The Use of Fuel Blends and Distributed Injection for Active Detonability Control in a PDE

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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 applications [1]. 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 [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 Number (ON) [3], (2) detonation run-up distance [3], (3) critical initiation energy [4], (4) limiting tube diameter [5], 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 persentage of iso-octane (by volume) in the iso-octane (iso-C$_8$H$_{18}$) – n-heptane (n-C$_7$H$_{16}$) 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-C$_7$H$_{16}$ – iso-C$_8$H$_{18}$ – air mixtures capable of providing auto-ignition and surface ignition data 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-C$_7$H$_{16}$ – iso-C$_8$H$_{18}$ 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.

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.

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

M	1.0			1.5			2.0		
H, km	0.0	3.0	10.0	0.0	3.0	10.0	0.0	3.0	10.0
P, bar	1.89	1.31	0.49	3.58	2.48	0.94	6.52	4.51	1.7
T, K	346	323	268	418	390	323	518	484	401

Methodology

The requirements to prospective PDE fuels in terms of the ON are theoretically analyzed by using the oxidation mechanism of n-C_7H_{16} – iso-C_8H_{18} – air mixtures [6,7,2]. The mechanism contains two blocks of reactions: (1) a semi-empirical block including reduction reactions of high hydrocarbons to C_1 – C_2-hydrocarbons and the reactions of high peroxides responsible for low-temperature oxidation, and (2) a detailed oxidation mechanism of C_1 – C_2-hydrocarbons.

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 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-C_7H_{16} – iso-C_8H_{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-C_7H_{16} – iso-C_8H_{18} oxidation mechanism.

Thus, the ON requirements for prospective PDE fuels/blends can be found by considering the behavior of triple systems, H_2O_2 – n-C_7H_{16} – iso-C_8H_{18} under operation conditions of a PDE.

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_p of a prospective fuel at T_w = 800 K should exceed 10 ms all throughout the chamber, i.e. $\tau_p \geq 10$ ms.

Since there are no general approaches to estimate energy requirements for detonation initiation, a simple consideration is used. As a criterion for detonation initiation and propagation, assume that the ignition delay of FAM behind an initiating blast wave, τ_i never exceeds a preset value, 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 H_2O_2 – n-C_7H_{16} – iso-C_8H_{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 $\tau_p \geq 10$ ms).

Based on the obtained requirements to blend ON, one can search the prospective fuels for a PDE.

Here, we restrict ourselves by considering $H_2O_2 - iso\text{-}C_8H_{18}$ blend. The aim of the computational example, presented below, is to estimate (1) the amount of H_2O_2 as the additive to the stoichiometric $iso\text{-}C_8H_{18}$ – 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 $H_2O_2 - iso\text{-}C_8H_{18}$ – air mixtures were calculated instead of solving the problem of surface ignition.

Table 2 presents the results of calculations for the conditions listed in Table 1. Shown in Table 2 are the minimum required values of M_i and the required range of β (volume fraction of H_2O_2).

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

M	1.0			1.5			2.0		
H, km	0.0	3.0	10.0	0.0	3.0	10.0	0.0	3.0	10.0
M_i	3.5	3.6	4.0	3.0	3.2	3.6	2.5	2.7	3.2
β, %	1–7.5	2.8-7.8	5–9.2	1–6.4	1.2–7	3.7–8.4	0.7–5.3	0.8–6	1.2–7.3

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 $H_2O_2 - iso\text{-}C_8H_{18}$ blending should be controlled.

In principle, if neglecting conventional constraints on fuel consumption and initiating energy supply, the addition of 5-5.3% (vol.) H_2O_2 to the stoichiometric $iso\text{-}C_8H_{18}$-air mixture, and the use of the initiating blast wave with $M_i \geq 4$ and the 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 $H_2O_2 - n\text{-}C_7H_{16} - iso\text{-}C_8H_{18}$ blends within the frame of the detonability concept based on the Octane Number. A simple example is considered that illustrates the approach.

References

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