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AN EFFICIENT AND CLEAN FUEL FOR HIGH TEMPERATURE PROCESS INDUSTRIES

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Abstract The use of energetic materials as a main fuel in high temperature process industries are not known to the scientific community as such. This paper highlights some of the features and advantages of using organic peroxides especially di-tert-butyl peroxide (DTBP) in high temperature process industries. The feasibility of using DTBP as a main or supporting fuel in process industries have also been justified with the help of Computational Fluid Dynamics (CFD) simulations. For peroxides requirement of less fuel and air for the same amount of heat flux has been shown. The resulted emission from the combustion of DTBP is also discussed.

Keywords Energetic materials, process industries, organic peroxide, di-tert-butylperoxide (DTBP), CFD simulation, emission.

INTRODUCTION

The demand of efficient and cleaner combustion of fossil fuels is increasing year by year [1]. On one side these fuel reserves are limited for use and on the other side the world's energy requirement has grown up continuously in the past couple of decades. The industries have also to obey the strict environmental protection regulations simultaneously in order to achieve a target of clean and healthy atmosphere. Altogether global demand and supply of energy has to be met in any way either by modifying the existing plant machinery and operation or to search for other fuel options and energy resources [1]. It seems that the energy, emission, economy and environment are to be kept in mind while deciding the fuel and means for combusting them. It is very common practice to use natural gas as a primary fuel in high temperature process industries e.g. glass, steel and cement etc. Since natural gas (methane) is a slow burning fuel therefore in order to meet the production requirement the fuel has to be burnt at a much faster rate e.g. in a form of a high pressure jet. The obvious consequence of the same is that the oxidizer e.g. air or oxygen in oxy-fuel combustion has to be increased in the same proportion. When used air a source of NO_x is

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introduced and when used pure oxygen a safe and cost effective operation has to be ensured.

The use of energetic materials as a main or supporting fuel in high temperature process industries is not known in the literature as such. Organic peroxides are such energetic materials the use of which more or less limited. Since their processing asks for the careful handling due to their distinct thermo chemical properties they considered to be costly and unsafe. They have been widely used in the polymerization process where they perform the job of initiating the chemical reactions [2]. Sometimes they have also been used as an additives or combustion improvers in certain applications. However, their use as a main or supporting fuel is not known to the community in general. BAM Federal Institute for Materials Research and Testing is continuing fundamental as well application oriented research on combustion of organic peroxides over the years [2, 3, 4, 5]. To highlight the advantages and limitations of using an organic peroxide especially di-tert-butyl peroxide (DTBP) in processing industries are some of the prime issues this paper address.

COMBUSTION CHARACTERISTICS OF KEROSENE AND DTBP

In order to compare the combustion characteristics of organic peroxides and hydrocarbon fuels same experimental conditions were established. DTBP as an organic peroxide and kerosene as hydrocarbon fuel were selected for reference fuels. In Figure 1, DTBP and kerosene are burning in an equal size of pan ($d = 0.06$ m) under similar surrounding conditions.

It was found that DTBP burns 15 times faster than kerosene and exhibit larger flames. The large flame lengths are the direct result of fast burning which enhances the fuel Froude number and consequently the visibility of the flame [2]. This higher fuel Froude number also implies the flame to appear like a low momentum diffusion flame.

In Figure 2 the maximum flame temperatures of DTBP and kerosene flames as measured by the thermographic camera are shown for various source sizes.

A difference of ~ 300 K can be seen between DTBP and kerosene flame temperatures. It is important to mention that both fuels are burning under atmospheric pressure. In order to achieve the same flame like DTBP, kerosene needs to burn with a 225 times higher pressure [7].



Figure 1. Flames of DTBP (left) and kerosene (right) ($d = 0.06$ m) [3]

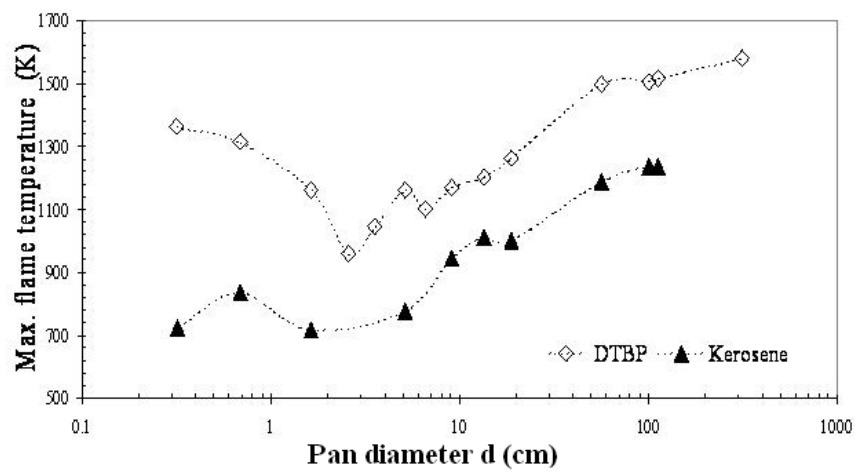


Figure 2. Measured flame temperatures of DTBP and kerosene [3, 5]

The obvious consequences are the higher amount of fuel and air followed by the large combustion chamber size and emissions thereon. On the other hand the fast combustion of DTBP can be achieved without even by applying any external pressure. At the same time the air supply will also be reduced due to the oxygen containment of the fuel. This fact will be supported by the CFD simulation in the next section of this paper. Fourier Transform Infrared measurements show that there is no NO_x production for the DTBP flame shown in Figure 1 [5].

CFD SIMULATION OF A MODEL COMBUSTION CHAMBER

CFD simulations have been performed for a model combustion chamber where a fixed output i.e. a radiative heat flux of 1 MW/m² (at the outlet) criteria is tried to achieve by varying the fuel and air flow.

Geometry, Mesh and Boundary Conditions

The model combustion chamber consists of inlets for fuel and air, a chamber for the combustion of mixtures and an outlet. The diameters for the fuel and air inlets are 0.05 m and 0.1 m, respectively. The chamber has a diameter of 0.2 m and a length of 1.8 m as shown in Figure 3. The unstructured meshes were generated with a total number of elements of 735,469. The boundary and mesh details are summarized in the Table 1 below.

The physics of the problem specified in the simulation can be obtained in Table 2. Methane is used as a reference fuel for hydrocarbon and DTBP as an organic peroxide. Steady state simulations with Ansys CFX-11 [8] were carried out for a convergence criteria of 10⁻⁴ for all residuals. A time step size of 0.01 s has been used in the simulations.

Table 1. Mesh and boundary conditions used in the simulation.

Part	Boundary conditions	Number of elements
Fuel flow	Inlet (methane 1 m/s, DTBP 0.5 m/s)	694
Air flow	Inlet (methane 0.5 m/s, 1 m/s, 5 m/s) (DTBP 0.5 m/s, 1 m/s)	2,703
Outflow	Outlet	1,094
Chamber	Adiabatic wall	21,782

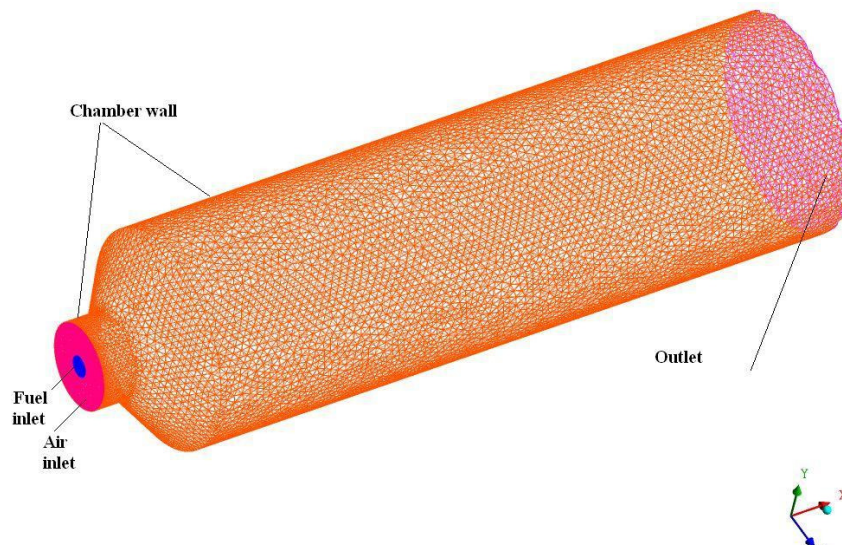


Figure 3. Geometry, mesh and boundary conditions of a model combustion chamber

Table 2. Details of the physics implemented in the simulation.

	Model	Remarks
Type of Simulation	Steady RANS	-
Turbulence	k- ϵ	-
Chemistry	Single step	Arrhenius equation
Combustion	Eddy dissipation	With model coefficient A = 4 and B 0.5
Radiation	P1	-
Buoyancy	Non-buoyant	-

Temperature predictions

The average center plane temperatures predicted by the simulations in combustion chamber is shown in Figure 4. DTBP combusts relatively faster than methane and produces the same flame temperatures ~ 1525 K with an inflow of half of that of methane. This can be further confirmed by the Figure 1 where the DTBP flame extends its length in the vertical

direction unlike kerosene which is driven by the buoyancy and widens horizontally. Another interesting thing to observe in Figure 4 is the jet-like flow of DTBP even with this half of the flow of fuel whereas at the same time methane tries to widen in the beginning and reacts slowly thereafter. It also justifies the reduction in the size of chamber as the temperature increases (fast combustion) distribution in case of a DTBP flame occurs at a shorter distance. This indirectly supports the assumption of less residence times of DTBP inside the chamber leading to less or negligible production of NO_x.

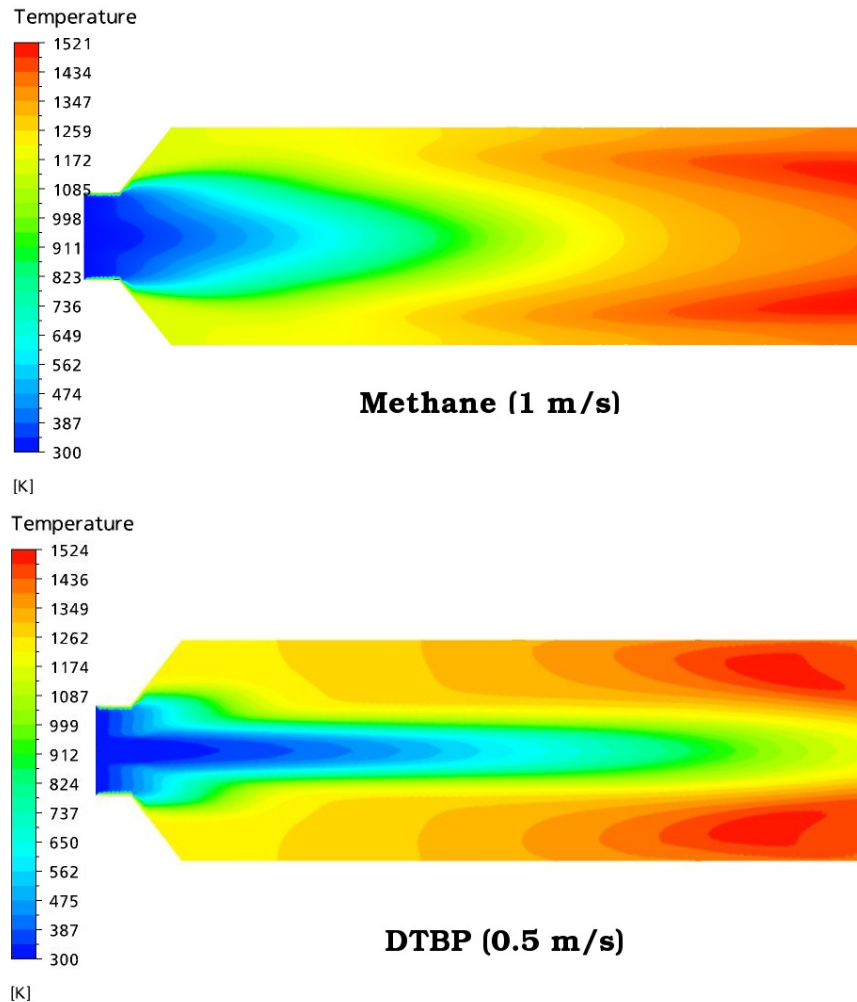


Figure 4. Temperatures predicted at the centre plane of the model combustion chamber for methane (top) and DTBP (bottom), respectively.

In order to get precise estimation of temperature distributions at radial locations along the center line of the chamber Figure 5 has been plotted. It can be seen in Figure 5 that methane flame (with a speed of 1 m/s) proceeds with a very slow speed and the temperature variation ranges ~ 300 K for instance at $x = 0.5$ m. The same for DTBP is ~ 600 K. That means the DTBP flame transfers heat much faster than methane and helps to avoid any local concentration of temperatures or hot spots. Consequently, a much lower amount of NO_x can be expected from a DTBP flame.

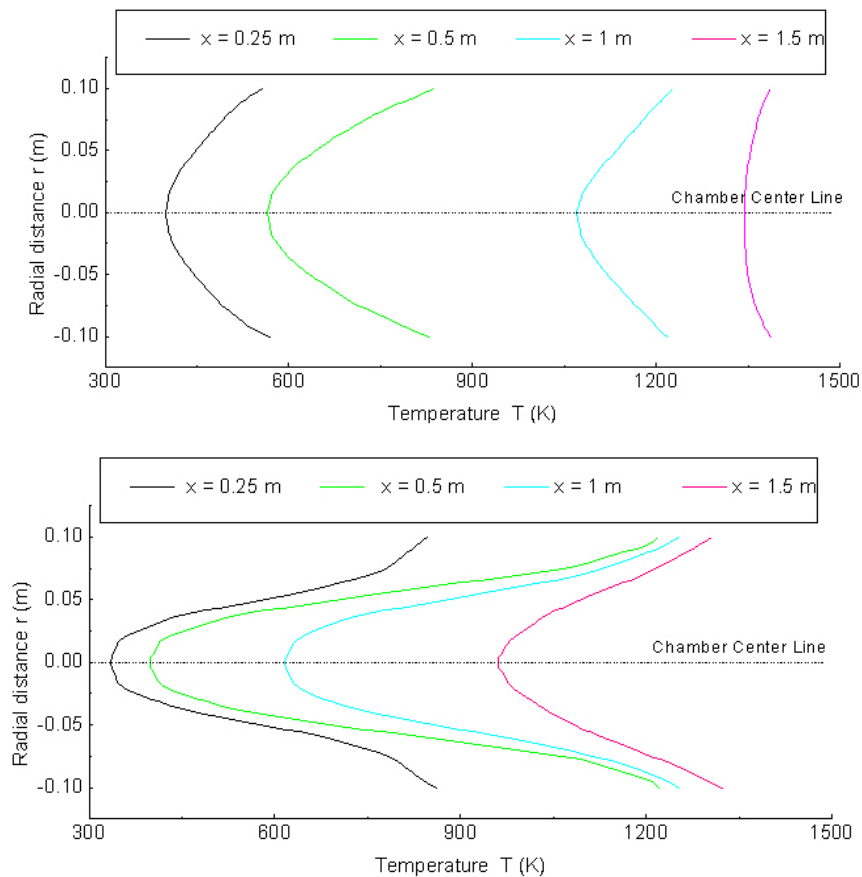


Figure 5. Temperature distributions along the centreline of model chamber for methane (top) and DTBP (bottom), respectively.

Looking to the flame characteristics in a model combustion chamber described before it can be shown for an industrial furnace also that peroxide i.e. DTBP needs half of the amount of methane for a fixed heat flux or

output. From Figure 4 it can be deduced that for peroxides the required furnace volume will be half of that of methane. Moreover, a jet like flow of DTBP flame provides the larger surface to be processed at the half of the flow rate of methane.

Heat radiation predictions

The radiation output from both methane and DTBP flames are shown in Figure 6. Methane meets the target criteria of $\sim 1 \text{ MW/m}^2$ at a speed of 1 m/s. On the other hand DTBP does so at a speed of 0.5 m/s. In Figure 6 it can be seen that fast progression of the DTBP flame also speeds up the radiation heat transfer for instance 0.84 MW/m^2 at a much shorter distances ($\sim 10\%$ to 15% shorter) than in case of methane.

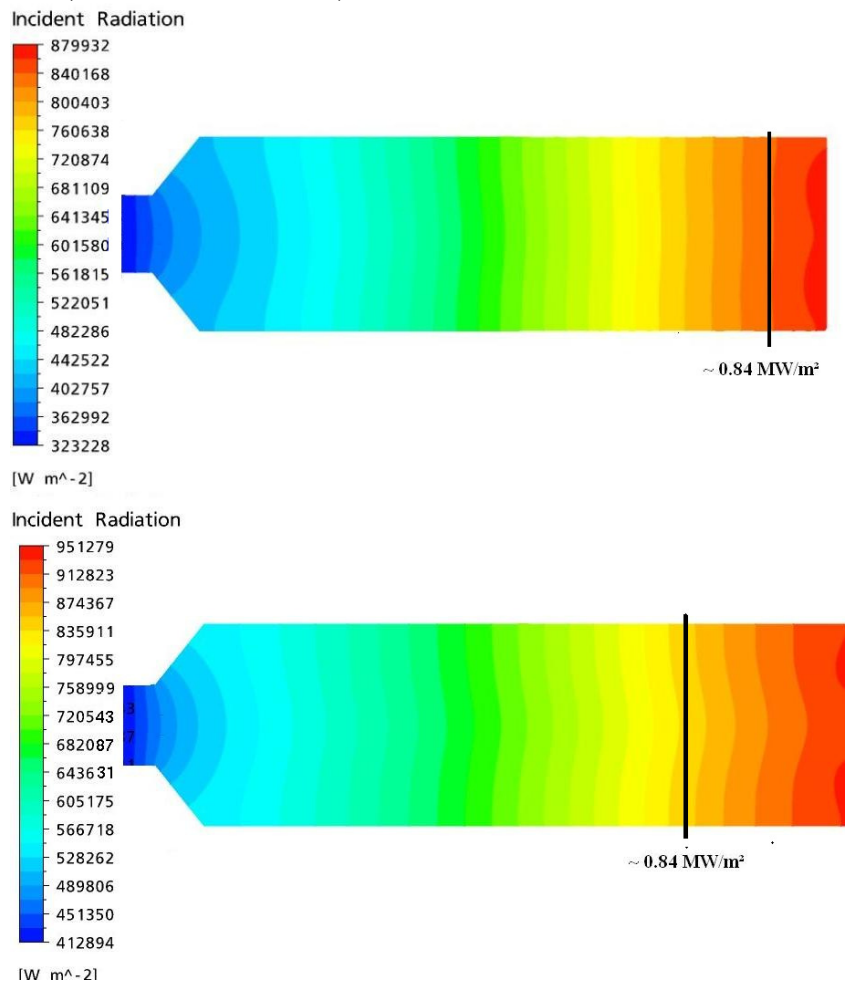


Figure 6. Radiation heat flux distributions at the centre plane of chamber for methane (top) and DTBP (bottom), respectively.

CONCLUSIONS

The diffusion flames of a hydrocarbon fuel and an organic peroxide (DTBP) were experimentally investigated and simulated with CFD. It is recommended to use DTBP as a main or supporting fuel in process industries to enhance the overall performance of the combustion process. It was found that DTBP needs half of the amount of methane to produce the same amount of heat flux. Furthermore, the flame characteristics investigated by CFD simulation supports the presumption that the DTBP flame provides less favorable conditions for NO_x formations. However, this needs the support of future simulations to study the NO_x predictions in much detail.

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REFERENCES

1. Baukal C. E., *Industrial combustion pollution and control*, CRC Press, 2003, ISBN 0824746945, 9780824746940.
2. Mishra K. B., *Experimental investigation and CFD simulation of organic peroxide pool fires (TBPB and TBPEH)*, BAM Dissertation Series 63 Berlin 2010, ISBN 978-3-9813550-6-2.
http://www.bam.de/en/service/publikationen/publikationen_medien/dissertationen/diss_63e_vt.pdf
3. Chun H., *Experimentelle Untersuchungen und CFD-Simulationen von DTBP-Poolfeuern*, BAM-Dissertationsreihe.Band 23, Berlin 2007, ISBN 978-3-981655-0-0.
http://www.bam.de/de/service/publikationen/publikationen_medien/dissertationen/diss_23_vt.pdf
4. Wehrstedt K.-D., Wandrey P. A., Experimental investigations of pool fires of organic peroxides, PTB Report No. PTB-W-54, PTB Brunswick, 97-108, 1993, ISBN 3-89429-359-4.
5. Mishra K. B., Wehrstedt K.-D., A more efficient and cleaner fuel for the processing industry, World patent, WO/2011/11026742, 2010.
<http://www.wipo.int/pctdb/en/wo.jsp?WO=2011026742>
6. Joshi M.L., Darien, I. L., Oxy-Fuel Combustion Firing Configurations, United States Patent 6 398 547B1, 2002.

11th Conference on Energy for a Clean Environment
Lisbon, Portugal, 5-8 July 2011

7. Ansys CFX-11 user manual, 2011.
8. Mishra K. B., Wehrstedt K.-D., Rocket propellants, Patent pending, 2010.