EVALUATION OF FUEL BLEND COMPOSITION FOR PDE APPLICATIONS

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Introduction

High thermodynamic efficiency of detonative combustion is an attractive feature for propulsion applications. 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 Hz. In view of the latter, a number of problems arise that deal with requirements of a PDE fuel: fast evaporation of liquid fuel and mixing with air, reliable detonation initiation in the fuel–air mixture (FAM) at relatively short distances (1–2 m), preventing premature ignition of FAM at hot surfaces and uncontrolled auto-ignition of FAM due to mixing with residual combustion products, 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 operating conditions. According to [1, 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 for detonability criteria. There exist several approaches based on the concepts of Octane Number (ON), detonation run-up distance, critical initiation energy, limiting tube diameter, etc. Since there is a vast variety of fuels that could be considered as candidates for PDE applications,

a general approach is needed for searching the optimum components of fuel blends.

In this paper, two approaches are used for this purpose, namely the modified Octane Number [1, 2] and the critical initiation energy [3, 4] approaches. These approaches are applied for assessing the required fuel detonability in a PDE of simple design. The assessments are made in terms of detonability of triple H_2O_2–n-C_7H_{16}–iso-C_8H_{18} blends in air under variable flight conditions of a PDE-driven vehicle. Note that jet propulsion kerosene can be considered to be made up of approximately 79% of high n-alkanes, 10% cycloalkanes and 11% aromatics [5]. In view of it, the hydrocarbons under study are capable of representing the behavior of kerosene.

Octane Number Approach

Within this approach, the detonability requirements to prospective PDE fuels are analyzed by using an oxidation mechanism of n-C_7H_{16}–iso-C_8H_{18}–air mixtures capable of providing auto-ignition and surface ignition data within a wide range of PDE operating conditions. 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 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 estimated by considering the behavior of triple systems, H_2O_2–n-C_7H_{16}–iso-C_8H_{18} under operation conditions of a PDE. Note that H_2O_2 is an easily detonable self-decomposing fuel [4]. Moreover, it is considered as an efficient ignition promoter in a wide range of temperatures and pressures. In the following this approach will be referred to as ON approach.

Critical Initiation Energy Approach

Within this approach, the detonability requirements for prospective PDE fuels are analyzed by using the thermo-chemical code

"SAFETY" [3–4]. The code provides data on the basic parameters of multifront detonation waves: propagation velocity D, pressure p_D, temperature T_D, cell size λ and critical initiation energy E^* for plane (E_1^*), cylindrical (E_2^*) and spherical (E_3^*) initiation, etc. The code is based on computing thermodynamically equilibrium detonation products and detonation cell size. For obtaining the cell size, comprehensively validated semi-empirical models are applied. In the following, this approach will be referred to as CIE approach.

Flight Conditions

Variations of inlet pressure and temperature in the detonation chamber of a PDE-driven supersonic vehicle have been examined in [1, 2]. It was shown that inlet conditions in terms of pressure p_0 and temperature T_0 vary from 0.5 to 6.5 bar and from 270 to 520 K, respectively, at flight Mach number up to 2 and altitude up to 10 km. Other important PDE operation parameters are the PDE channel length L, operation frequency f and the permitted wall temperature T_w. Restrictions on engine weight and available on-board energy for repeated detonation initiation are the most important PDE design constraints. Parameters that influence engine weight and energy consumption are the PDE channel diameter d and the detonation initiation energy E^*.

Application

Conditions of the previous section imply that the available time for expansion of detonation products through a nozzle, and fuel injection and mixing with air is about f^{-1}. Time taken for detonation initiation and propagation along the detonation chamber can usually be neglected if $L/D = o(f^{-1})$. For the operation frequency $f \sim 100$ Hz and typical hydrocarbon–air mixtures $(D \sim 1600$–1800 m/s) this condition is met at $L < 1.6$–1.8 m. Thus, the premature ignition delay τ_{pi} of a prospective fuel at wall should exceed f^{-1} all throughout the chamber, i.e. $\tau_{pi} > f^{-1}$. In the procedure of evaluating FAM composition this is the first requirement to be met. The ON approach can be used to determine the range of premixed FAM compositions meeting the requirement

$$\tau_{pi}(p_0, T_0, \Phi, B) > f^{-1} \tag{1}$$

Table 1 Estimated molar fractions (β) of H_2O_2 in stoichiometric H_2O_2–n-C_7H_{16}–air and H_2O_2–iso-C_8H_{18}–air mixtures that meet the requirements to the resistance of the blended fuels to premature ignition in a PDE at various flight conditions (M and H are the flight Mach number and altitude, respectively)

No.	M	H, km	H_2O_2–n-C_7H_{16}–air β, %	H_2O_2–iso-C_8H_{18}–air β, %
1	1.0	0.0	< 5.6	< 7.5
2	1.0	3.0	< 6.1	< 7.8
3	1.0	10.0	< 7.5	< 9.2
4	1.5	0.0	< 4.4	< 6.4
5	1.5	3.0	< 6.2	< 7.0
6	1.5	10.0	< 6.8	< 8.4
7	2.0	0.0	< 2.0	< 5.5
8	2.0	3.0	< 3.8	< 6.0
9	2.0	10.0	< 6.6	< 7.4

in terms of inlet conditions (p_0, T_0), fuel–air ratio Φ and blending ratio $B = H_2O_2{:}n\text{-}C_7H_{16}{:}iso\text{-}C_8H_{18}$ in H_2O_2–n-C_7H_{16}–iso-C_8H_{18} blend.

First, consider a case when the PDE weight constraint is dominant. Then the other requirement to prospective FAM compositions is that they are readily detonable in the channel of diameter d. This requirement can be expressed in terms of the limiting tube diameter $d^* \approx \lambda/\pi$:

$$d \geq d^*(p_0, T_0, \Phi, B) \tag{2}$$

To estimate d^* at given p_0, T_0, Φ, and B, the CIE approach can be used. Thus, if both constraints (1) and (2) hold simultaneously, then the premixed FAM of fuel–air ratio Φ and blending ratio B can be considered as appropriate to a given PDE under inlet conditions (p_0, T_0). Corresponding energy requirements for detonation initiation can then be estimated by using the CIE approach.

When the on-board available energy is the dominant constraint for PDE design, the following relationship should be met:
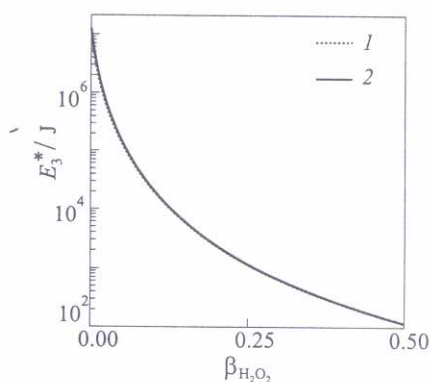
$$E_i \geq E^*(p_0, T_0, \Phi, B) \tag{3}$$

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Figure 1 Estimated variation of the critical energy for spherical detonation initiation with the molar fraction of H_2O_2 for n-C_7H_{16}–H_2O_2 (*1*) and *iso*-C_8H_{18}–H_2O_2 (*2*) blends of stoichiometric fuel–air composition with respect to hydrocarbon fuel
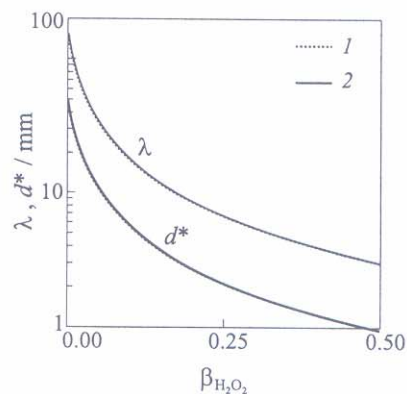
Figure 2 Predicted variation of the detonation cell size λ and the limiting tube diameter d^* with the molar fraction of H_2O_2 for n-C_7H_{16}–H_2O_2 (*1*) and *iso*-C_8H_{18}–H_2O_2 (*2*) blends of stoichiometric fuel–air composition with respect to hydrocarbon fuel

where E_i is the initiation energy. Again, if both constraints (1) and (3) hold simultaneously, then the premixed FAM of fuel–air ratio Φ and blending ratio B can be considered as appropriate to a given PDE under inlet conditions (p_0, T_0). The channel diameter should anyway satisfy the constraint (2).

When both weight and available energy restrictions in PDE design are important, minimum values of d and E_i should be taken in constraints (2) and (3).

The calculation procedure has been applied for two specific examples dealing with the behavior of premixed stoichiometric H_2O_2–n-C_7H_{16}–air and H_2O_2–*iso*-C_8H_{18}–air mixtures at various flight conditions. Table 1 shows the estimated molar fractions of H_2O_2 in the mixtures that meet the constraint (1) at maximum wall temperature of 800 K. Figure 1 shows the estimated variation of the critical detonation initiation energy E_3^* with the molar fraction of H_2O_2 in the mixtures at normal conditions.

Clearly, the addition of H_2O_2 results in decreasing the initiation energy by a few orders of magnitude. In terms of the critical initiation energy, the mixtures under study with 5% and 20% of hydrogen peroxide appear to be equivalent to stoichiometric ethylene–air and hydrogen–air mixtures, respectively. Figure 2 shows the predicted variation of the detonation cell size and the limiting tube diameter for the blended fuels depending on the molar fraction of H_2O_2. Joint consideration of Table 1 and Figs. 1 and 2 indicates that depending on the flight Mach number and altitude both the initiation source strength and the blending ratio B should be properly controlled. Application of the procedure to nonpremixed two-phase compositions is also discussed.

Acknowledgments

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