Research on Detonation of Liquid Hydrogen-Oxygen by Numerical Simulation

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1 Introduction

There are some combustors in engineering that work by burning liquid hydrogen and oxygen. Extremely high pressure peaks can occur during the ignition process and possibly cause serious problems if the combustor isn't well designed. When very high ignition pressure peaks occur, it is difficult to obtain abundant details about the flow field due to the very short ignition process. The extremely high ignition pressures are a big potential risk to the combustors, thus it is important to understand the fundamental mechanisms and find an approach to eliminating associated risks. The aim of the paper is to investigate the mechanism of the extremely high ignition pressure peaks by numerical simulation, which are performed by a Reynolds Average Navier-Stokes method in the framework of the commercial software ANSYS FLUENT [1]. The development of more advanced approaches for capturing the details of the flow physics, such as implicit Large Eddy Simulations [2], are under development and results will be presented in a future paper.

Although the duration of the ignition process is very short for a liquid hydrogen-oxygen combustor, extremely complex physical and chemical processes occur. Besides the motion of the continuous phase, the associated physical and chemical processes include atomization, the motion, collision, breakup and vaporization of droplets, the interaction between droplets and the continuous phase, chemical reaction, deflagration, detonation, and etc.

Because the simulation problem is so complex, it is impossible to treat all those related factors equally. To reveal the mechanism, only the major influence factors should be involved, which is implemented by reasonably choosing appropriate models and ignoring the minor factors.

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2 Methods and Models

The Euler-Lagrange approach has been employed for modeling the multiphase flow. The droplet trajectories are computed individually at specified intervals during the fluid phase calculation. The Reynolds-averaged Navier–Stokes equations is used to model the fluid phase, and the pressure-based transient PISO solver (Pressure-Implicit with Splitting of Operators) is applied to solve the Navier-Stokes equations. Discrete phase models and the chemical reaction model are also incorporated.

2.1 Assumptions

As described in the introduction, the ignition process is very complex. To make the simulation viable, the following assumptions (and simplifications) have been made:

1. The heat transfer between the combustor and the outside environment is not taken into account, so the wall is considered as an adiabatic wall. The effect of thermal radiation is also ignored.
2. The specific process of liquid film breaking is not considered. The droplet sizes and velocity distribution are directly defined at the nozzle outlet. The secondary breakup of droplets is ignored.
3. The influence of virtual mass force, Basset force, pressure gradient force, Magnus force, Saffman force and other factors on droplets is ignored. Gravity is also ignored.

2.2 Discrete Phase Models

Discrete phase models include spray nozzle model, droplet evaporation model and the interaction between the continuous phase and the discrete phase.

ANSYS FLUENT supports common injection types, including single, group, solid-cone, and etc. Which injection type to choose is problem-specific.

Droplet evaporation is modeled by a convection/diffusion-controlled control model, which is suitable for evaporation processes, where the evaporation rate is high and the effects of surface convection is important. The motion of the droplet is treated by a Lagrangian method. The exchange of mass momentum and energy occurs between the droplet and the continuous phase.

2.3 Chemical Reaction Model

Table 1: Chemical reaction constants

species	reactions	$k_r = A_r T^{\beta_r} \exp\left(-\frac{E_r}{RT}\right)$		
		$A_k / \left(\left(\mathrm{cm}^3 \cdot \mathrm{mol}^{n-1}\right) \cdot \mathrm{s}\right)$	B_k	$E_k / \left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)$
H2 O2 OH O H H2O	H2+O2=OH+OH	1.7×1013	0.00	201.5
	H+O2=OH+O	1.42×1014	0.00	68.62
	H2+OH= H2O +H	3.16×107	1.80	12.68
	H2+O=OH+H	2.07×1014	0.00	57.53
	OH+OH=H2O+O	5.50×1013	0.00	29.29
	H+OH+M=H2O+M	2.21×1022	-2.00	0.00
	H+H+M=H2+M	6.53×1017	-1.00	0.00

In the chemical reaction part of the simulation, both a laminar flamelet model and an eddy dissipation concept (EDC) model have been tested for a straight pipe with one end closed, filled with stoichiometric hydrogen-oxygen gas mixture. The simulation results show that detonation does not occur with the EDC

model. The laminar flamelet model can simulate the detonation successfully. The laminar flamelet model is applied to carry out the simulation of the whole ignition process, although the steady-state operating simulation results of many combustor simulation cases indicate that the flame structure is qualitatively more accurately captured with the EDC model.

The detailed chemical reaction mechanisms[3] adopted is the 6-species, 7-reaction (6s7r) model, where the species include H2, O2, OH, O, H and H2O. The chemical reaction constants are shown in Table 1.

3 Simulation Case

In actual engineering, there is a liquid hydrogen-oxygen combustor with very extremely high ignition pressure peaks. Although during the steady operating state, the pressure in the combustor is about 3.1 MPa, the measured transient pressures during the ignition process are about 200 MPa and could even reach as high as 400 MPa with certain propellant mixing ratios. Additionally, the time span between the hydrogen-oxygen injection and the measurement of very high peak pressures is also extremely short, approximately 200 ms.

To carry out 3D simulation of the combustor, a 3D grid for the combustor was created. The geometry of the combustor is very complex containing many small holes and screws. To guarantee grid quality, a fine unstructured grid containing more than 900,000 grid points, was implemented.

The spray nozzle for liquid oxygen is centrifugal, which can be modeled by a solid-cone injection type in ANSYS FLUENT. Since the secondary breakup of droplets is not considered, the mean diameter of droplets is defined to be less than the estimated value, 50 μm, and the velocity is 40 m/s. The spray nozzle for liquid hydrogen is of plain-orifice type, and in ANSYS FLUENT the surface injection type can be used to model it. The mean droplet diameter is defined as 100 μm , and the velocity is 74 m/s.

Due to the initial temperature in the combustor chamber, approximately 300 K, which is very high compared to the extremely low temperatures of liquid hydrogen and oxygen, liquid hydrogen and oxygen droplets keep vaporizing very quickly all the time along their respective trajectories, thus forming a mixture of gas hydrogen, gas oxygen, liquid hydrogen droplets, liquid oxygen droplets and other gas components that exist before the injection of liquid hydrogen and oxygen. When the mixture develops until it is near the bottom of the combustion chamber, where the temperature is about 1800K, the mixture ignites and forms flames moving upwards, droplet vaporization accelerates and deflagration to detonation transition (DDT) occurs. The practical test measured very high peak pressures at both the top and lower part of the combustor at almost the same time.

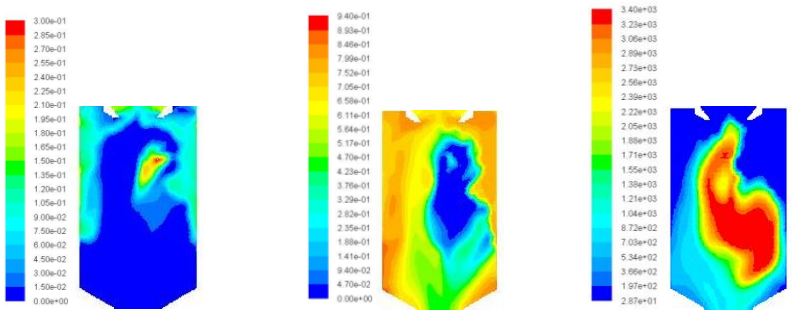

Figure 2. Left and middle: hydrogen and oxygen mass fraction distribution; right: temperature distribution

The strength of detonation wave is closely related to the mixing ratio, initial temperature and pressure of the mixture. Figure 2 shows the mass fraction distribution of hydrogen and oxygen and the temperature

distribution of the flow field just before detonation. For a large part of the mixture, the mixing ratio is in the vicinity of 4.0, which is within the detonable range of hydrogen-oxygen[4-6], from 1.78 to 90.67 with 8.0 being the stoichiometric ratio. The temperature of a large proportion of the mixture is very low, about 30 K. The initial pressure in the combustion chamber is about 1.4 MPa.

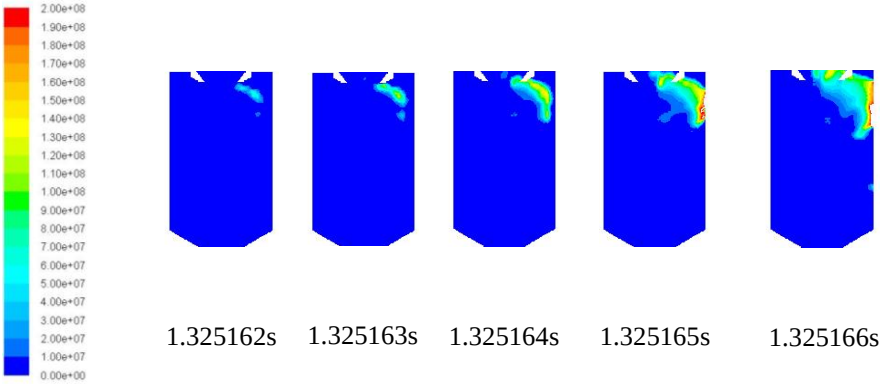

Figure 3. Propagation of detonation wave

Figure 3 shows the development of detonation wave. As can be seen, the detonation wave first appears near some position close to the top of the combustion chamber. Following that, the detonation wave propagates through mixture, which features mixing ratios within the detonable range. Very high pressures occur at the top and the middle position of the combustion chamber simultaneously, and the speed of detonation wave is as high as 5000 m/s. Pressures at some positions can be as high as 200 MPa.

4 Conclusion

The occurrence of strong detonation waves is due to the fact that the ignition flame is located at the bottom of the combustion chamber. As a result, hydrogen and oxygen droplets at extremely low temperatures evaporate rapidly and accumulate in large quantities in the combustion chamber. They subsequently form a hydrogen-oxygen mixture at very low temperature (30 K), high initial pressure (1.4 MPa) and mixing ratio of 4.0. The strong detonation wave is due to the combination of three main factors: low initial temperature, high initial pressure and appropriate mixing ratio. The simulation results are also consistent with the calculation results of CJ detonation theory[5,7]. To eliminate detonation, the ignition position can be change to some position near the head of the combustor, so that hydrogen-oxygen mixture cannot accumulate.

References

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