Numerical Simulation of Pulse Detonation Engine Working Process Initiated by Small Energy

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0 Introduction

A pulse detonation rocket engine (PDRE)^[1-3] is a new-concept propulsion system utilizing repetitive detonations to produce thrust or power. It has many potential advantages such as low specific fuel consumption, high thrust weight ratio, simple structure, light weight, small size et al. Besides the experimental research, numerical simulation is also a very important method in researching the PDRE, and it always provides a cheap and efficient way.

In the simulation studies, some researchers adopted direct ignition with high temperature and pressure zone^[4, 5]. Some other researchers^[6, 7], whereas, took ignition energy into consideration, and then used the indirect initiation of small energy, but employed small zone of high-temperature to replace small energy. The simulations are different from the practical spark plug with initial ambient temperature. In addition, they did not consider the initial flow velocity at the ignition moment in detonation chamber and this neglect makes above numerical simulations far from the reality.

In this study, a pulse detonation engine simulative model of two-dimensional working process was established which combined with CFD software and boundary conditions control program. A whole pulse detonation engine working cycle was calculated. The working cycle contains filling, ignition by small energy under the condition of initial flow velocity of the mixture, propagation and purging processes. Experiments under the same conditions have been done to prove the correctness of the simulation.

1 Governing equations

The governing equations for inviscid, reacting, thermally perfect gases are the inviscid Euler equations with reactive source terms. The equations may be written as:

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = H$$

where Q is a conservation vector, E and F represents the flux vector of x and y directions, and H is the source term vector. And they are given by:

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	$\left(\rho_{1}\right)$		$\left(\rho_{1}u\right)$		$\left(\rho_{1}v\right)$		(ω_1)
	ρ_2		$\rho_2 u$		$\rho_2 v$		ω_2
	:		•		:		:
Q =	$ ho_{ns}$	<i>E</i> =	$\rho_{ns}u$	<i>F</i> =	$ ho_{ns}v$	H =	ω_{ns}
	ρи		$\rho u^2 + \rho$		ρиν		0
	ρv		ρиν		$\rho v^2 + \rho$		0
	$\left(\rho e_{t}\right)$		$\left(u(\rho e_t + p)\right)$		$v(\rho e_t + p)$		0

Here, u, v are respectively the gas velocity in x direction and y direction. ρ is tota gas density. p is the gas pressure determined by the ideal gas law. e_t is the total energy per unit mass of gas. ω_k is mass production rate for the component. The details of the definitions are given in [8].

2 Experimental setup and simulation model

2.1 Experimental setup

The schematic of PDRE experimental setup is shown in Fig.1. The engine consists of three parts, the first is mixing ignition section, for mixing the oxidizer and fuel; the second is Shchelkin acceleration section, including a Shchelkin spiral, which is used to accelerate DDT process; the third is propagation section for detonation wave. Solenoid valves were used to control the intermittent supply of oxidizer, fuel and nitrogen. In experiment, oxidizer was supplied by inlet1 and fuel by inlet2; after being injected into the detonation tube, the oxidizer and fuel rapidly mixed and were ignited in the mixing ignition section. The spark plug igniter of automobiles was employed to ignite the mixture, and the ignition energy was set as 50mJ. Dynamic piezoelectric pressure transducers were used to survey the pressure history along the detonation tube. The ambient pressure and temperature were around 0.1MPa and 300K, respectively.



Fig.1 Schematic of PDRE experimental setup

2.2 Simulation model and assumptions

The schematic of PDRE numerical simulation model is shown in Fig.2. The engine simulation model is constituted by main detonation chamber and exit flow field. The main detonation chamber was completely in accordance with the experiment model of the geometric design, easy to verify with the experimental results. The role of the exit flow field is to provide PDRE working environment, such as temperature and pressure.



Fig.2 Schematic of PDRE simulation model

In simulation, the Shchelkin spiral was replace by 3mmX3mm solid square. In order to reduce the computation of the simulation, the fuel atomization process had been ignored, and the fuel and oxidizer premixed model was directly used. Furthermore, the axis boundary condition was used and only the zones above the axis were calculated.

A basic PDRE working cycle includes filling, detonation and purging processes, and the detonation process is proceeding when the valves closed. Furthermore, the detonation process can be divided into ignition process and propagation process. The ratio of each working process time to the engine working cycle time is defined as duty cycle. In this paper, both in the experiment and simulation, a whole cycle of the PDRE working at 10Hz frequency was studied, and the duty cycles of filling, detonation and purging processes were set as 0.5, 0.1 and 0.4 respectively.

In simulation, before the engine start to work, we assumed the exit flow field was filled with static air, with the pressure and temperature of 0.1MPa and 300K, respectively. At the initial moment of filling process, the filling mixture was set to be stoichiometric state, and the mixture initial temperature was set to be 300K. When the mass fraction of fuel in the outlet of detonation chamber was greater than 80% of the stoichiometric mixture, the chamber was assumed as fully filled with stoichiometric mixture, and the valve closed.

In order to initiate detonation by small energy, as shown in Fig.2, a 4mm diameter circular ignition zone defined by CFD software was set near the close end. The spark ignition zone was filled with detonative mixture with the pressure and temperature of 0.1MPa and 300K, and the ignition energy was set as 50mJ, the same as in the experiment. As soon as the detonation chamber had been fully filled, the ignition module was started, and the calculation of DDT process begun.

When the detonation wave exited the detonation chamber, and a little time later when the chamber internal pressure closed to atmospheric pressure, the purging process was started. The component of purging mixture was changed to be nitrogen with temperature of 300K, which to purge the hot detonation products within the detonation chamber and prevent high temperature combustion products from contacting with the fresh detonable mixture of next working cycle.

All the above changes were controlled by the user defined function (UDF) program, written by the authors.

During the simulation, the solid walls were assumed as adiabatic and inviscid walls, the outside of the computational domain boundaries were assumed as pressure-far-field boundary.

3 Results and Discussion

In this study, the gaseous mixture of kerosene and oxygen detonation was simulated at first, and the results were compared with the experiment results and NASA CEA results, to validate the simulation and grid generation methods.

Because of the propane has similar characteristic as gasoline and the mixture of propane and air are difficult to produce detonation^[9]. Therefore, using the same methods the propane and air detonation was simulated, to investigate DDT process in detail.

3.1 Simulation of gaseous mixture of kerosene and oxygen detonation

When the chamber was fully filled, as the figure of flow velocity in the detonation chamber presented, which was not shown here, the maximum flow velocity was nearly 45m/s before ignition.

Fig.3 gives the simulation parameters at different time. The left figure presents the temperature of first part of inner chamber. The right one presents the pressure profiles in the detonation chamber axis. It can be observed form the left figure that after ignition, within 0.200ms, the ignition zone temperature rose slowly, mainly because the spark plug was undergoing the processes of discharging, releasing energy, heating and ionizing the mixture. And because of the ionization and temperature rose, the Arrhenius rate of chemical reaction increased, which led to more energy releasing, and in turn the same zone temperature rose up. From 50.201ms to 50.700ms the temperature nearly increased 100K per 0.100ms, at the same time, the Arrhenius rate of chemical reaction rose, but still at a low speed. After 50.811ms the Arrhenius rate of chemical reaction increased rapidly, and the temperature of the same zone also rose sharply. At 50.817ms the maximum temperature in chamber was nearly 5000K,

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much higher than actual temperature. This was due to the assumptions of the ideal gas equation of single-step reaction and disregarded of the thermal dissociation of products and heat loss to wall. Our further work is to overcome this imperfection.

As can be seen in the right figure of Fig.3, before 50.811ms the chamber maximum pressure remained constant about 0.1MPa. At 50.817ms the first pressure steep rise generated, the maximum pressure sharp rose to 0.7MPa. 0.002ms later another pressure steep rise turned up, the pressure spike sharply rose to 2.3MPa. As it can be observed form Fig.5, at 50.821ms the high pressure and high temperature zone spread to the whole end and a deflagration flame formed. Accelerated by Shchelkin acceleration section, the deflagration was ready to turn to be a detonation. Moreover, from Fig.6 it can be observed that the detonation wave pressure spikes were stable at around 2.5MPa. Additionally, by measuring the time of the detonation wave travelling across the two pressure transducer locations with a fixed distance, the velocity of the detonation wave can be determined. After a simple calculation, the velocity of the detonation has been successfully formed.



Fig.3. Simulation Parameters at different times. Left: Temperature of inner chamber. Right: Pressure profiles at the detonation chamber axis.



Fig.4 Experimental pressure profiles. Left: Experimental pressure profiles with the operation frequency of 10Hz Right: Enlargements of the first pressure spike in the left figure of Fig.4.

Experimental pressure profiles are shown in Fig.4. The left figure presents pressure profiles with the operation frequency of 10Hz. The enlargements of its first pressure spike were shown in right one.Pressure1 and pressure2 are the pressure profiles of pressure transducer1 and 2 locations, respectively. It can be observed that all the pressure peak values were greater than 1.8MPa, and the

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average value was around 2.1MPa. And the velocity of the detonation wave was determined as around 1700m/s.

From Fig.3 and Fig.4, we can figure out the velocity difference of simulation and experiment is only 62m/s, 4% of the experiment one; and there is only 0.4MPa pressure discrepancy between simulation and experiment. In conclusion, under the same ignition condition, the simulation and experiment results agree well, and this validates that the simulation and the grid generation methods and implies that they can be used in the simulation of a whole PDRE working cycle.

3.2 Simulation of propane and air detonation References

Using the same simulation and grid generation methods, the detonative mixture of propane and air was simulated. During the study, we tried a number of initiation energy and found it must be larger than1J and 3J would be a perfect one.



Fig.5 Contours of temperature and pressure. Left:Temperature isograms of the detonation chamber at different time. Right: Pressure isograms of detonation chamber.

The left figure of Fig.5 presents the temperature isograms of detonation chamber at different time. The right one gives the pressure isograms of detonation chamber. From Fig5, at 53.783ms the detonation C-J pressure at x=0.68m increased to 1.779MPa; the local temperature was 2930K. And the wave velocity increased to 1797.5m/s. Compared with the results of NASA CEA (Chemical Equilibrium and Applications) code as follows: $p_{C-J}=1.831MPa$, $T_{C-J}=2821.4K$, $v_{C-J}=1796.6m/s$, the discrepancy between calculation and the CEA results is smaller than 4% of the CEA results. The comparative results prove the simulation methods are suit for detonation simulation, the DDT process can be captured, and detonation have been formed.



Fig.6 Profiles of density along the axis at different time

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Profiles of density on the axis at different time are shown in Fig.6. The density spike locations present the compression wave locations. And because of the shock wave characteristic of detonation, every density along the axis at the detonation wave location certainly has a sharp peak, and the maximum values are stable around a constant. As can be seen from Fig.11, the density spikes ascended to 6.0 Kg/m3 at 53.783ms and then maintained around the value. As analyzed above, the detonation wave was formed at 53.783ms with the location of 0.68m.

The DDT process can be observed from Fig.5~6: the gas mixture temperature and the pressure slowly increased before 53.522ms because of the ignition and then the deflagration formed. The pressure increase to 0.6MPa and the first steep rise turn up owing to the superposition of the compression wave at 53.522ms and the density is up to 3.4Kg/m³. As the simulation proceed to 53.762ms, the pressure increased to 1.332MPa and the pressure increased to 1.792MPa with the density of 6.0Kg/m³ at 53.783ms when the detonation wave finally turned up. The pressure fell to 1.633MPa and then turned to be a steady value after the detonation wave propagated for 0.003ms. When the pressure spike was 1.792MPa, the distance between this location and the ignition zone (0.68m) was regarded as the DDT distance, and the time 3.783ms was considered as DDT time.

4 Conclusions

- (1) The numerical simulation of a whole working cycle of PDRE which used kerosene (propane) as fuel and oxygen (air) as oxidizer, spark plugs as ignition energy as 50mJ (3J) has been achieved.
- (2) The temperature presented linear increase basically and the pressure rise steppedly after ignition. High-temperature and high-pressure zone is formed at about 0.8ms after ignition in kerosene and oxygen detonation.
- (3) The results of numerical simulation and experiment results are well agreed with each other, which proves the methods of numerical simulation and grid generation in this paper are suitable for simulating the complete working cycle of pulse detonation engine. Using the methods, the DDT process can be simulated, and the DDT distance and DDT time can be accurately obtained.

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