

APPLICATION OF FUEL BLENDS FOR ACTIVE DETONATION CONTROL IN A PULSED DETONATION ENGINE

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Abstract

Reliable operation of a pulsed detonation engine (PDE) can be attained by adopting a controlled charge concept based on the in-chamber blending of several fuels exhibiting different detonability. Detonability of fuels is characterized by the Octane Number. For examining Octane Number requirements of a PDE, dealing with fuel detonability and resistance to premature ignition, a semi-empirical oxidation mechanism for hydrogen peroxide – *n*-heptane – *iso*-octane blends is applied. The concept is examined in the example of two fuels: *iso*-octane and hydrogen peroxide.

Introduction

High thermodynamic efficiency of detonative combustion is the attractive feature for propulsion applications¹. Detonative combustion of fuel-air mixtures can be attained in either oblique or propagating detonation waves. In a pulsed detonation engine (PDE) fuel is supposed to burn in a propagating detonation wave, which is repeatedly generated at a closed end of a detonation chamber at a characteristic frequency of 100-200 Hz. In view of the latter, a number of problems arise that deal with requirements to a PDE fuel: (i) fast evaporation of liquid fuel and mixing with air, (ii) reliable detonation initiation in the fuel-air mixture (FAM) at relatively short distances (1–2 m),

(iii) preventing premature ignition of FAM at hot surfaces and uncontrolled auto-ignition of FAM due to mixing with residual combustion products, (iv) ensuring performance stability under variation of the flight Mach number and altitude.

It is hardly possible that a single fuel could meet the above requirements within a wide range of PDE operation conditions. According to Ref.2, these requirements could be met if the concept of controlled in-chamber blending of two fuels exhibiting different detonability is employed.

For assessing the required detonability of fuel blends there is a need in a detonability criterion. There exist several approaches based on the concepts of (1) Octane Number³ (ON), (2) detonation run-up distance³, (3) critical initiation energy⁴, (4) limiting tube diameter⁵, etc. Since detonability of fuel blends in terms of approaches (2) to (4) is poorly studied both experimentally and theoretically, the ON concept appears the most appropriate for the assessments. This concept is usually applied to assess the detonability of a test fuel in a piston engine in terms of the percentage of *iso*-octane (by volume) in the *iso*-octane (*iso*-C₈H₁₈) – *n*-heptane (*n*-C₇H₁₆) blend that matches the test fuel in allowable compression ratio.

Theoretically, the detonability requirements to prospective PDE fuels can be analyzed by using an oxidation mechanism of *n*-C₇H₁₆ – *iso*-C₈H₁₈ – air mixtures capable of providing auto-ignition and surface ignition data

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within a wide range of PDE operation conditions. To widen the range of fuels to be tested, in particular those exhibiting essentially higher detonability in air than *n*-heptane (i.e. fuels exhibiting “negative” ON), the range of ON should be significantly extended. It is implied that, experimentally, the detonability of a test fuel in terms of ON could be assessed by a standard procedure using a piston engine.

Studied in this paper is a possibility of meeting the requirements to PDE fuels by applying the controlled in-chamber blending of two fuels exhibiting different detonability. To extend the range of ON considered, hydrogen peroxide has been chosen as an additional reference fuel. The advantage of hydrogen peroxide is that it is present in the oxidation mechanism of an *n*-C₇H₁₆ – *iso*-C₈H₁₈ blend, and it exhibits a large negative ON.

Operating Conditions of a PDE

Table 1 shows the estimated variations of inlet pressure *P* and temperature *T* in the detonation chamber of a PDE-based supersonic vehicle.² Examination of Table 1 shows that at flight Mach number *M* = 2.0 the inlet conditions in the chamber may range from 520 K and 6.5 bar at sea level (*H* = 0) to 400 K and 1.7 bar at altitude *H* = 10 km. The effect of changing the flight Mach number on the inlet air temperature and pressure can be seen in the range of operation conditions at 10 km, where they vary from 270 K and 0.5 bar at *M* = 1.0 to 400 K and 1.7 bar at *M* = 2.0.

Table 1: Estimated variations of pressure and temperature in the detonation chamber of a PDE-based supersonic vehicle

No.	<i>M</i>	<i>H</i> km	<i>P</i> bar	<i>T</i> K
1	1.0	0.0	1.89	346
2	1.0	3.0	1.31	323
3	1.0	10.0	0.49	268
4	1.5	0.0	3.58	418
5	1.5	3.0	2.48	390
6	1.5	10.0	0.94	323
7	2.0	0.0	6.52	518

8	2.0	3.0	4.51	484
9	2.0	10.0	1.70	401

Repeatable propagation of detonation waves in the detonation chamber will obviously result in considerable heating of confining walls. Premature ignition of FAM is expected to arise at wall temperatures exceeding 600-800 K, providing that the duration of the PDE operation cycle is longer than the characteristic ignition delay.

Taking into account the dependence of physical and chemical processes in PDE on temperature, pressure, and FAM composition one realizes that special measures should be undertaken in order to ensure stable performance.

Detonability of Heavy Hydrocarbon Fuels

Quite a limiting number of experiments is available in the open literature on detonability of heavy gaseous fuels and vapors in air. The comparison of cell size data for stoichiometric fuel-air mixtures for the alkane family⁶⁻¹¹ shows that fuels larger than ethane exhibit very similar cell size of 40–70 mm at atmospheric pressure. Stoichiometric mixtures of high alkanes (propane, hexane, octane, decane, etc.) in air typically require 100–300 kJ (about 22–65 g of high explosive) for detonation initiation.^{6-8,11} Vapor of liquid fuel JP-4, considered as a candidate for PDE applications, shows the detonation properties (cell size and initiation energy) similar to hexane.¹⁰ Aerolite, which is the gaseous fuel issued from a solid propellant gas generator, is also considered a prospective fuel for PDE.¹² Its estimated ignition delay at temperatures relevant to detonation initiation in typical hydrocarbon–air mixtures (1400–1500 K) is less than 10 μs.¹² Extensive experimental data on ignition delays of motor fuels within wide ranges of temperatures and pressures are presented elsewhere.¹³ These can be used for estimating the detonation cell size and the critical initiation energies by using simple correlations for the dynamic parameters of detonation. The effect of ignition (detonation) promoters on self-ignition of heavy hydrocarbon fuels in shock waves was studied in Ref. 14,15. These studies have demonstrated that addition of *iso*-propyl nitrate, methyl nitrate, cyclo-hexyl

nitrate, N_2F_4 , NO_2 and other promoters to the fuel in amounts of about 15% and lower results in a reduction of the ignition delay by up to an order of magnitude in the range of ignition delays below 1 ms.

Detonability of fuel sprays in air has been studied to even lesser extent than that of gases and vapors.^{9,16-18} Extensive experimental work on detonability of JP fuels (JP-4, JP-8, JP-10), currently performed in Boeing-Phantom Works in view of their applicability to PDE¹⁹. The study⁹ unambiguously shows the important role of vapor phase in detonability of fuel sprays of such primary reference hydrocarbons as hexane and decane. Hexane and decane have a vapor pressure of about 130 Torr and 1.5 Torr at 20 °C, respectively. In aerosol cloud form, these fuels did not detonate when initiated by a high explosive charge of 850 g. Detonation of hexane cloud was possible only at a delayed triggering of the initiator (exceeding 150 ms after fuel dispersion) allowing for vaporization of fuel droplets. Detonation of decane could not be initiated at any delay times. Under similar conditions, sensitive liquid fluids such as propylene-oxide and nitrated hydrocarbons were detonated easily in aerosol form. Propylene-oxide has high vapor pressure (~ 450 Torr at 20 °C) and, at time the cloud was detonated, the fuel was most likely in a vapor phase. However, the nitrated hydrocarbon fuels tested had very low vapor pressure and thus detonated in the aerosol form. Dabora [Ref. 17] reports that pure kerosene sprays are non-detonable in air. However, addition of 10–20% (by weight) nitrated hydrocarbons (propyl nitrate or butyl nitrate) to kerosene allowed to detonate lean fuel–air mixtures in a laboratory detonation tube of 5.08 x 5.08 cm square cross-section and 2.75 m long. Fuel–air ratios tested were 0.3, 0.44, and 0.59. Initial fuel droplet size was 780 μm. Detonation was initiated by a shock wave of Mach number 3.5 providing the initiation energy of about 50 J/cm².

Experimental findings¹⁷ allow us to suggest a simple approach to estimating the detonability requirements to a PDE fuel. In his experiments, temperature and pressure of the fuel-air mixture behind the initiating shock wave were well-defined and equal approximately 1000 K and 14 bar. At these conditions, ignition delay of pure kerosene exceeds 50 ms, and ignition delay of butyl nitrate is about 0.1 ms [Ref. 13]. Butyl nitrate and propyl nitrate are easily

ignitable fuels and their action as promoters can be explained on both thermal basis and on increasing the radical pool that accelerates the initial oxidation rate of the kerosene–promoter blend. It is thus reasonable to assume that the ignition delay of 0.1 ms behind the initiating shock wave is a conservative requirement for the fuel blend to be detonable. Since the detonability of gaseous heavy hydrocarbons in terms of the detonation cell size is quite similar, it is hoped that the “0.1 ms” criterion is applicable to various fuel blends.

Approach

Since there exists a vast variety of fuels which could be considered candidates for PDE applications, a general approach is needed for searching the optimum components of fuel blends. Here, it is proposed that the requirements to prospective PDE fuels are formulated in terms of the ON.

The ON requirements for the prospective fuel are theoretically analyzed by using the oxidation mechanism of *n*-C₇H₁₆ – *iso*-C₈H₁₈ – air mixtures.^{20,21,2} The mechanism contains two blocks of reactions: (1) a semi-empirical block including reduction reactions of high hydrocarbons to C₁ – C₂-hydrocarbons and the reactions of high peroxides responsible for low-temperature oxidation, and (2) a detailed oxidation mechanism of C₁ – C₂-hydrocarbons.

The first block of reactions contains 29 reactions with 26 reactants (C₈H₁₈, C₈H₁₇O₂H, C₈H₁₇O₂, C₈H₁₇O, C₈H₁₇, C₇H₁₆, C₇H₁₅O₂H, C₇H₁₅O₂, C₇H₁₅O, C₇H₁₅, C₆H₁₂, C₆H₁₁, C₂H₅, C₂H₄O₂, C₂H₃, CH₄, CH₃O₂H, CH₃O₂, CH₃O, CH₃, CO₂, H₂O, HO₂, OH, O₂, H). These reactions describe cool flames and two-stage auto-ignition under certain critical conditions. They include competing reactions (separately for *iso*-C₈H₁₈ and *n*-C₇H₁₆) which ensure transition from low-temperature to high-temperature oxidation mechanism.

The second block of reactions is the detailed oxidation mechanism of C₁ – C₂-hydrocarbons containing 255 elementary reactions with 30 species (some of them similar to those in the first block), described in detail in [Ref. 20]. This mechanism was modified for applying to a wider range of initial pressures, from sub-atmospheric to 100 bar.

Verification of the kinetic mechanism for $n\text{-C}_7\text{H}_{16} - iso\text{-C}_8\text{H}_{18} - \text{air}$ mixtures was made earlier^{21,22} by comparing predicted auto-ignition delay times with available measurement data. The ignition delay time was calculated by assuming homogeneous, isochoric, adiabatic ignition process, and was obtained from temperature histories, as well as the histories of alkyl peroxide radical concentration. The ignition delay time was defined as the time interval required for the rate of temperature rise to reach the value of 10^7 K/s. Some alternative definitions of the ignition delay time were also checked.²¹ The induction time of a cool flame was defined as the time interval required for the concentration of alkyl peroxide to reach a maximum value. It was shown^{21,22,2} that the kinetic mechanism provides a good agreement with measured ignition delays and the concentration histories of basic species within wide ranges of initial pressure (1–100 bar) temperature (650–1200 K), and fuel-air ratio (0.5–2). Three reduced reaction mechanisms containing (1) 27 reactions and 18 species, (2) 23 reactions and 16 species, and (3) 21 reactions and 13 species were developed.²²

To widen the range of fuels to be tested as candidates for PDE, in particular those exhibiting essentially higher detonability in air than n -heptane (i.e. fuels exhibiting “negative” ON), the range of ON is extended by considering hydrogen peroxide as a reference fuel, in addition to n -heptane (ON = 0) and iso -octane (ON = 100). The ON rating of H_2O_2 can be readily estimated. Linear extrapolation of τ (ON) curves, showing the dependence of the auto-ignition delay τ on $n\text{-C}_7\text{H}_{16} - iso\text{-C}_8\text{H}_{18}$ blending for various P and T , results in large negative ON for H_2O_2 . The advantage of H_2O_2 as an additional reference fuel is that this compound is intrinsically present in the $n\text{-C}_7\text{H}_{16} - iso\text{-C}_8\text{H}_{18}$ oxidation mechanism. Thus, the ON requirements for prospective PDE fuels/blends can be found by considering the behavior of triple systems, $\text{H}_2\text{O}_2 - n\text{-C}_7\text{H}_{16} - iso\text{-C}_8\text{H}_{18}$ under operation conditions of a PDE. Note that H_2O_2 is an easily detonable self-decomposing fuel.²³ Moreover, it is considered as an efficient ignition promoter^{14,24,25} in a wide range of temperatures and pressures.

Application

Consider a simplified example, which illustrates the application of the concept. For the sake of definiteness, the length of the PDE detonation chamber is taken 1 m, the frequency of detonation initiation 100 Hz, and the wall temperature T_w is assumed to be less than 800 K. Fuel injection is distributed along the chamber.² These conditions imply that the available time for expansion of detonation products through a nozzle, and fuel injection and mixing with air is about 10 ms. The time taken for detonation initiation and propagation along the detonation chamber can usually be neglected. Thus, the premature ignition delay, τ_{pi} of a prospective fuel at $T_w = 800$ K should exceed 10 ms all throughout the chamber, i.e. $\tau_{pi} \geq 10$ ms.

Since there are no general approaches to estimate energy requirements for detonation initiation, a simple “0.1 ms” criterion, discussed above, is used. This criterion assumes that for the detonation to be initiated the ignition delay of FAM behind an initiating blast wave, τ_i never exceeds 0.1 ms, e.g. $\tau_i \leq 0.1$ ms, during the PDE operation cycle.

If one specifies the Mach number of an initiating blast wave, M_i , it becomes possible to estimate the composition of the triple $\text{H}_2\text{O}_2 - n\text{-C}_7\text{H}_{16} - iso\text{-C}_8\text{H}_{18}$ blend meeting the above requirements in terms of the ignition delay both behind the initiating blast wave and at hot surfaces (i.e. $\tau_i \leq 0.1$ ms and $\tau_{pi} \geq 10$ ms). Based on the obtained requirements to blend ON, one can search the prospective fuels for a PDE.

Here, we restrict ourselves by considering $\text{H}_2\text{O}_2 - iso\text{-C}_8\text{H}_{18}$ blend, as an example. The aim of the computational example, presented below, is to estimate (1) the amount of H_2O_2 as the additive to the stoichiometric $iso\text{-C}_8\text{H}_{18} - \text{air}$ mixture and (2) the strength of the initiating blast waves to meet the constraints mentioned above. As a conservative estimate for an ignition delay at hot surface, auto-ignition delay of $\text{H}_2\text{O}_2 - iso\text{-C}_8\text{H}_{18} - \text{air}$ mixtures were calculated instead of solving the problem of surface ignition.

Figures 1 to 9 show the predicted dependencies of the ignition delay τ_i , and of premature ignition delay τ_{pi} at $T_w = 800$ K on the volume fraction of H_2O_2 , β , in a stoichiometric $iso\text{-C}_8\text{H}_{18} - \text{air}$ mixture. The values of τ_i in Figs. 1 to 9 were calculated for the PDE operation conditions 1 to 9 (see Table 1), respectively. Horizontal dashed lines

in Figs. 1 to 9 correspond to the conditions $\tau_i = 0.1$ ms and $\tau_{pi} = 10$ ms. Vertical dashed lines show the amount of H_2O_2 -additive to the stoichiometric $iso-C_8H_{18}$ – air mixture, at which the conditions $\tau_i = 0.1$ ms and $\tau_{pi} = 10$ ms are achieved. Clearly, the allowable amount of H_2O_2 -additive is that between the two vertical dashed lines. Table 2 summarizes the results of calculations. Shown in Table 2 are the minimum required values of M_i and the required range of β for PDE operation.

It follows from Table 2 that the required strength of the initiating blast wave decreases with flight Mach number and increases with altitude, ranging from 2.5 at $H = 0$ and $M = 2.0$ to 4.0 at $H = 10$ km and $M = 1.0$. The minimum required amount of H_2O_2 decreases with M and increases with H , ranging from 0.7% at $M = 2.0$ and $H = 0$ to 5% at $M = 1.0$ and $H = 10$ km. The maximum allowable amount of H_2O_2 decreases with M and increases with H , ranging from 5.3% at $M = 2.0$ and $H = 0$ to 9.2% at $M = 1.0$ and $H = 10$ km. These ranges show that, depending on the flight Mach number and altitude, both the initiation source strength and $H_2O_2 - iso-C_8H_{18}$ blending should be controlled.

Table 2: Estimated minimum Mach numbers of initiating shock waves, M_i and the percentage of H_2O_2 , β (vol.) in a stoichiometric $iso-C_8H_{18}$ – air mixture that meet the requirements to fuel blend detonability and to resistance to premature ignition in a PDE

No.	M	H, km	M_i	β , %
1	1.0	0.0	3.5	1.0–7.5
2	1.0	3.0	3.6	2.6–7.8
3	1.0	10.0	4.0	5.0–9.2
4	1.5	0.0	3.0	1.0–6.4
5	1.5	3.0	3.2	1.1–7.0
6	1.5	10.0	3.6	3.7–8.4
7	2.0	0.0	2.5	0.7–5.5
8	2.0	3.0	2.7	0.8–6.0
9	2.0	10.0	3.2	1.1–7.4

In principle, if neglecting conventional constraints on fuel consumption and initiating energy supply, the addition of 5–5.5% (vol.) H_2O_2 to the stoichiometric $iso-C_8H_{18}$ -air mixture,

and the use of the initiating blast wave with $M_i \geq 4$ and the shock compression phase duration $\tau_+ > \tau_i$ will meet the requirements outlined above for the whole range of PDE operation conditions.

Conclusion

Distributed in-chamber blending of fuels, exhibiting different detonability, allows to control detonation in a PDE in a wide range of inlet conditions. Detonation and premature ignition timing of prospective PDE fuels/blends can be estimated by examining the reaction kinetics of triple $H_2O_2 - n-C_7H_{16} - iso-C_8H_{18}$ blends within the frame of the detonability concept based on the Octane Number. A simple example is considered that illustrates the approach.

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