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Diffusive burning characteristics of peroxy-fuels

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ABSTRACT

The diffusive burning characteristics of four peroxy-fuels (usually known as liquid organic peroxides) and one hydrocarbon fuel are experimentally investigated targeting alternative fuels (or as additives to conventional fuels) for the future. Measurements are performed in form of pool fires with pool diameters in the range between 1 cm and 1 m. Mass, momentum and energy transfer studies are carried out by measuring the mass burning rate, flame length, flame temperature and radiation heat transfer across the liquid fuel and gaseous flame. It has been shown that comparatively much less mass of peroxy-fuels and pressure drop (required to maintained the flow) of fuel are required to produce a given heat flux. The momentum delivered by the peroxy-fuel vapours are order of magnitude higher than for hydrocarbons making the visibility of flame to be 4–5 times larger. A heat balance analysis shows that the total heat release rate of a peroxy-fuel fire is contributed equally by convection and radiation. Finally, the three E's (Efficiency, Economy and Emission) are discussed in the context of present experimental results followed by some recommendations concerning safe handling of the proposed fuels.

1. Introduction

The US Energy Information Administration projects that by 2035 the worlds global energy consumption to be more than doubled of 1990s [1]. Fossil fuels (liquid, solid and gaseous) will fulfil majority of this excess demand followed by renewables and nuclear [1]. Clearly, combustion will be the major mode of energy conversion from these fuels at least in the coming decades. The result of increased volume of combustion will have huge environmental impact in terms of emissions which are either directly or indirectly contributing towards global warming [2].

In this article the possibilities to utilise organic peroxides as alternative fuels in industrial combustion processes for an efficient combustion and to reduced environmental impacts are investigated.

Organic peroxides belong to energetic materials and are liable to exothermic decomposition. Some commercially available products may decompose explosively, particularly if confined [3]. Only few of these are able to propagate a detonation or a deflagration. However, for such organic peroxides this characteristic is suppressed by adding appropriate diluents and/or the use of suitable packagings. As initiators, additives and combustion improvers they are well known [4–7]. Since liquid organic peroxides have not been actually used in combustion processes yet as main fuels as such from here onwards they will be called as peroxy-fuels. Although there are some investigations done before on organic peroxides [4,5] they do not inform much about the combustion properties of the same. The detailed investigations on the combustion (non-premixed) characteristics of peroxy-fuels to the authors best knowledge were reported in [8–10]. The objective was to investigate the safety aspects of peroxy-fuel pool fires. The laboratory- and field-scale fires with different peroxy-fuels were performed and the fire characteristics, e.g. mass burning rate, flame length, flame temperature and heat flux due to radiation were measured and were also simulated [8–10].

The next anticipated issue is related to the efficiency, economy and emissions (the three E's). Undoubtedly, they are relatively more efficient than hydrocarbons. The exact estimations of costs are not possible to report now. However, depending on experience there should be a remarkable saving in overall costs. Emissions are expected to be much lower than in case of hydrocarbons for the reasons stated in Section 4.5.

This paper is organised to address above issues in bit detail based on experimental facts given in the respective sections emphasising the conserved quantities.

2. Peroxy-fuels

There is a wide variety of peroxy-fuels that can be explored for their potential utilisation in various combustion applications. In this particular study, the discussion is limited only up to four peroxy-fuels listed in Table 1. Their full names are as follows: INP: Di-(3,5,5-trimethylhexanoyl) peroxide, TBPEH: tert-Butyl

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Table 1
Properties of investigated peroxy-fuels and kerosene.

Type of fuel→ Parameter↓	INP	TBPEH	TBPB	DTBP	Kerosene Jet A-1
Formula	$C_{18}H_{34}O_4$	$C_{12}H_{24}O_3$	$C_{11}H_{14}O_3$	$C_8H_{18}O_2$	–
Molar mass (g/mol)	314.5	216.32	194.2	146.2	–
Active oxygen (%)	5.09	7.40	8.24	10.94	–
Enthalpy of combustion (ΔH_c) (MJ/kg)	30.1	34.5	30.1	36.6	43.1
T_{SADT} [3] (K)	293	308	338	358	–
Air to fuel ratio (–)	10.7	10.52	9.23	10.86	15
$\dot{m}''_f$ (kg/m^{2}s) (d = 1 m)	4.22	0.78	0.62	0.29	0.07

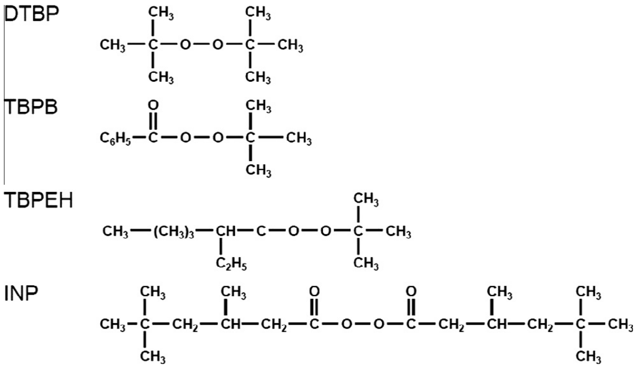

Fig. 1. Chemical structures of the investigated peroxy-fuels.

peroxy-2-ethylhexanoate, TBPB: tert-Butyl peroxybenzoate, DTBP: Di-tert-butyl peroxide.

Peroxy-fuels contain at least one O–O bond in their chemical structure which is more or less easy to break [6] (Fig. 1). Upon thermal decomposition they release a complete range of products. The major decomposition products, e.g. of DTBP are acetone and ethane [9]. The interesting thing in the structure of DTBP is the symmetry and the associated protection of the O–O bond given by the two tert-butyl groups (+I-effect) which stabilise the molecule and influence significantly the combustion process and makes it different from the others. In contrast, such a stabilisation effect does not exist in case of INP, e.g. due to the length of the side chains and the influence of the two carbonyl groups (−I-effect) with the consequence that the so called self-accelerating decomposition temperature (SADT) is lower (see Section 3.2). Based on their structure, the (thermal) stability of TBPB and TBPEH is between DTBP and INP [11,12].

3. Experiments

3.1. Description and procedure

The combustion characteristics of four different peroxy-fuels and one hydrocarbon fuel, i.e. kerosene are measured (in form of pool fires) (Table 1). The arrangement is shown in Fig. 2. The liquid fuels were filled in pan sizes ranging from d = 0.01 m to 1 m and were ignited by a hand torch. The average mass loss (burning) rate (kg/(m^2 s)) was measured by a weighing instrument. The weighing instrument was kept on a stable steel table. In measurements we recorded the loss of fuel with time. It was seen that the total amount of peroxy-fuel was consumed in much (~10 to 300 times) lesser time than that taken by kerosene. The average flame lengths were determined by using video and thermographic images, respectively. A number of thermocouples were located at the flame axis and heat flux sensors (at various distances from fire) were located on the ground to measure the heat flux (due to radiation).

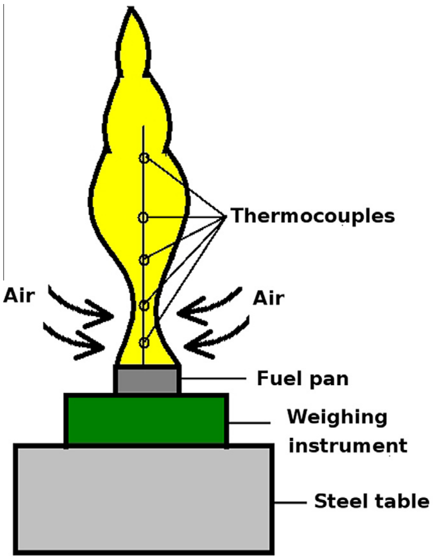

Fig. 2. Experimental set-up.

3.2. Safety issues

The regulations for safe storage and transportation of hydrocarbons depend on many factors. Most importantly prevention from fire and explosion hazards. Safety distances from fire hazards are given in terms of thermal radiation (according to NFPA: 5 kW/m^2 for skin burn injury) whereas overpressure (5 kPa, typical pressure for glass breakage) determines the explosion strength. Please see [10,13,14] for more details.

Apart from above there are some standards developed for the safe handling (storage and transportation) of peroxy-fuels. The most widely followed norm is based on the Self-Accelerating Decomposition Temperature (T_{SADT}) [3,10,11]. It is the lowest temperature at which the self-accelerated decomposition of peroxy-fuels in a defined packaging start. These T_{SADT} values for the investigated peroxy-fuels are listed in Table 1. It is recommended that the processing of peroxy-fuels is occur preferably below this temperatures.

3.3. Uncertainty in measurements

A detailed uncertainty analysis of the measured data is not carried out in the present study. However, it has been approximated (Table 2) based on the measurement data available in [8–10,15]. The correct estimation of emissivity, convective heat transfer coefficient and sensitivities of heat flux sensors to cross wind conditions are the key parameters to be addressed in future.

4. Result and discussions

The results are presented with an objective to highlight the average values of conserved quantities, i.e. mass, momentum and