame, (III) Non-Luminous Cool Flame and (IV) Rapid Reaction. These were distinguished using a combination of visual evidence as well as the reading of the gas phase thermocouple (T_4). Qualitatively the differences between these modes are summarized in Table 3. This classification is limited mainly to qualitative descriptors since the temperature rises and timescales for the same ignition mode can vary substantially between two different fuels or even different compositions of the same fuel. For instance mode III ignition events for n-Decane were seen to produce a temperature rise of 50-200°C on timescales of 1.5-3.5 minutes for various fuel volumes while for Jet A these events were only capable of 25-70°C temperature increases on similar timescales. A representative series of images showing the time progression of each of the first three ignition modes

Table 3: Classifications of various ignition behaviors observed in ASTM-E659

Ignition Mode	**Name**	**Luminosity**	**Temperature Rise (ΔT)**	**Timescale for reaction**
I	Ignition	Large	Large	5 sec - 2.5 mins
II	Cool Flame	Small	Small	15 sec - 4 mins
III	Non-Luminous Cool Flame	None[a]	Large	1 - 5 mins
IV	Rapid Reaction	None	Small	30 sec - 2 mins
-	Non-Ignition	None	<15°C	> 4 - 5 mins

[a] Faint glow only visible to naked eye and small puff of smoke

is shown in Fig. 2. In events classified as mode I, the images show that the initial explosion progresses rapidly and the flame quickly expands out the top opening of the flask before burning out. For mode II events, it was typically observed that the ignition event is less energetic and the flame remains confined to the interior of the flask indicative of a low pressure rise which is consistent with the measured low temperature rise. Mode II was primarily observed in compounds with high ignition temperatures ($> 400°$C) including the aromatics and Isocetane. Mode III ignition events were more prevalent in heavier hydrocarbon species and were indicated by a brief and very dim glow visible to the naked eye only in complete darkness. Alternatively, a puff of smoke escaping from the flask could also be observed in these cases and was much easier to record with the current setup as shown by the series of images for mode III in Fig. 2. Mode IV was similarly non-luminous but was distinguished by a much smaller temperature rise and shorter timescale for the peak temperature to be reached as compared to mode III. These events were observed primarily for multi-component mixtures including the Jet A blends and surrogate fuels.

The thermocouple traces accompanying each of these ignition cases are shown in Fig. 2. The difference between the initial gas temperature and the peak temperature measured by T_4 is defined as the peak temperature rise. In some cases the visual evidence alone was not sufficient to distinguish between ignition modes I and II so the thermocouple trace was used for classification. Mode II ignition was always characterized by a longer ignition delay time as well as a lower peak temperature as compared to mode I events for the same fuel. Mode III also had a far longer timescale than the other modes which further distinguished it from the other modes. Mode IV was unique in that the reaction delay occurred on a similar timescale as that of a normal mode I ignition but resulted in a very small temperature spike, in some cases comparable to non-ignition cases.

The results of the ASTM-E659 ignition testing are presented here for each of the Jet A batches and surrogates studied. These data are summarized for each fuel by separate plots containing each ignition test as a data point in the temperature-composition space. Also plotted are the reported AIT values from the literature sources discussed in section 1.1. However, these numbers are always reported as a global minimum with no associated composition given so these values are plotted as constant lines across the compositional domain. The peak temperature rise during each test (ΔT) was also recorded and is shown here for two fuels. Tests were also performed with the molecular components of each surrogate as well as n-Hexane but complete results are not presented here.

A global equivalence ratio (ϕ) was defined in order to more easily compare results from fuels of different structure and molecular weight by putting the seemingly arbitrary fuel volumes into context. This ϕ is defined based on the vapor space for each fuel sample as if the fuel mass were fully vaporized and mixed homogeneously with air and is calculated by the equation

$$\phi = \frac{m_{fuel}/(\rho_{air}V_{flask})}{(F/A)_{stoich}} \tag{1}$$

where m_{fuel} is the fuel mass, V_{flask} is the flask volume, ρ_{air} is the air density, and $(F/A)_{stoich}$ is the stoichiometric fuel to air mass ratio. Using this parameter, it is much easier to see what the effect of having a fuel rich ($\phi > 1$) or fuel lean ($\phi < 1$) mixture is on the ignition behavior and to interpret the different ignition modes.

3.2 Alkanes & Aromatics

Three normal alkanes (n-Hexane, n-Decane, and n-Dodecane) and three aromatic compounds (1,2,4-Trimethylbenzene(TMB), Toluene, Trans-decalin) were studied along with one branched

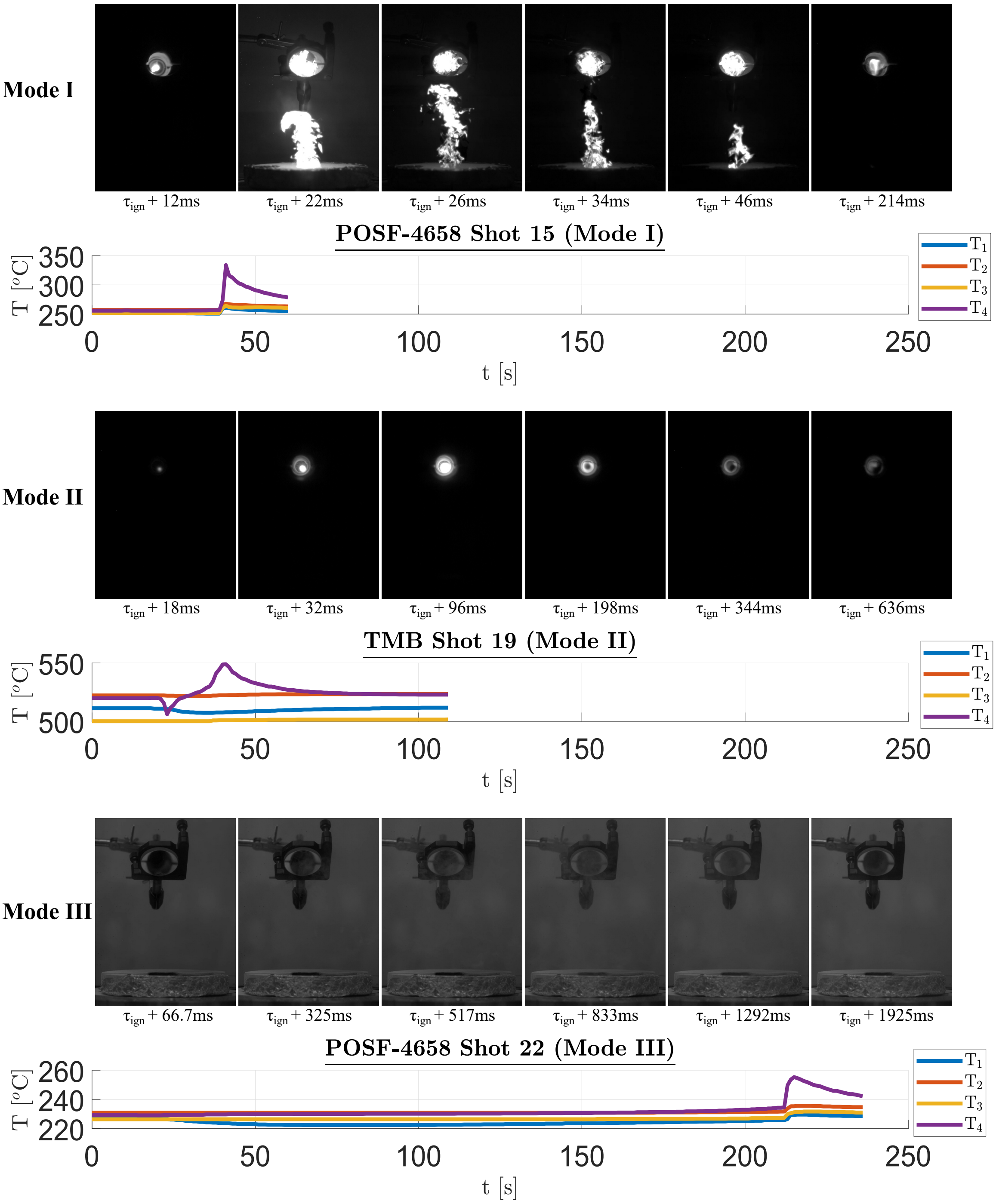

***Fig. 2**: Representative ignition events for 3 distinct ignition modes: (I) Ignition, (II) Cool flame, (III) and Non luminous cool flame (Note these correspond to POSF-4658 Shot 15, TMB Shot 19, and POSF-4658 Shot 22)*

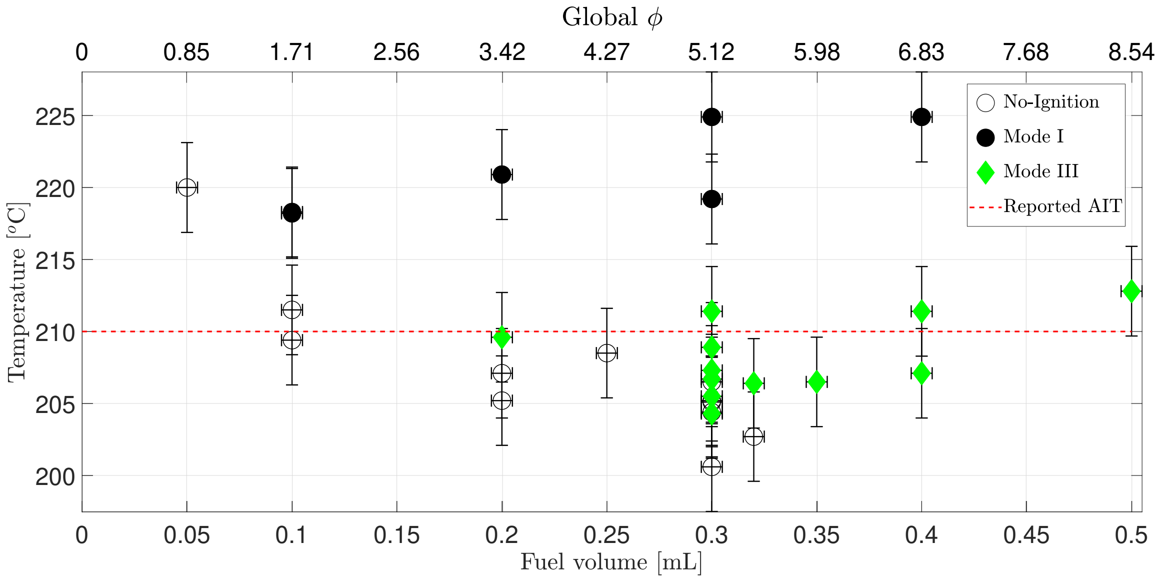

***Fig. 3**: n-Alkane representative ignition test results (n-Decane)*

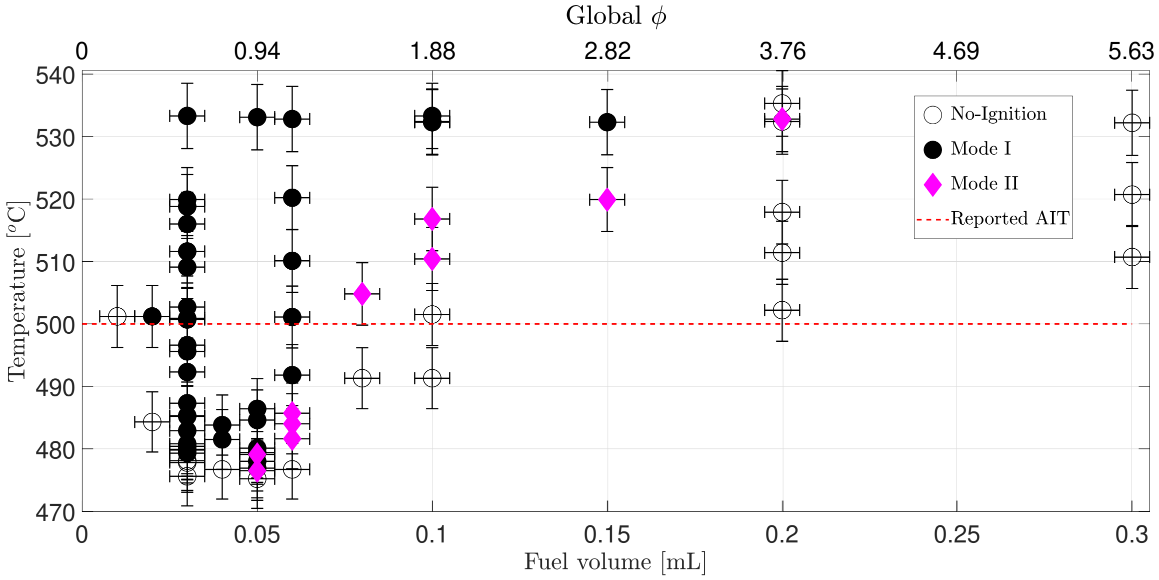

***Fig. 4**: Aromatic representative ignition test results (1,2,4-Trimethylbenzene)*

alkane (2,2,4,4,6,8,8-heptamethylnonane, more commonly known as Isocetane). These compounds were chosen for study because they are the molecular components for both of the surrogate fuels (Aachen and JI). n-Hexane was also chosen for study due to extensive previous work from our group on n-Hexane ignition in various test conditions, see Boettcher et al. (2012, 2013), Mével et al. (2014), Coronel et al. (2018), Mével et al. (2019). Some representative results of n-alkane and aromatic ignition results are shown in Fig. 3 and Fig. 4 respectively. The influence of fuel volume on AIT seen in these figures is a result of the complex dynamics associated with the fuel injection, vaporization and mixing processes which can create an inhomogeneous mixture within the combustion chamber with pockets that may be beyond the rich or lean flammability limits. These effects require further study in the present geometry in order to fully understand the influence of these processes on AIT. The global minimum AIT measured from each of the fuels as well as the corresponding test conditions are also summarized in Table 4 for convenience. The n-alkanes studied showed generally lower AITs than Isocetane and the aromatics which is consistent with the connections made between chemical structure (branching, unsaturation) and AIT as laid out in Affens et al. (1961). The n-alkanes also generally exhibited lower ignition temperatures at more fuel rich conditions where mode III ignition events became dominant. Isocetane also followed this trend but with mode II ignition becoming dominant at fuel rich conditions. The TMB and Toluene showed an opposite trend in that the minimum AIT was generally observed at near stoichiometric or slightly lean conditions with increasingly great difficulty igniting at rich conditions. Additionally mode II ignition rapidly became dominant at even slightly rich conditions for both of these aromatics. The exception to these trends for the aromatic fuels was the Trans-decalin which became more easily ignited at rich conditions with a far lower AIT around 240°C. In addition Trans-decalin exhibited all four ignition modes with mode II and III both becoming dominant at rich conditions and mode IV ignition being observed only at lean conditions near the ignition threshold. The temperature rises measured were also far higher for the n-alkanes than Isocetane or any of the aromatics.

3.3 Multi-component fuels

The multi-component fuels examined in this study were Jet A fuel standards (POSF-4658 and POSF-10325) and surrogate jet fuels from the literature (Aachen and JI). Some of the observed ignition behaviors of these fuels can be attributed to characteristics of their molecular components. As summarized in Table 1, these fuels are effectively entirely composed of alkanes and aromatic compounds with the alkanes being present in much larger proportions than the aromatics (approximately 3-4 to 1) so the alkane ignition behavior is expected to dominate.

POSF-4658 is a Jet A blend which has been examined extensively by a number of researchers, see Edwards (2017). Fig. 5 (a) shows the ignition results obtained in this study for this blend. Mode III and mode IV events are observed in the rich and lean regimes respectively which is similar to the behavior of the simple fuels. There is a good agreement between these experimental results and the reported Jet A AIT value ($T = 229.0°\mathrm{C} \pm 3.1°\mathrm{C}$ vs 232°C). This relatively low AIT can likely be attributed to the alkane dominant composition of Jet A since alkanes generally exhibit AITs in this range while aromatic compounds tend to be much higher. Fig. 5 (b) shows temperature rises around 100°C while the mode III and IV events exhibit far lower temperature increases.

POSF-101325 shows substantially similar ignition behavior to POSF-4658, which is consistent with the modest differences in composition between the two fuel blends (Table 1). The POSF-10325 ignition data shown in Fig. 6 is similar to Fig. 5 (a) but has a few minor differences. One of these differences is in the lean regime where the mode IV ignition occurs at slightly lower temperatures than for the POSF-4658. Peak temperature rises for all ignition modes are also similar to those seen for POSF-4658 so are not included here. The minimum AIT is also similar to that found for POSF-4658.

The Aachen surrogate is a simple two component blend which seems to capture the general trends from the Jet A batches while missing some details like mode IV events in the lean regime as seen in Fig. 7 (a). Mode III events are generally well captured in the rich regime with this mode extending to higher temperatures for richer compositions as was seen for Jet A. The Aachen surrogate also exhibits relatively lower ignition temperatures than those seen for Jet A samples as well as the reported value ($T = 219.0°\mathrm{C} \pm 3.1°\mathrm{C}$ vs 232°C). The peak temperature rises (not shown) are also

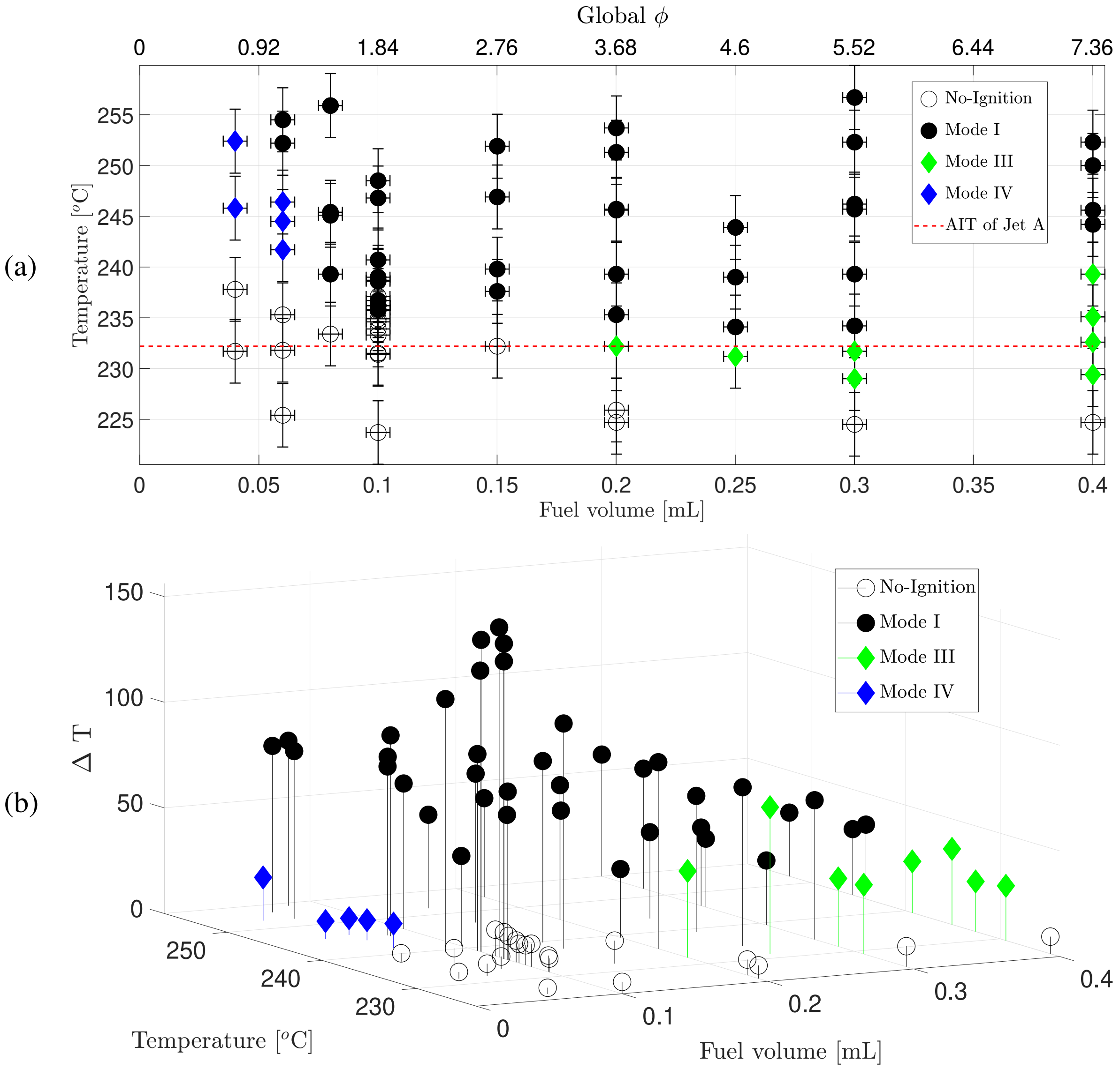

Fig. 5: *(a) POSF-4658 (Jet A) ignition testing results (b) Peak temperature rise*

quite similar to that of the two Jet A batches.

The more complex JI surrogate consisting of 4 components does a much better job at reproducing the ignition behaviors found in the Jet A samples. Fig. 8(a) shows the existence of mode IV events in the near stoichiometric regime along with the mode III events being maintained in the rich regime. However, these mode IV events occur at slightly richer compositions than observed for Jet A. Fig. 8(b) shows another difference in that the temperature rises measured for JI are much lower than those seen in either of the Jet A samples as shown by Fig. 5(b). The minimum AIT measured here is also much more consistent with the reported value as well as that measured for the Jet A samples ($T = 228.3^\circ\text{C} \pm 3.1^\circ\text{C}$ vs 232°C).

The global minimum AIT measured from each of the fuels as well as the corresponding test conditions are summarized in Table 4 and compared to some values reported in the literature. The differences between present results and literature values range from 1 to 7%, comparable to or

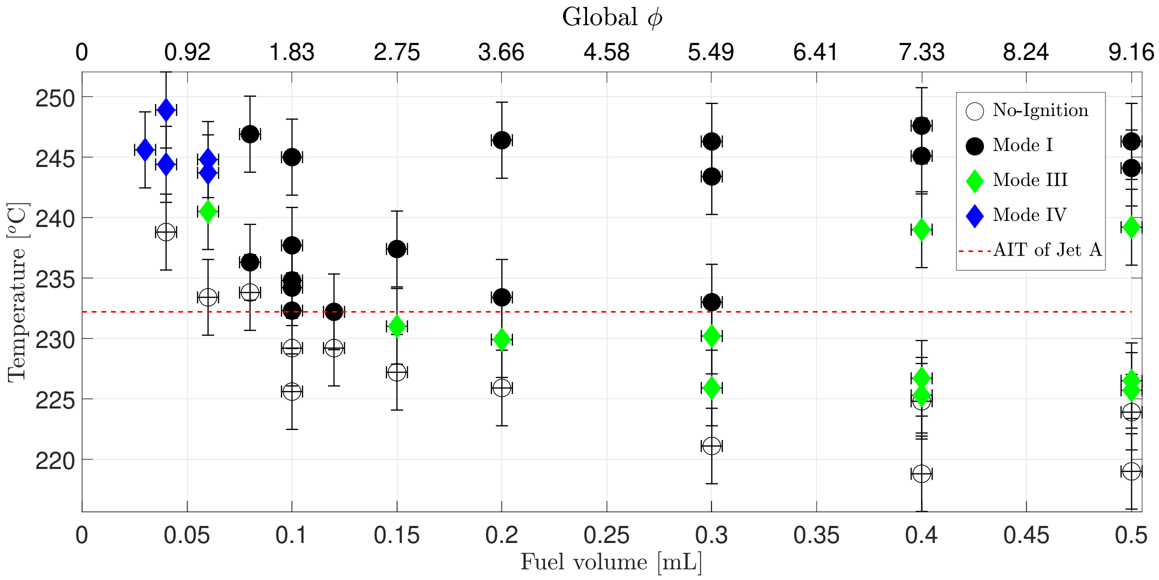

***Fig. 6**: POSF-10325 (Jet A) ignition testing results*

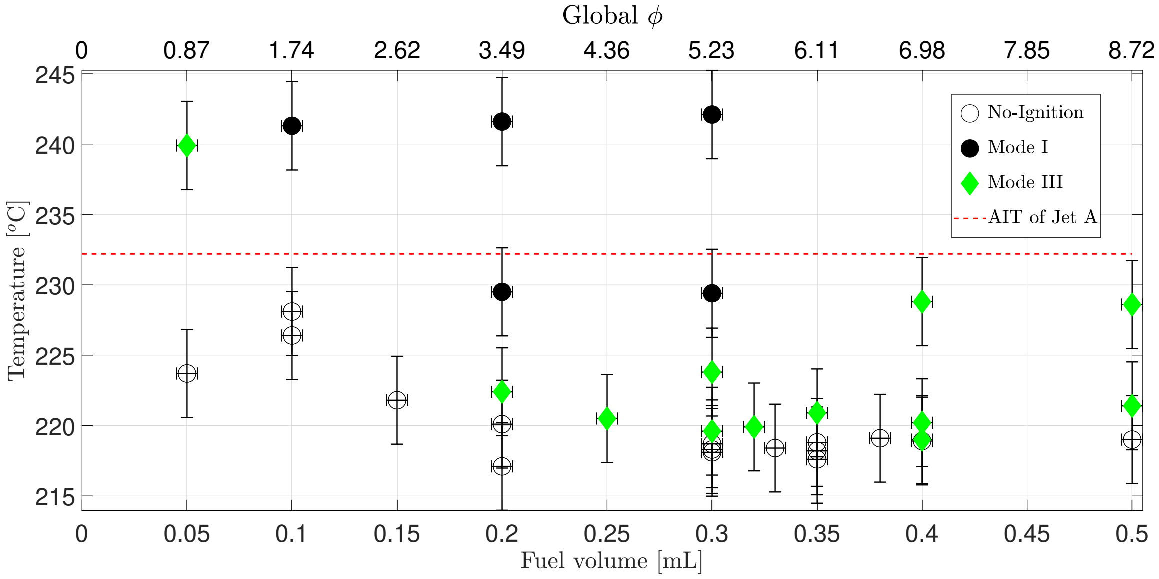

***Fig. 7**: Aachen surrogate ignition testing results*

larger than the estimated uncertainty of $\pm 1\%$.

4 Conclusions

The very low-temperature thermal ignition regime is important to industrial safety for commodity fuels but presents many challenges for combustion experimenters and modelers. In concert with related efforts in our laboratory, we have examined the potential for using surrogate fuels with simple and well-controlled composition rather than samples of Jet A which can have wide variability in properties. As a first step in determining the applicability of surrogates for very low temperature Jet A thermal ignition studies, we have examined the ignition behavior in the ASTM-E659

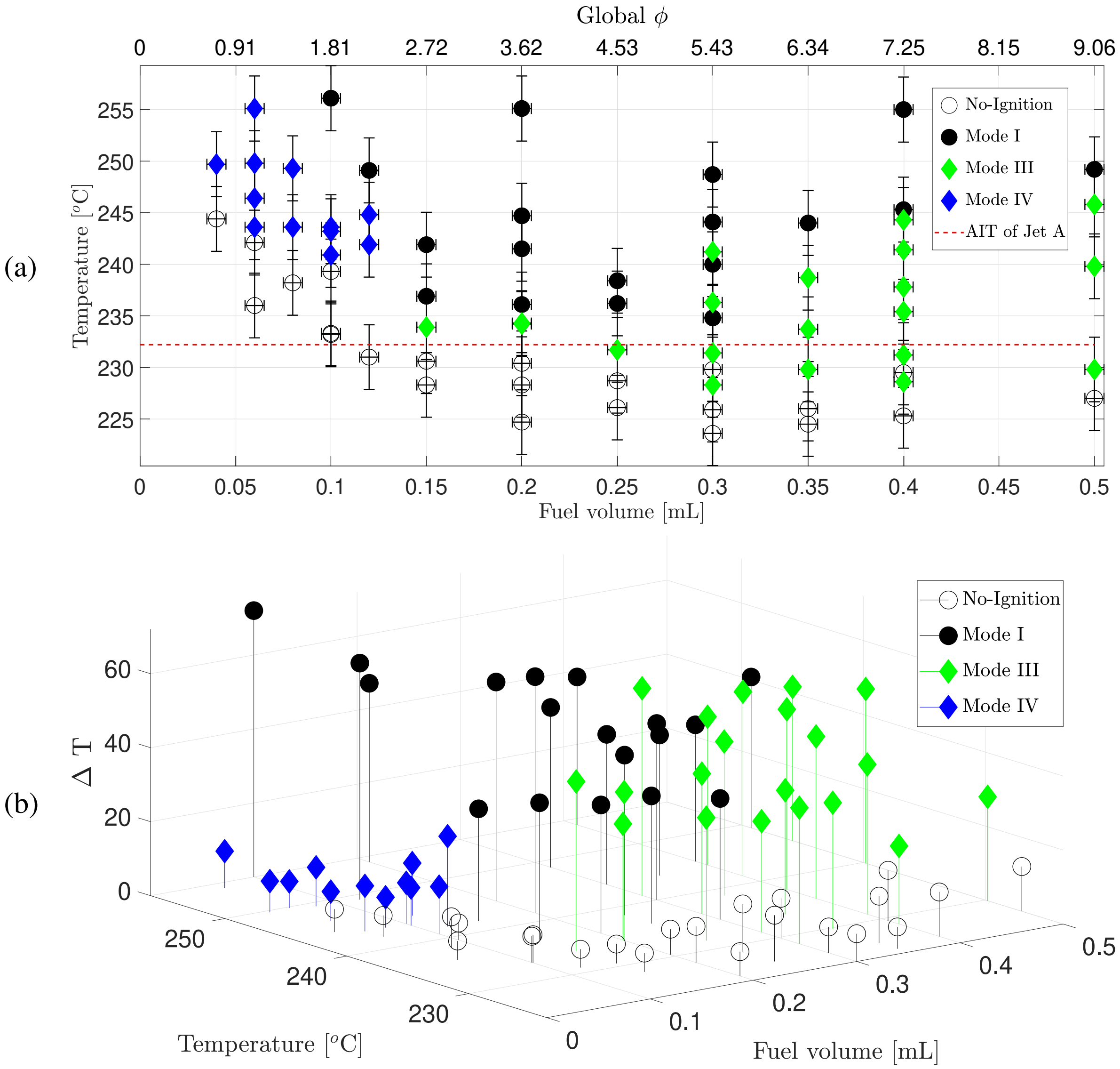

Fig. 8: *(a) JI surrogate ignition testing results (b) Peak temperature rise*

apparatus for two Jet A surrogates, and two standardized batches of Jet A.

Four distinct ignition modes were observed near the AIT threshold and were characterized using the limited diagnostic tools possible in the ASTM-E659 test. Experimental results were compared with reported minimum AIT numbers from literature sources with some data obtained showing significant discrepancies with reported AIT numbers. The multi-component fuels exhibited ignition characteristics that appear to be dominated by n-alkanes which is consistent with the predominance of alkane components in these fuels. The two Jet A batches studied showed very similar ignition behavior across the parameter space while both the Aachen and JI surrogates were able to reasonably replicate most of the Jet A ignition trends with composition and temperature. The JI surrogate did however exhibit much better agreement for ignition thresholds in comparison with Jet A than the Aachen surrogate and was even able to reproduce the existence of mode IV ignition events which the Aachen surrogate could not.

Table 4: Summary of measured minimum AIT values and corresponding test conditions

		Measured			Literature
	Fuel	**Fuel Volume [mL]**	**Global ϕ**	**Minimum AIT [°C]**	**Reported AIT [°C]**
Alkanes	n-Hexane	0.10	1.56	235.3 ± 3.1	225[a] (236[b])
	n-Decane	0.30	5.12	204.3 ± 3.1	210[ab]
	n-Dodecane	0.30	5.24	202.2 ± 3.1	203[a]
	Isocetane	0.40	7.36	395.2 ± 4.1	-
Aromatics	1,2,4-Trimethylbenzene	0.05	0.94	476.5 ± 4.8	500[ab]
	Trans-decalin	0.25	5.04	239.5 ± 3.1	255[a]
	Toluene	0.06	1.09	508.2 ± 5.0	480[ab]
Multi component	POSF-4658	0.30	5.52	229.0 ± 3.1	232[c]
	POSF-10325	0.40	7.33	225.3 ± 3.1	232[c]
	Aachen Surrogate	0.40	6.98	219.0 ± 3.1	-
	JI Surrogate	0.30	5.43	228.3 ± 3.1	-

[a] NFPA (1991) ; [b] USCG (1999) ; [c] FAA (2018)

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