Learning from the Brachina beetle – combustion of methane in a heart–shaped combustor

M. Forman[1], A.C. McIntosh[2]

[1]Brno University of Technology, Czech Republic
email: premf@dt.fme.vutbr.cz
[2]Energy and Resources Research Institute
Department of Applied Mathematics
University of Leeds
Leeds LS2 9JT, United Kingdom
email:a.c.mcintosh@leeds.ac.uk

Abstract

A numerical study of a heart–shaped reaction chamber is presented. The chamber design is modelled on the Brachinus defense apparatus, and extended for the combustion of a methane-air mixture. The aim is to study the pressure focusing mechanism used in the naturally occurring combustor with a view to possible application as a re-light device for gas-turbines. Using the heart–shaped design of the reaction chamber the CFD calculation with single step Arrhenius chemistry has been carried out for the Brachinus apparatus and also for a methane-air stoichiometric mixture on a scaled up geometry. In both cases the reaction is set up by suddenly increasing the temperature of the reaction chamber walls.

Keywords: pulse combustion, single step chemistry, CFD,Brachinus

Introduction

There are many modern devices which have been inspired by designs found in nature. It is, however, not so typical for combustion science to find an inspiration in the world of living creatures. Such an exception is Brachinus (commonly called the Bombardier beetle) found in Africa, South America and Asia. Work by Eisner at al. [1, 2] has shown, that the pulse combustion principle is used by certain Brachina beetles. These beetles use a spray of hot chemicals ejected at high frequency from an opening at the tip of their abdomen. The beetle responds to the attack of predators (usually ants, spiders, frogs and birds) with a $100°C$ hot spray of hydroquinone and hydrogen peroxide solution in water which is then partially evaporated within a few milliseconds and ejected from a rear nozzle which the beetle aims towards the enemy. This study uses the findings of Eisner and Aneshansley [1, 2]. The reaction mechanism of the beetle – Hydroquinone and Hydrogen peroxide – is described and used successfully in an initial CFD simulation. The discharge mechanism of the Brachinus has been shown to be very effective, and to try to gain better understanding of this phenomenom, a numerical study of the reaction chamber design was performed using the Brachinus geometry, but with combustion of methane and air under stoichiometric conditions. It may be advantageous to use the methane–air mixture in small heart-shaped combustors for re-light purposes.

Chemistry of the Brachina beetle

The whole apparatus of the Brachina is shown on the Fig. 1. It consist of two sets of reservoirs with reactants and reactions vessels leading into one nozzle at the tip of the beetle. In the reservoir, the aqueous solution of reactants is stored. The mixture of hydroquinone and hydrogen peroxide is introduced from the reservoir by muscles into the combustion chamber squeezing the reservoir and opening the valve again be means of attached muscles. Once the reactants are present in the combustor, the enzyme catalysts (a mixture of catalases and peroxidases) are introduced through the combustor walls. An extremely fast catalytic reaction then takes place. The reaction mechanism can be described with the global chemical reaction:

$$C_6H_4(OH)_2(aq) + H_2O_2(aq) \quad \longrightarrow \quad C_6H_4O_2(aq) + 2H_2O(l) \tag{1}$$

The enthalpy of the overall reaction (eq.1) is $\Delta H_1 = -203.0kJ/kmol$.

In [1] the mass of ejected liquid and gases is reported to vary from $0.1mg$ to $0.5mg$ for a single discharge. While the reactant storage and delivery system is driven by muscle contraction, the reaction vessel is rigid. From the spectrographic measurements reported by Eisner [2] the following data can be shown: the average discharge duration is $11.9ms$; the mean frequency of the pulses is found to be $531Hz$; the average velocity of the spray emerging from the beetle tip is $11.63m/s$ (ranging from 3.25 to $19.5m/s$). Eisner also reports, that the spray can reach as far as 2 to 3 centimeters.

Methods and modelling

The beetle defense system with the hydroquinone – hydrogen peroxide mixture has been modelled along with a parallel calculation using a methane–air mixture, but with a scaled up geometry. For both cases a single step global chemistry equation with Arrhenius kinetics was proposed for the description of reactions. The flow is assumed to be transient and fully compressible with an axial line of symmetry (no variation in tangential direction). For spatial differencing, a second order scheme CCCT was used, and for the time domain a fully implicit scheme with quadratic differencing (second order scheme) was used. For solving the set of equations, the commercial software package CFX was used.

Both cases were modelled with Lewis number Le equal to unity with constant heat capacity and viscosity.

The geometry of the computational domain is shown in Figure 2. The discharge part of the domain (part c - see Fig. 2) is confined to a cone shape for better convergence.

As a first step for modelling the beetle discharge mechanism, a simple solution of reactants in the gas phase was chosen. The exothermic reaction is started by raising the temperature of the wall to $100°C$. The time step was chosen according to Courant-Friedrichs-Lewy criterion to be 2.5×10^{-7} sec. Very little data are available about the catalytic kinetics of hydroquinone – hydrogen peroxide. So initially a single step Arrhenius type equation was used:

$$\frac{\mathrm{d}\,[C_6H_4(OH)_2]}{\mathrm{d}\,t} = [C_6H_4(OH)_2] \times [H_2O_2] \times AT^{\beta} exp\left(\frac{-E_a}{RT}\right), \qquad (2)$$

where the pre-exponential A is 3.3×10^{-7}, activation energy E_a is $5.8 \times 10^7 Jkmol^-1$ and the temperature exponent $\beta = 2.0$.

For the calculations with methane-air, a scaled up geometry was used (described below). For the kinetics, a global single step reaction [3] was used with values of Arrhenius pre-exponential $A = 1.3 \times 10^8$, activation energy $E_a = 2.02 \times 10^8 Jkmol^-1$ and exponents -0.3 and 1.3 for fuel and oxygen concentrations respectively. The mixture was ignited by suddenly increasing the combustor wall temperature to $1800K$. For resolution of pressure disturbances, the same time step as with hydroquinone mixture was used.

Results and Discussion

Beetle discharge mechanism:

The simple gas phase calculations showed that the pressure waves forming during ignition are focused on to the centre of the chamber as well as the propagating reaction front. Hot products follow the pressure propagation and approximately $0.2mg$ of hot products are ejected out from the chamber. The frequency of pressure disturbances is 3 times higher then the frequency reported from experiments on Brachinus. Calculations with different time steps show, that the history of the discharge mass flux is sensitive to pressure fluctuations. The results of the gas phase calculations show that the pressure focusing mechanism causing the discharge of the products from the chamber is similar to that of the beetle. Currently further numerical work is in progress to model the two phase flow with the reactants dissolved in water which is evaporated during exothermic reaction. We believe that by using this approach, we can find agreement with experiments in frequency and also in mass flux discharged from the chamber.

Methane-air case:

The methane-air mixture was used as a medium for study of different features of design of the bombardier beetle. Four main configurations are shown: two geometry variants (G1 and G2) and two ignition arrangements (W1 and W2). To study the effect of the main design parameters, the ratio of a and b parameters shown on Fig. 2 has been varied as in Table 1.

As it is shown later in the figures, the effect of widening the chamber on combustor performance is quite strong. To illustrate the effect of location of ignition on the combustor wall, two variants are presented for both geometries. In case W1, only the front part of the chamber has the elevated temperature for igniting the mixture (see Figure 2). However in case W2, the complete surface of the combustor is used for ignition. We first examine the effect of the different geometries. The most significant parameter for comparing the geometries was mass flux out from the chamber. In Figure 3 the mass flow through the nozzle is shown for geometries G1 and G2, for both ignition arrangements. From this Figure, we can see, that the outflow from the wider geometry G1 is greater shortly after ignition and it is caused by the pressure rise in the combustor. The total mass-flux from the domain is shown in Table 2 for all cases (integrated for the first 10 ms). There is a very small variation in mass flux from the combustor for different ignition configurations W1 and W2.

Figure 4 shows the pressure history for both geometries in the centre of the combustor. Data are shown only for case W1. No significant difference was recognized for the different ignition configurations. From this figure we can clearly see the main difference in behaviour of the two geometries. In the wider geometry G1, the pressure is accumulated and increases by about 34 percent in the centre of the chamber. In the case of the more narrow geometry G2, the maximum increase of pressure is approximately 4.6 percent, but higher frequency oscillations are recognised. The higher pressure in geometry G1 also increases the temperature due to the compression. In case W1, the flame is pushed from the rear of the combustor to the nozzle, while in the case W2 the flame front propagates into the volume and then towards the nozzle. There is another feature of this geometry, that plays a role in the propagation of the flame. As the flame propagates from the wall, due to the pressure field, hot products are sucked along the wall out from the combustor. The results show that the wider reaction chamber provides better discharge characteristics. Temperature contours for time $8ms$ and $10ms$ on Figure 5 show the formation of the discharged products. The red colour represents the maximum temperature of $2250K$.

Further work using single step chemistry data for the methane-air mixture from ignition delay experiments [4] is currently being carried out to obtain an accurate reaction rate and consequently the pressure field at the ignition stage.

Variant	a [mm]	b [mm]	c [mm]	b/a
Brachinus	14	6.8	60	0.48
G1	34	18	300	0.53
G2	25	12	300	0.48

Table 1: Combustor Geometry Parameters; Brachinus -geometry with beetle chemistry; G1 and G2 - geometries for methane–air combustion

	W1	W2
G1	5.4129e-5 kg	5.2101e-5 kg
G2	3.2797e-5 kg	3.6281e-5 kg

Table 2: Overall mass flux from the combustor

Conclusions

The initial study of the Brachina discharge apparatus with gas phase flow and single step chemistry has been described. The main features of the mechanism have been discussed. The Brachina discharge mechanism has also been investigated for a scaled up geometry with methane-air combustion, which does suggest a possible use for the Brachina apparatus as a re-ignition device.

Acknowledgment

The work was supported by the Marie Curie Training site programme.

References

[1] Eisner T. Widom M. Widom B. Aneshansley D. J. Biochemistry at 100°c: Explosive secretory discharge of bombardier beetles (brachinus). *Science*, 165:61–63, July 1969.

[2] Aneshansley D. J. Eisner T. Spray aiming in the bombardier beetle: Photographic evidence. *Proc. Natl. Acad. Sci. USA*, 96:9705–9709, August 1999.

[3] Dryer F.L. Westbrook, Ch.K. Chemical kinetic modeling of hydrocarbon combustion. *Prog. Energy Combustion Science*, 10:1–57, 1984.

[4] Freeman W.G. Cowel L.H. Lefebvre, A.H. Spontaneous ignition delay characteristics of hydrocarbon fuel/air mixtures. *NASA report No. CR-175064*, 1986.

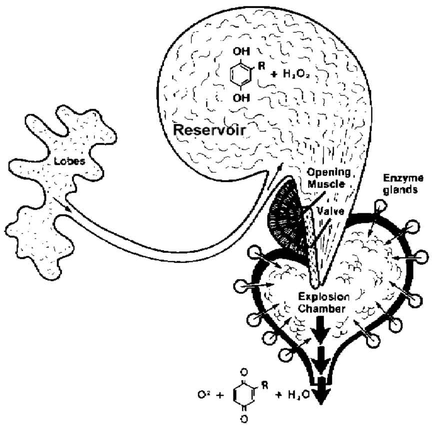

Figure 1: The defence aparatus of the Brachina Beetle

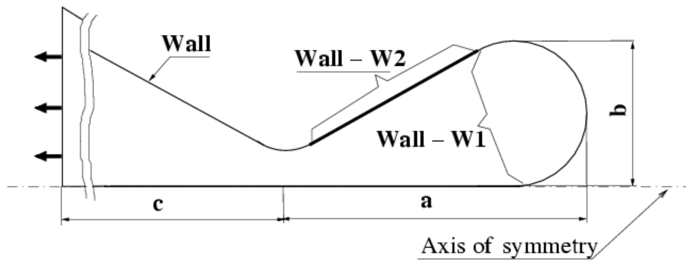

Figure 2: Geometry of the computational domain for all cases (for values see Table 1)

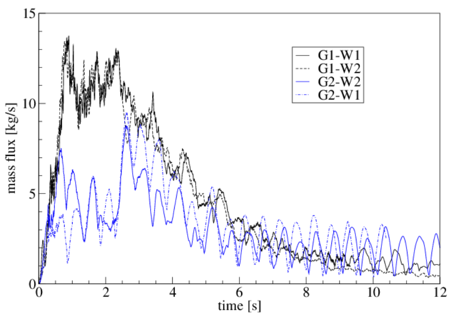

Figure 3: Mass flow time history at nozzle for ignition arrangements W1 and W2 comparing two geometries G1 and G2

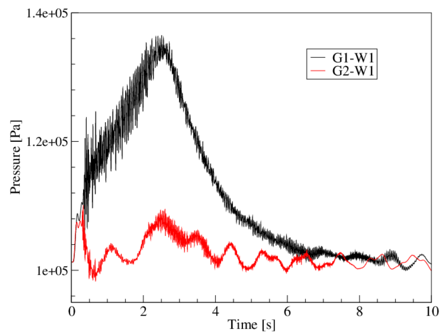

Figure 4: Pressure time history at nozzle for two geometries G1 and G2

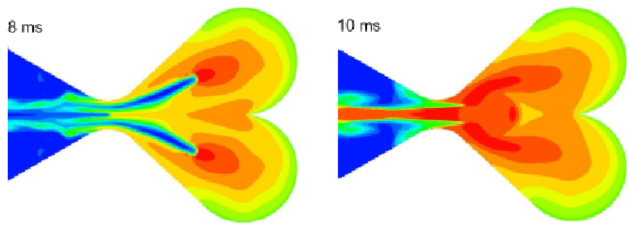

Figure 5: Temperature contour plots for methane-air combustion at 8 and 10ms. Geometry G1 and ignition configuration W1 (ignition only on back wall).