Spinning Detonation : Experiments and Simulations

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1 Introduction

The elementary structure of the detonation front is composed of three shock waves : incident, transverse and Mach stem [1]. The intersection of these waves called triple point delimits high pressure zones of very different amplitude which are experimentally visualized by traces on smoked plate.

It was established that the detonation cell size measured by this technique in self-sustained detonations (generally close to CJ) is an intrinsic characteristic of a given gaseous mixture. So it does not depend on the geometric configuration in which detonation propagates unless the cell size is about the order of the limiting characteristic dimension of the tube (its diameter for instance).

Close the limit of the detonation propagation in cylindrical tube, the detonation front is only composed of one triple point which follows a spinning trajectory. If the ratio between the cell size and the limiting dimension of the tube still increases, there will be detonation failure. This phenomenon is particularly important from safety point of view and needs some fundamental studies.

Recent numerical studies on spinning detonation was performed by Hayashi et al. [2] on the detonation propagation in H_2/Air mixture confined in a square cross-section tube using detailed kinetic in a $3mm^3$ volume. Tsuboi et al. [3] carried out simulations in a similar case with a circular cross section tube.

To study the spinning detonation, we have choosen an undiluted CH_4/O_2 mixture where heat release occurs in one global step in contrast to two-step heat release provided by very fast first reaction followed by slow second reaction step [4, 5]. The CH_4/O_2 stoichiometric mixture exhibits the largest cell size among usual C_nH_m/O_2 mixtures, therefore it allows us to compare directly numerical simulation with experiment. After introducing the experimental device and the numerical method used, we will present some comparisons between experiment and numerical results.

2 Experimental Study

The experimental device consists of a detonation tube of 52mm inner diameter and 18m length. A 0.5m long high pressure section containing a C_2H_2/O_2 mixture is used to initiate the tested mixture. Two 3m spaced series of three Kistler 603B pressure gauges (1µs rise time) positionned 25cm apart check the steadiness of the detonation wave at the end of the tube. The accuracy on velocity is about 20m/s (i.e. 1%).

The global activation energy of $CH_4 + 2O_2$ mixture is 50–55kcal/mol and for an initial pressure of 50mbar the shock front temperature, T_{ZND} , is about 1800K. We measured a cell size λ of about 25mm for self-sustained detonation propagation at $P_0 = 200mbar$ in agreement with results of Pedley et al. [6]. As Ea/RT_{ZND} is high ($\simeq 18$), detonation cell pattern is very irregular.

We obtained the spinning detonation regime by decreasing the initial pressure down to 50mbar.

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3 Numerical Method

We used 3D unsteady code solving Euler equations. The scheme is explicit with FCT technique [7]. The chemical kinetic has a single step $A \rightarrow B$ given by an Arrhenius global reaction :

$$\frac{d[B]}{dt} = Z\rho^n (1 - [B])^n e^{-\frac{Ea}{RT}}$$

The order of reaction n was set to 1.1 and preexponential factor Z was ajusted to $10^{10}(SI)$ in order to get numerical cell size λ_{num} almost equal to the above mentionned experimental value for $P_0=200mbar$.

The cartesian grid has $1000 \times 50 \times 50$ cells with a homogeneous grid size of 1.04mm in the leading part of the wave. It adapts itself in the direction of propagation (x) that is why the computational area in the 52mm diameter tube spreads up to 12m.

According to Djebaïli Chaumeix et al. detailed kinetic scheme [8], the calculated ZND induction length in a $CH_4 + 2O_2$ mixture at $P_0=50mbar$ is about 4mm. This length agrees well with our reaction zone thickness since we count at least 4–6 grid cells in high gradient concentration zones. Figure 1 shows the profiles of burned gas concentration and density in axial plane and a front view of pressure for the detonation run distance of 9m. Some unburned gas pockets behind the front are put in evidence due to the spinning transverse wave creating shear layer.



Figure 1: CH_4/O_2 spinning detonation simulation at t=3.830ms a) Instantaneous concentration field of burned gas in the cross-section y=0 Black line : $0.054kg/m^3$ density isocontour White lines : 0.01 and 0.99 burned gas concentration isocontours b) Instantaneous density field in the cross-section y=0 c) Front view of pressure isocontours (above 3bar)

Figures 1 to 3 represent three successive instants showing the counter-clockwise spinning front propagation. By comparing Fig. 1 and Fig. 2, we can see the layer of preshocked fresh mixture ahead of th reaction front. Despite the pressure is maximal at the bottom of the cross-section axial plane at t=3.833ms (Fig. 2), it is not strong enough to ensure ignition of the fresh mixture just ahead of the detonation. As a result, the detonation front propagates transversally in the layer of preshocked and preheated mixture which itself propagates in the longitudinal direction. The existence of unburned pockets shows that the reaction zone length is quite important.



Figure 2: CH_4/O_2 spinning detonation simulation at t=3.833ms (Same layout as in Figure 1)



Figure 3: CH_4/O_2 spinning detonation simulation at t=3.836ms (Same layout as in Figure 1)

4 Comparision between Experiments and Simulation

4.1 Detonation Velocity

The theoretical velocity of the self-sustained detonation in $CH_4 + 2O_2$ mixture at $P_0 = 50mbar$ is 2262m/s. Calculated mean detonation velocity is close to D_{CJ} since the tube losses are ignored, while experimental value is at least 4% lower than the ideal velocity.

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4.2 Pressure and Detonation Shape

Pressure signals (Fig. 4) are very typical for spinning detonation and depend on the relative position of the pressure gauge to the spin. We remark after the first pressure peak of the incident detonation front another strong peak corresponding to the head of the transverse spinning detonation wave followed by periodic jumps of decreasing amplitudes. We notice a reasonable agreement between numerical and experimental pressure signals. Because the numerical code does not take into account losses, some difference appears in the amplitude beyond $50\mu s$.



Figure 4: Numerical and experimental pressure signals of a spinning detonation



Figure 5 shows a 3D view of the spinning detonation structure. We can notice the transverse spinning wave and the spiral shape of elevated overpressure behind the front.

Figure 5: Isocontours of pressure at t = 4.700 ms

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4.3 Spin Pitch

Experimental and numerical soot traces are respectively presented in Fig. 6 and 7. The helix angle is $45^{\circ} \pm 3^{\circ}$ in both cases. Experimental tests show a spin pitch between 15cm to 17cm while the numerical one ranges from 15cm to 19cm.

The track of numerical spinning wave appears as a band of variable thickness as in experiment which is typical for systems with high reduced activation energy E_a/RT_{ZND} . Nevertheless, the grid resolution is not sufficient to observe some fine structure inside the band and near the track of the helix.



Figure 6: Experimental soot traces for $CH_4 + 2O_2$ mixture at $P_0 = 50mbar$.



Figure 7: Numerical soot traces at $P_0 = 50mbar$ (i.e. the maximum pressure history recorded in the plane y=-0.026m). The band size is about 3mm thick in the left record and 6mm in the right one.

5 Conclusion

The present work reports on the simulation of a spinning detonation propagation in real experimental conditions. The spinning detonation in stoichiometric methane/oxygen mixture is well modeled with a one step Arrhenius chemical kinetics in spite of its high reduced activation energy. Reasonable agreement is obtained between simulation and experiments results on the detonation pressure history, the front structure, the spin pitch and the slope of trace.

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