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CHARACTERISTICS INVESTIGATION OF COMBUSTION PROPERTIES OF ELECTROFUELS FOR AEROSPACE APPLICATION

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Abstract

Alternative fuels, such as so-called electrofuels, could be a long-term answer given the increase in air traffic and the need to reduce emissions. When referring to electrofuels, it is meant that they both use renewable energy for fuel synthesis and emit no carbon dioxide. In this study, five prospective electrofuels—n-octane, methanol, methane, hydrogen, and ammonia—are compared to traditional Jet A-1 fuel and considered with regard to their potential use as aviation fuels. There are three key points that are highlighted. The technological approaches, energy efficiency, and level of maturity or research required for the manufacture of the electrofuel are outlined. The physical-chemical characteristics are contrasted with regard to specific energy, energy density, and characteristics that are important for fuel combustion, such as autoignition delay time, adiabatic flame temperature, laminar flame speed, and extinction strain rate. Except for n-octane, the results indicate that the physical and combustion properties are markedly different from those of jet fuel. The findings outline how the various electrofuels perform in relation to crucial factors like fuel and air mass flow rates. The outcomes also aid in identifying the mixing characteristics of each electrofuel's exhaust gas. N-octane manufactured synthetically is viewed as a potential option for an electrofuel in the future, even with a drop-in capability. The result indicate that the autoignition delay period and laminar flame speed percentage errors for the elecrtofuels and conventional fuels are 23% and 12% respectively. For the other fuels, further questions need to be investigated before they may be used as electrofuels in aircraft. Future hydrogen-ammonia combinations may be particularly intriguing, but research in this area is still in its early stages.

Keywords: Aviation, Autoignition, Combustion, Electrofuel, Greenhouse, Hydrogen, Storage,

1. INTRODUCTION

A totally sustainable aviation future calls for the use of energy sources that are based on renewable resources and have zero impact on the environment. Both local and greenhouse gas emissions should be avoided. In theory, aviation powered by electricity would be a possibility, however battery packs ability to store direct electrical energy is severely constrained. Utilizing electrofuels as an alternative to conventional fuels for aviation is a possibility [1]. The fuel can be viewed as an energy carrier in the sense that, on the ground, the electrical energy is stored in the fuel with a high energy capability by synthetically creating fuel with the aid of electricity. The energy required for flight is then provided by this fuel inside the aircraft through combustion processes. Such electrofuels could be viewed as CO_2-neutral if the ground-based storage process of the fuel results in no emissions of greenhouse gases (basically CO_2) or other emissions, which, at least ideally, might be possible by using renewable power sources like wind or solar-based electricity. This is clear for such energy-carrying fuels with no carbon content (such H_2 or HN_3), but it holds true (at least in theory) even for electrofuels having a hydrocarbon structure. However, because the carbon is removed from the atmosphere during the manufacturing of this fuel, it can still be considered CO_2-neutral. Electrofuel combustion does not eliminate all combustion pollutants, including soot particles, nitrogen oxides (NOx), carbon monoxide (CO), and unburned hydrocarbons (CxHy). Due to the fact that these electrofuels will be created synthetically, new degrees of freedom in their design and selection may be available, which might drastically lower local combustion emissions as well. The fuel might permit lean premixed combustion in place of non-premixed combustion in existing air-engines that operate with a significant excess air-to-fuel ratio (lean combustion). Lean premixed combustion prevents soot particle emissions while also significantly reducing NOx emissions [2]. To avoid pre-ignition or a flashback of the flame into the mixing zone, great care must be taken in this situation. Since the two stages required to achieve entirely renewable and fully CO_2-free aviation.

These fuels may be referred to as drop-in fuels, if they were produced using green power, yet they may have characteristics that were somewhat similar to those of the present aviation fuels (Jet A, Jet A-1, and JP-8). They can be included into the current aviation engines, perhaps with some adjustments to accommodate the slightly different features. The use of drop-in fuels is viewed as the first step toward an electro-based sustainable aviation industry. [3] Provides an overview of recent developments in conventional drop-in fuels. The combustion engines also need to be rebuilt, if different fuels were to be employed. The development of new air engines would need to put a lot of work into this, since other difficulties outside the aero-thermochemical characteristics need to be taken care of. However, this opens up a lot more room for novel combustion ideas and potentially new engine architectures.

Alternative fuels have been used in aviation for some time. Ammonia (HN_3) was used as the fuel in various activities that had already been researched in the 1960s [4-6]. The main findings were that although ammonia combustion is technically feasible, it is constrained by a small ignition range and has poor flame stability. Ammonia and oxygen could be burned as a potential solution. Here, a military supersonic research aircraft called the X-15 was powered by a rocket engine [7] using liquid oxygen and anhydrous ammonia as fuel [8]. However, it appears that this choice is not appropriate for general aviation use. Mixing HN_3 with other, more reactive fuels is an alternative. More recently, this was explicitly investigated in a micro-gas turbine using HN_3 /kerosene and HN_3 /CH_4 fuel mixes [9-10].

The use of hydrogen as an aviation fuel has also been researched for many years for high-speed air transportation aircraft [11-15], including concerns about airport safety [16]. The first experimental cryogenic aircraft, the Tupolev Tu-154 [17] in the 1980s, which was powered by liquefied hydrogen and natural gas, served as the proof of concept for the use of hydrogen in aviation. [18] Discusses a comparison between hydrogen and hydrocarbon aviation fuels. Further work on the use of hydrogen for aviation engine were done by [19-27]. With regard to hydrogen in aviation [28] provide a good review.

Examples of comparative research for various fuels are those [29] and [30]. [31] Provide a fairly recent review of sustainable alternative aviation fuels. For example, [22] conducted a life cycle analysis comparing liquid hydrogen and liquid natural gas, while [32] compared hydrogen, ammonia, methanol, ethanol, and liquefied natural gas for aircraft. The most recent study comes to the precise conclusion that aircraft powered by ammonia and hydrogen may have a positive influence on the environment.

This study compares various fuels that could be used as electrofuels in aviation in a first-order approximation with regard to their synthesis, combustion characteristics, and effects on the combustion chamber and turbine of the aircraft engine. The study will concentrate on the fundamental aero-thermochemical difficulties and only sometimes bring up other factors like constructional restrictions, safety, production factors, and costs.

The definition of electrofuels and the synthesis of five potential electrofuels n-octane, methanol, methane, hydrogen, and ammonia—come first in the remaining section of this study. Then, the distinctive combustion characteristics of five chosen electrofuels are contrasted with those of regular jet fuel. The autoignition delay time, adiabatic flame temperature, laminar flame speed, and extinction strain rate are computed numerically and examined for the comparison. In a comparison discussion, the key findings are gathered in the form of an assessment matrix, along with any prospective benefits and drawbacks, and issues that require more analysis and research. In that regard, this study might be viewed as being in a rather early stage of scientific discussion. Within the Earth's finite environment, problems about the limited fuel resources and the environmental effects of energy use, specifically in aviation, have become more and more important to people.

Electricity is expected to play a major role in sustainable transportation in the future, including aviation, as we move away from fossil fuels and toward renewable energy sources. The small amount of energy that can be stored on board in batteries makes employing electric power for transportation (and aviation in particular) a major difficulty. Even with anticipated advancements, batteries' physical limitations will prevent their energy density from exceeding that of chemical fuels. Electrolysis is a method that stores electrical energy within the molecules of gaseous or liquid fuels. The idea behind this strategy is commonly known as power-to-gas or power-to-liquid, with compatible fuels being referred to as electrofuels.

A decoupling between the time and place of production and use is achievable with electrofuels since they may be thought of as energy storage, which is a key distinctive attribute of electrofuels in comparison to the erratic availability of wind power and photovoltaics. Electrofuels can also be easily transported and stored, which is beneficial for use in aviation. The current study concentrates on the use of electrofuels with combustion.

Due to the difficulties in using hydrogen as a fuel, molecular hydrogen is typically used as a chemical intermediate to create more manageable liquid or gaseous fuels, such as methane ("power-to-gas") and longer chained hydrocarbons (power-to-liquid) from carbon dioxide, or to create ammonia from nitrogen (power-to-ammonia). Fundamentally, all of these substances can be described as molecular hydrogen transporters. All these method using hydrogen to create energy is called Power-X technology. Combining electrolytic hydrogen synthesis with a subsequent catalytic conversion of the hydrogen gas with carbon dioxide or nitrogen is shown in Figures 1. The respective catalytic conversions often call for comparatively extreme pressure and temperature conditions because of the chemical stability of the carbon dioxide and dinitrogen molecules and the accompanying high activation barrier of these reactions.

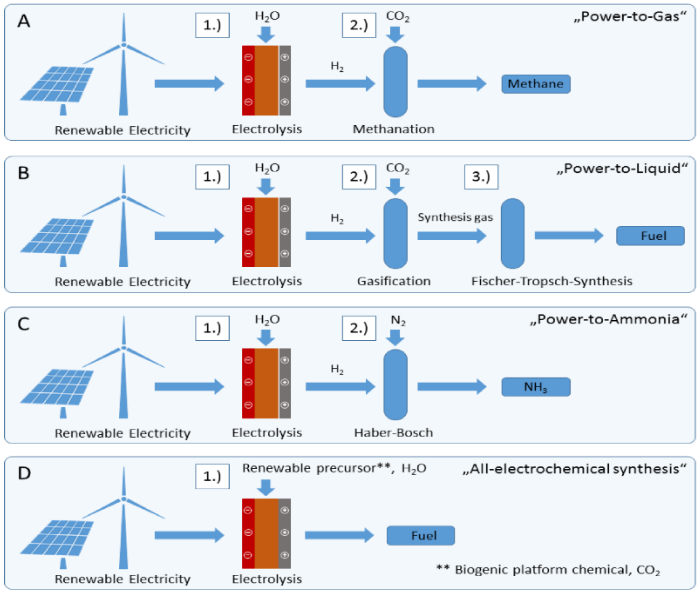

Figure 1: Schematic representation of the power-to-X technologies described: (A) Power-to-Gas, (B) Power-to-Liquid, (C) Power-to-Ammonia, and (D) All-Electrochemical Synthesis. [33]

The power-to-gas process (Figure 1A) often entails the methanation of hydrogen and carbon dioxide, in the exothermic process: $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$. Compared to hydrogen, methane is significantly simpler to store and transport. Methane is already a well-established fuel for ground transportation due to its accessibility from fossil resources (natural gas). Compared to other innovative fuels, infrastructure and motor optimizations are at a high level, which is a significant benefit. Methane can be used either as a compressed gas (compression of 200–250 bar) or in a liquefied state (boiling point of -161.5 °C). The power-to-liquid method (Figure 1B) is used to create longer chained hydrocarbons. A portion of the electrolytic hydrogen is needed in the first stage to convert carbon dioxide to carbon monoxide. The latter creates syngas, the precursor to the ensuing Fischer-Tropsch synthesis, when combined with more hydrogen. Fuels with desired qualities can be produced by varying operational factors including syngas composition, pressure, and temperature, as well as the catalyst system. The power-to-ammonia method (Figure 1C) offers the possibility of a completely carbon-free fuel and the utilization of nitrogen, one of the most prevalent elements in our atmosphere, as a hydrogen carrier. The widely used Haber-Bosch method is currently the industry standard for producing ammonia. If hydrogen is created by steam reforming from fossil fuels, the Haber-Bosch process has an energy efficiency of about 60%. Instead of using water electrolysis as a sustainable production method, the method is much less efficient (38.5%) [34]. Another method is the relatively recent solid state ammonia synthesis (SSAS), which electrochemically converts molecule-level nitrogen to ammonia. Elevated reaction temperatures in the range of 80 to 650 °C appear to be necessary because of the high activation barrier. The SSAS procedure has an overall energy efficiency that can reach 66% [34]. Compared to hydrogen, ammonia is simpler to store. It liquefied at a pressure of 10.3 bar [35]. Combustion's use of ammonia is a subject that has received relatively little study. Various ideas have been put forth, such as using ammonia as a drop-in fuel for diesel engines, burning it directly, or converting it to hydrogen before combustion. If every component is designed specifically for the ammonia motor, efficiency ratings of 65% are suggested [36]. Given the aforementioned information, well-to-wheel efficiency would range from 25.0 to 42.9%. Ammonia's low energy density, which even in its liquid form is only one-third that of conventional gasoline or kerosene, its chemical corrosivity, which necessitates the use of new materials for storage tanks and fuel lines, and its toxicity are its three main drawbacks as a fuel.

2. METHODOLOGY

2.1. Comparison of Physico-Chemical Fuel Properties

Five sample electrofuels, n-octane, methanol, methane, hydrogen, and ammonia—are chosen for this study based on the mentioned synthesis techniques. Regarding a few chosen features that are crucial for their possible use as sustainable aviation fuels, they are compared to conventional jet fuel (Jet A-1). See table 1.

Table 1: Comparison of physical and chemical properties of Jet A-1 and different potentials elecrofuels (L= Liquified; * at 15 °C; † at 20 °C; ‡ at boiling point) [37].

Physical Properties	**Jet A-1**	**nC_8H_{18}**	**CH_3O**	**LCH_4**	**LH_2**	**LNH_3**
Flash point (°C)	38	12	11	--	--	--
Autoignition temperature (°C)	210	205	455	595	560	630
Energy density (MJ L^{-1})	34.2	33.2	15.9	21.2	8.4	13.6
Density (g cm^{-3})	0.808^{*}	$0.70^{\dagger}$	$0.796^{\dagger}$	0.58	$0.071^{\ddagger}$	$0.73^{\ddagger}$
Boiling point (°C)	176	126	65	−162	−252	−33
Melting point (°C)	−47	−57	−98	−182	−260	−77.7
Vapor pressure at 20 °C (hPa)	3	14	129	N/A	N/A	8573
Lower explosive limit (vol %)	0.6	0.8	6.0	5.0	4.0	15.0
Upper explosive limit (vol %)	6.5	6.5	50.0	15.0	77.0	28.0
Mass fraction of hydrogen (-)	N/A	0.16	0.13	0.25	1.00	0.18
Mass fraction of carbon (-)	N/A	84	0.38	0.75	0.00	0.00
Mass fraction of oxygen (-)	N/A	0.00	0.49	0.00	0.00	0.82

The flash point of a liquid fuel—the lowest temperature at which its vapors will ignite in the presence of an external ignition source—is a crucial characteristic. As a matter of safety, jet fuel has a flash point that is higher than ambient temperature to lessen the possibility of a fire starting. Since the fuel vapor can no longer be ignited, the flash point shouldn't be too high. The autoignition temperature is another characteristic that specifies the temperature at which the fuel will self-ignite in the presence of an oxidizer without the need for an external ignition source. The minimum and maximum fuel concentrations in the air that the mixture can burn at are known as the lower and upper explosive limits, respectively. The pressure of vapor above the liquid phase is referred to as vapor pressure. The fuel supply in the fuel line can be interrupted by a phenomenon known as vapor lock if the vapor pressure is too high, which can result in a transition from the liquid to gas phase. Vapor pressure and boiling point go hand in hand. To avoid the fuel from freezing during flights at high altitudes, the melting point should be low. Mass-based specific energy and volume-based energy density serve to quantify the fuel's chemically stored energy. The range of an aircraft is significantly impacted by both of these attributes. While the second one establishes the capacity of the tank system, the first one defines the weight for the required fuel.

Physical characteristics comparisons reveal that n-octane and jet fuel are very comparable. The specific energy, energy density, autoignition temperature, lower explosive limit, and higher explosive limit are all almost the same. Small additions of mixable hydrocarbon-based fuels with high energy densities can be used to modify other attributes like flash point, vapor pressure, and boiling point. These factors make it possible to utilize a mixture based on n-octane as a drop-in fuel in a conventional engine instead of regular fuel. As a result, the aircraft only needs to be slightly modified in this situation. Other environmentally friendly electrofuels including methanol, methane, hydrogen, and ammonia would call for at least some adjustments to the aircraft's fuel system, tank system, and engine. Their low volumetric energy density, which necessitates larger tank systems, is those fuels' main disadvantage. Because the information for methane, hydrogen, and ammonia is based on liquid fuel, the tank system must either be under high pressure or be cooled down by cryogenic tanks. Only a 10 K temperature difference between the inside of the cryogenic tank and the atmosphere at a 10-km altitude is needed for cryogenic liquid ammonia, whereas greater than 100 K and greater than 200 K temperature differences are required for cryogenic liquid methane and hydrogen, respectively. The data for a 10-km altitude ($T = -50$ °C, $p = 26{,}436$ Pa) are: cryogenic liquid ammonia ($T = -60$ °C, $P_{vap} = 21{,}892$ Pa); cryogenic liquid methane ($T = -178$ °C, $P_{vap} = 20{,}145$ Pa); and hydrogen ($T = -275$ °C, $P_{vap} = 20{,}447$ Pa)

3. RESULTS AND DISCUSSION

Engine performance is affected by the content and characteristics of the fuel during combustion and emission. By doing numerical simulations with in-depth reaction processes for the examined electrofuels, certain fundamental combustion parameters, such as autoignition delay time (τ), adiabatic flame temperature (T_{ad}), laminar flame speed (S_L) and extinction strain rate (a) are calculated.

With the help of the open-source Cantera [38], which is integrated into a Python script to carry out parallel computations, simulations with intricate finite-rate chemistry are carried out. The autoignition delay periods were calculated using simulations of a zero-dimensional perfectly stirred reactor with set time steps of 1×10^{-7}–1×10^{-6} s at a constant pressure p of 2.5 MPa and for fresh gas temperatures Tu of 1000–1500 K. The criteria for autoignition occurrence is defined by the maximum of heat release rate. The adiabatic flame temperature T_{ad} and laminar flame speed S_L are computed for air/fuel equivalence ratios λ of 0.9–1.8, fresh gas temperature Tu of 650 K and pressure p of 2.5 MPa using the one-dimensional freely-propagating flame model with an adaptive grid refinement control and multicomponent transport. To reduce computation time, the Soret effect is disregarded. The greatest axial velocity gradient is the extinction strain rate a, which is determined using the one-dimensional counterflow diffusion flame model. The boundary conditions are considered to be plug-flow. The fuel and oxidizer's input temperatures and mass flow rate area densities are established at1 300 K and 1kg m^{-2} s^{-1} respectively. The 20 mm gap between the fuel and oxidizer inlets is predetermined. The scaling criteria of [39] are used to improve the convergence behavior and decrease the computational burden of the counterflow flame simulations.

A validation is carried out in order to draw conclusions about the computations' predictability. An indirect method is used to validate the computations because there is a dearth of experimental evidence for the conditions and mixture compositions indicated above in the literature. Table 2 lists the experimental datasets from [40-58] that was employed.

Table 2: Experimental data used in the study

Autoignition Delay Time					**Laminar Flame Speed**				
S/N	**Mixture**	**λ (-)**	**T_u (K)**	**p (MPa)**	**S/N**	**Mixture**	**λ (-)**	**T_u (K)**	**p (MPa)**
01	Jet A/air	1.00	934–1220	2.2–5.1	17	Jet A/ai	0.60–1.39	473	0.
02	Jet A/air	1.00	990–1222	2.0	18	Jet A/air	0.76–1.43	400	
03	Jet A/air	1.00	978–1230	4.0	19	Jet A/air	0.74–1.43	400	
04	$nC_8H_{18}/O_2/Ar$	1.0	1265–1455	0.2–0.4	20	Jet A/air	0.77–1.43	400	
05	nC_8H_{18}/air	1.0	1025–1260	2.0	21	nC_8H_{18}/air	0.67–1.43	353	
06	$CH_3OH/O_2/N_2$	1.0	1013–1207	2.0	22	CH_3OH/air	0.67–1.43	298	
07	$CH_3OH/O_2/N_2$	1.0	963–1124	3.1	23	CH_3OH/air	1.00	450–570	
08	$CH_3OH/O_2/Ar$	1.0	996–1276	0.9–1.1	24	CH_4/air	0.77–1.43	298	
09	$CH_3OH/O_2/Ar$	1.0	999–1296	4.6–5.0	25	CH_4/air	0.77–1.43	298	
10	$CH_4/O_2/Ar$	1.0	1418–1656	2.0 [71]	26	CH_4/air	0.71–1.43	300	
					27	H_2/air	0.20–2.00	298	
					28	$H_2/O_2/He$	0.50–1.18	298	
					29	$H_2/O_2/He$	0.50–1.18	298	
					30	NH_3/air	0.80–1.20	298	
					31	NH_3/air	0.90–1.20	298	

In order to validate the mechanisms at atmospheric conditions, as well as at high temperatures (up to 2085 K) and pressures (up to 5.1 MPa). Figure 2 displays the validation results.

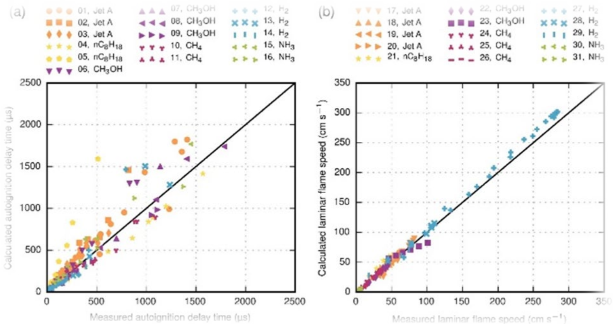

Figure 2. Comparison of calculated and experimental data (**a**) Autoignition delay time; (**b**) Laminar flame speed.

Figure 3. Illustrates the simulation outcomes for various fuels. According to inverse temperature between 1100 and 1500 K, the autoignition delay time is plotted using logarithmic scale.

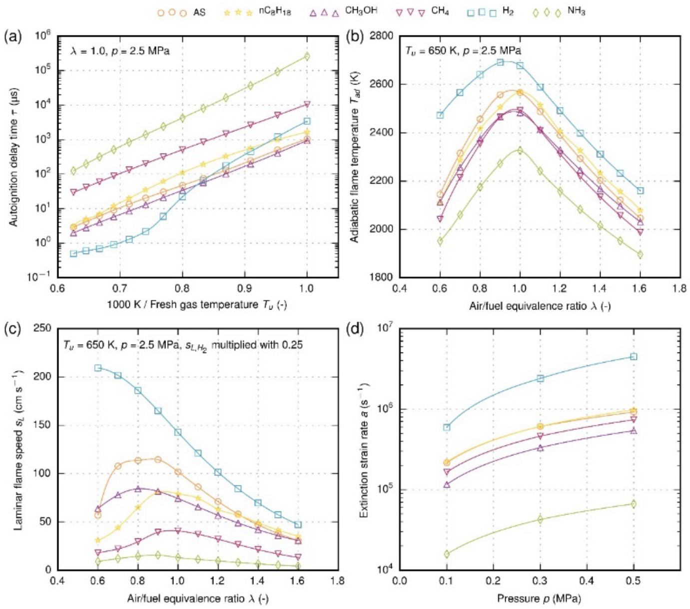

Figure 3. Combustion properties of different (**a**) Autoignition delay time; (**b**) Adiabatic flame temperature; (**c**) Laminar flame speed; (**d**) Extinction strain rate

The response rate or ignition energy can be inferred from the ignition delay time. For instance, higher ignition energy is required for fuels having a long autoignition delay time in order to start the ignition as rapidly as possible, which is crucial for starting an engine after a flameout. In comparison to n-octane, ammonia and methane have the longest autoignition delay times, followed by jet fuel. Methanol has a significantly shorter autoignition delay time, whereas the temperature of the reactants has a significant impact on the hydrogen self-ignition behavior. Premixed combustion in aircraft engines might be possible with longer autoignition delay durations.

For autoignition delay durations and laminar flame speeds, the mean absolute percentage error for all mechanisms is within around 23% and 12%, respectively, of the experimental data, where the deviation is higher. [59-63] Provide additional support for further validations in this work.

4. CONCLUSION

The fundamental combustion properties, such as the autoignition delay time, adiabatic flame temperature, laminar flame speed, and extinction strain rates, were computed using a complete reaction mechanism and contrasted to a conventional jet fuel. The findings shown that all of the investigated electrofuels, with the exception of n-octane, have combustion characteristics that are extremely unlike to those of jet fuel. For a combustion chamber under aircraft operating condition, numerous significant parameters were determined for a constant cruise operating point. The mass flows of air required for combustion and for cooling the hot gases produced during combustion are roughly same, but the mass flows of the fuel vary because of their varying specific energies. More research is required in this area, where mixture techniques (ammonia/hydrogen mixture) may be of particular interest. Combustors must be designed to match the fuels. This necessitating fundamental investigation into flame stability and emission. If the combustion were based on more sophisticated methodologies, like lean premixed or partially-premixed combustion, it would be possible to lower the emission of soot and nitrogen oxide, despite the fact that this procedure will need a lot of work. In order to meet necessary safety margins for combustion stability, flashback studies and reignition studies are required.

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