Aerospace Science and Technology 56 (2016) 148–154

Contents lists available at ScienceDirect

Aerospace Science and Technology

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Mixing and combustion modeling of hydrogen peroxide/kerosene shear-coaxial jet flame in lab-scale rocket engine

Sen Li [a,*], Yifei Ge [b], Xiaolin Wei [a], Teng Li [a]

[a] State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, No. 15 Beisihuanxi Road, Beijing, 100190, China
[b] University of Chinese Academy of Sciences, Beijing 100190, China

ARTICLE INFO

Article history:
Received 11 June 2016
Received in revised form 2 July 2016
Accepted 17 July 2016
Available online 22 July 2016

Keywords:
H_2O_2
Kerosene
Shear-coaxial jet
Combustion
Plume

ABSTRACT

H_2O_2/kerosene bipropellants are effective alternatives for toxic propellants currently in use. The complex H_2O_2/kerosene turbulent flow and combustion chemical reaction are modeled, the atomization, evaporation and mixing are investigated, the characteristics of the complex chemical reaction path of kerosene at different stages in combustion chamber are analyzed, and the profiles of static pressure, temperature and Mach number of exhaust plume are provided. During the kerosene injection, the spray angle is 13°, the atomization and evaporation occur and complete simultaneously, the lasting time of atomization is about 1 ms, and the maximal vaporization rate reaches 1.5×10^{-6} kg/s. The combustion chamber can be divided into the following three zones: rapid high-temperature pyrolysis zone, oxidization zone and equilibrium flow zone. The initial excitation of kerosene reactions is crucial link, and the hydrogen abstraction reactions are the dominant reactions in the high pyrolysis. These peak values of static pressure, temperature, Mach number along plume axis almost evenly distribute, and the interval distances are about 32 mm along the centerline of axis.

1. Introduction

Green and nontoxic hypergolic H_2O_2/kerosene bipropellants are promising candidates as effective alternatives for toxic propellants currently in use [1]. Rocket-grade H_2O_2 (concentration $\alpha \geq 85\%$) is decomposed into a high-temperature ($T \geq 1000$ K) and oxygen-rich steam as it comes in contact with a catalyst medium. This leads to an automatic ignition with a liquid fuel in a bipropellant engine without a requirement for a separate ignition unit.

Previously, a test of 100N-thrust laboratory scale H_2O_2/kerosene rocket engine was performed. Due to high-pressure and high-temperature environment in the combustion chamber, the processes of kerosene spray, atomization, vaporization, mixing and chemical reaction were very difficult to be diagnosed, and the combustion chamber pressure and the exhaust plume image were only monitored.

The process of H_2O_2/kerosene combustion is very complex. Since the turbulence and the chemical reactions not only interact with each other but also with the spray processes [2], the presence of the liquid phase complicates the situation. An improved understanding of the physical and chemical processes occurring in liquid rocket engines is required to ensure the stability, reliability, and efficiency of the engines.

In the study, in order to discover the complex process of H_2O_2/kerosene combustion in rocket engine, based on the previous test, the complex gas–liquid turbulent flow and combustion chemical reaction are modeled, the atomization, evaporation and mixing are investigated, the characteristics of the complex chemical reaction path of kerosene are analyzed, and the profiles of static pressure, temperature and Mach number of exhaust plume are provided.

2. Lab-scale rocket engine configurations and experimental conditions

In the previous experiment, the rocket engine consists of silver screen catalyst bed, injector, combustion chamber and nozzle, as shown in Fig. 1. The length and inner diameter of combustion chamber are 100 mm and 25 mm, respectively. The inner diameters of the nozzle throat and nozzle exit are 7.5 mm and 15 mm, respectively. The above detailed configurations are mentioned in the following computing domain of combustion.

H_2O_2 and kerosene were pressurized with a regulated nitrogen gas manifold system. The propellants were controlled by a pneumatic actuator operated using a solenoid valve. 90% H_2O_2 was decomposed into high-temperature mixture of water vapor and

* Corresponding author.
E-mail address: lisen@imech.ac.cn (S. Li).

http://dx.doi.org/10.1016/j.ast.2016.07.008
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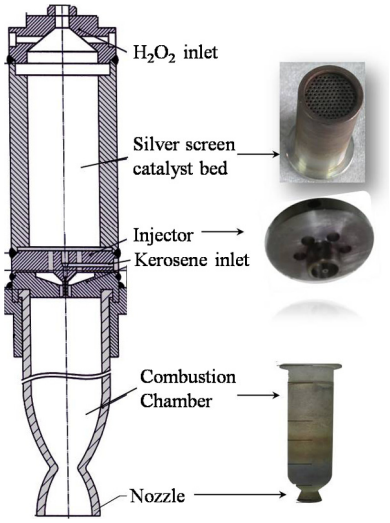

Fig. 1. Schematic of the experimental engine.

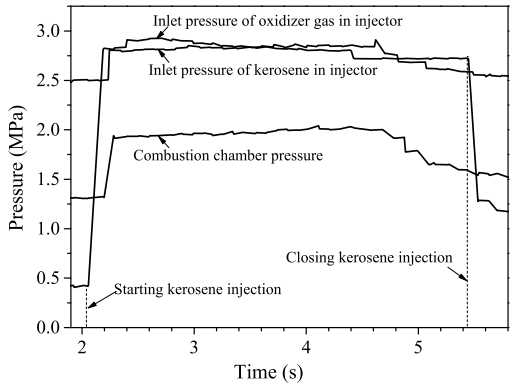

Fig. 2. Operating pressures of injector and combustion chamber in the experiment.

oxygen (mass concentration: 42.3% O_2, 57.7% H_2O; 1030 K) when it passed through the silver screen catalyst bed, and the decomposed stream was used as oxidizer.

The operating pressures of injector and combustion chamber were measured in the experiment, as shown in Fig. 2. At the injector inlet, the operating pressures of kerosene and oxidizer are about 2.8 MPa, and mass flow rates of kerosene and oxidizer are 7 g/s and 43 g/s, respectively. In the experiment, H_2O_2 was injected 2 s before kerosene was injected, and kerosene injection lasted for 3.5 s. The combustion chamber pressure was measured, and it was about 2 MPa. Since the combustion residence time is less than 10 ms in combustion chamber, the heat transfer through the chamber wall can be ignored, and the wall is considered as adiabatic wall in the simulation.

In the experiment, China No. 3 aviation kerosene was employed, the measured mass fractions of various components were listed in Table 1 [3]. Guided by Dagaut's three-component surrogate [4], Fan et al. [5] given the surrogate fuel consisted by mole of 49% *n*-decane, 44% 1,3,5-trimethylcyclohexane, and 7% *n*-propylbenzene.

3. Model description

3.1. Kerosene injection and spray break-up model

The CFD code Fluent is used in the study, a "Plain Orifice Atomiser" (POA) model is used to model the high-speed liquid injection into a gaseous atmosphere. The model is suitable to simulate

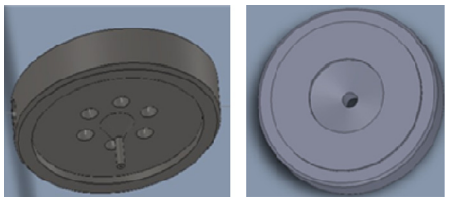

Fig. 3. View on the coaxial injection head.

kerosene injector with a long and thin orifice, and the orifice connects a high pressure reservoir of kerosene within the injector to the high-pressure steam of the decomposed hydrogen peroxide in the combustion chamber (see Fig. 3). Using the POA model enables the injection and subsequent atomization of the kerosene jet to be modeled without the need to create complicated mesh geometry. The main parameters used in the case modeled here are as follows: inner diameter of kerosene tube: 0.7 mm; tube length: 5 mm; mass-flow rate of kerosene: 7 g/s.

The "wave" model in Fluent is used to model kerosene spray break-up. The wave model of Reitz [6] considers that the break-up of an injected liquid is induced by the relative velocity between the liquid and gas phases. Once the spray breaks up into droplets, the penetration of the spray depends mainly on the aerodynamic drag of the droplets. This model is chosen for this study. To take into account the turbulence effects, the realizable k–ε turbulence model is used.

3.2. Eulerian–Langrangian Discrete Phase Model (DPM)

In the study, Eulerian–Langrangian Discrete Phase Model (DPM) is used, the flow of discrete fluid droplets is introduced to treat with an Eulerian description and the other with a Lagrangian approach. At the interface between the phases, the partial pressure of the vapor is considered equal to the saturated vapor pressure calculated at the liquid temperature. The rate of vaporization is governed by the gradient diffusion.

3.3. Thermodynamic model

The equation of state employed in the present study is the Peng–Robinson (PR) cubic equation, which is used in the Lagrangian/Eulerian description:

$$P = \frac{RT}{V-b} - \frac{a}{V^2+2bV-b^2} \tag{1}$$

where R is the universal gas constant and V is the molar volume. Terms a and b are coefficients that account for attraction and repulsion effect among molecules. Details of the application of these equations can be found in Ref. [7].

3.4. Combustion model

The combustion in liquid rocket propulsion typically occurs in the flamelet regime of turbulent combustion [8,9], which enables the use of the flamelet model for turbulent spray diffusion flames. Thus, the combustion is modeled by a Flamelet approach including non-equilibrium effects and a PDF-treatment to take into account turbulent combustion. In the flamelet model used in the non-premixed combustion model, the turbulent diffusion flame is considered as an ensemble of laminar flamelets, and chemical reactions and heat transfer occur in a thin layer. The thermochemistry calculations are preprocessed and then tabulated for look-up in the CFD code. Interaction of turbulence and chemistry is