

Research on the Application of Steady Laminar Flamelet Model Used in Two-phase Supersonic Combustion

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A numerical study was conducted to explore the computational accuracy and efficiency of steady laminar flamelet model used in two-phase supersonic combustion flow field. The combustion flow field of a double-cavity scramjet was simulated, in which liquid phase was described by the disperse particle method (DPM) with secondary break-up process. The results obtained show that the steady laminar flamelet model can decouple the equations of chemical reacting source terms and flow, and this model also can consider a detailed reaction with less computational resources. Moreover, the comparison of the numerical results with flame structure image and wall pressure distributions of the experiment show good agreement. And the detail of flow field calculated is accurate. This model greatly reduces the computational amount, and can facilitate engineering applications.

1. Introductions

Scramjet is one of the ideal power devices to realize the hypersonic flight in the atmosphere, and the complex supersonic combustion process has been the focus of the researchers (Kazmar, 2005; Van-Wie et al., 2005). Due to the complex flow and chemical reaction process, the turbulent combustion model is more complicated than that of low speed laminar combustion.

The finite rate combustion model based on multi component N-S equations is widely used in engineering. However, with the increase of the composition, the calculation cost increases significantly. There are mainly two kinds of method to solve such problems: first one is to simplify the complex reaction mechanism into one-step reaction (Zhou et al., 2007), or two-step reactions (Wang and Hou, 2007; Xu and Cai, 2002), but the over-simplified chemical reaction mechanism will reduce the accuracy of combustion simulation; and the second one is to use High Performance Computer to complete scramjet flow simulation with multi-step reactions (Yang et al., 2009), the high requirements for hardware and the longer calculation cycle limit its application in engineering. Peters (Peters, 1986) has proposed the flamelet model according to the study of the laminar diffusion flame. The model is based on the assumption of rapid chemical reaction, which can consider a reaction mechanism in detail, and avoid the coupling process of species' transport equations and chemical kinetics. This model improves the computational efficiency. Although the flamelet model is limited by the specific combustion mode, most of the turbulent combustion in reality is consistent with this hypothesis (Williams et al., 2000). At present, the flamelet model is mainly used to solve the problem of gaseous combustion in the field of super combustion, and has achieved some results (Fureby et al., 2010, Terrapon et al., 2010).

The kerosene which is commonly used is a complex liquid mixture at normal atmospheric temperature. There are still many problems in the study of this fuel (Liu, 2009). The chemical reaction of gaseous kerosene is usually calculated with one-step reaction, or simplified as the main intermediate product further, such as ethylene and methane (Yin and Yu, 2006). Besides, under the condition of supersonic combustion, ignoring or simplifying the process of atomization evaporation will cause errors, so how to consider the combustion process of liquid fuel is a necessary issue. Ldeinde (Ladeinde, 2009) believes that the flamelet model has become one of the hot spots in the study of supersonic turbulent diffusion combustion.

It is rarely reported that the steady laminar flamelet model is used to study the flow field of liquid fuel, so the simulation of a cavity scramjet experiment with kerosene fuel by Pan (Pan et al., 2011) was performed to explore

the feasibility, the accuracy and computational efficiency of the method, and expand the range of the flamelet model in supersonic turbulent diffusion combustion, aiming to solve the large amount of calculation problem in the two-phase supersonic combustion numerical study.

2. Physical model and governing equations

The flow field is solved based on the spatial filtered N-S equations, and the LES model is used to model the turbulent pulsation term in the momentum equation, then the combustion and the two phases are treated by the steady laminar flamelet model and DPM model respectively.

2.1 The steady laminar flamelet model

The basic hypothesis of the flamelet model is that the reaction time scale is small enough, and the chemical reaction takes place in a thin layer, which is mixed with its equivalence ratio. Under this assumption, the structure of the reaction zone is still laminar, and the diffusion transport occurs in the direction perpendicular to the equivalent mixing surface. Based on this, the scalar transport equations can be transformed into a coordinate system in an independent variable, mixture fraction Z . The flamelet model can be written as:

$$\frac{\partial Y_i}{\partial \tau} - \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} - \dot{m}_i = 0 \quad (1)$$

τ is time; ρ is density; \dot{m}_i is reaction rate; χ is scalar dissipation, which represents the rate of stretch in a mixed fractional space, usually given in the form of:

$$\chi = 2D(\nabla Z)^2 \quad (2)$$

Here, D is eddy dissipation rate. Other scalars such as temperature and enthalpy can also be got with the formula (1). The mixture fraction Z is a very important physical quantity in non premixed combustion. The definition is adopted by Masri (Masri et al., 1990).

$$Z = \frac{f_C / (mW_C) + f_H / (nW_H) + 2(Y_{O_2,2} - f_O) / (v_{O_2} W_{O_2})}{f_{C,1} / (mW_C) + f_{H,1} / (nW_H) + 2(Y_{O_2,2} - f_O) / (v_{O_2} W_{O_2})} \quad (3)$$

Here, f_C , f_H and f_O are mass fraction of carbon, hydrogen and oxygen; W_C , W_H and W_{O_2} are the corresponding molecular weight, and subscript 1 and 2, indicate the inlet parameters of the fuel and oxidizer flow respectively. In the process of rapid combustion reaction, the steady laminar flamelet model is usually adopted, which means the time item in formula (1) is neglected:

$$\rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{m}_i = 0 \quad (4)$$

The solution of formula (4) is just the function of scalar dissipation rate and boundary conditions; when the physical process is given, the boundary condition is determined, so the equations can be parameterized by a scalar value. The flamelet can be calculated in advance according to these parameters.

The steady state solution of the flamelet equations can be written in the form of $\phi(Z, \chi_{st})$, and PDF (Probability Distribution Function), is taken into account for the of turbulence effect:

$$\tilde{\phi} = \int_0^1 \int_0^\infty \phi(Z, \chi_{st}) P(Z, \chi_{st}) dZ d\chi_{st} \quad (5)$$

χ_{st} is assumed to be the δ -function, Z is a β -function distribution, the formula (5) can be expressed as:

$$\tilde{\phi} = \int_0^1 \phi(Z, \chi_{st}) \beta(Z; \tilde{Z}, \tilde{Z}^{n_2}) dZ \quad (6)$$

All the variables $\tilde{\phi}$ are calculated in advance using the detailed reaction mechanism and the flamelet equations, according to the formula (6). In the calculation, the solver only deals with the continuity equation, the momentum equation and the scalar transport equation of the three parameters. Other variables such as concentration, temperature and chemical source terms of each component were obtained by look-up table.

2.2 DPM model

It is assumed that the effects of the drop volume fraction on the continuous phase are neglected. The droplets are divided into representative groups, each with the same position, velocity, temperature and diameter. The interactions of mass, momentum and energy of two phases are added to the equations of two phases as the source forms. The liquid phase's equations are:

(1) Droplet motion equation

$$\begin{aligned} \frac{d\mathbf{u}_p}{dt} &= F_D(\mathbf{u} - \mathbf{u}_p) + \mathbf{g}(\rho_p - \rho) / \rho_p + \mathbf{F} \\ F_D &= \frac{18\mu C_D}{\rho_p d_p^2} \frac{Re_p}{24} \end{aligned} \quad (7)$$

Here, u_p , ρ_p and d_p are velocity, density and diameter of droplets; Re_p is droplet Reynolds number; C_D is drag coefficient; F is other forces.

(2) Droplet trajectory equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}_p \quad (8)$$

(3) Mass and energy exchange equation of droplets

The mass balance equation of the droplet in evaporation and boiling:

$$m_p(t + \Delta t) = m_p(t) - N_i A_p M_{w,i} \Delta t \quad (9)$$

$$h_{fg} \square dm_p / dt = h A_p (T_x - T_p) \quad (10)$$

When the temperature is lower than the evaporation temperature, the temperature equation is:

$$m_p c_p dT_p / dt = h A_p (T_\infty - T_p) \quad (11)$$

The temperature rise equation above the evaporation temperature:

$$m_p c_p dT_p / dt = h A_p (T_\infty - T_p) + h_{fg} \square dm_p / dt \quad (12)$$

Here, m_p , c_p and A_p are of the mass, the specific heat of specific pressure and the surface area liquid droplets, respectively. $M_{w,i}$ is the molar mass of the component, T_∞ is the temperature of the gas phase, h is the convective heat transfer coefficient, and h_{fg} is the latent heat of the liquid phase.

3. Calculation model and boundary conditions

The sizes and the calculation conditions of the model engine are given according to Pan (Pan et al., 2011). The reaction mechanism of kerosene combustion is the 17 components for the 30 steps reaction from the NASA Lanley Center (Molnar et al., 2003).

3.1 Computational model and meshing

The engine geometry is shown in Figure 1(Pan et al., 2011). The inlet area of the combustion chamber is 54.5mm*75mm, and the length of the combustion zone is about 592 mm. The upper and lower concave cavities are respectively D15L7A45 and D10L5A45 (the depth of the cavity is D=10mm, the length/depth is L/D=5, and the angle of the back wall is A=45 degrees). Kerosene is injected into the combustion chamber through the wall of the vertical holes, and there are three 0.5mm diameter nozzle on the upper wall, with fuel equivalence ratio 0.18, one 0.5mm diameter hole on the bottom, with the equivalent ratio of 0.07. The distance between the injectors and the front wall of the very cavity is 10mm. Figure 1 gives the location of the pressure measuring point and the position of the middle section in the test.

The mesh of the model is structured, and the nozzle and wall surface are locally refined. The total number of grids is about 2 million.

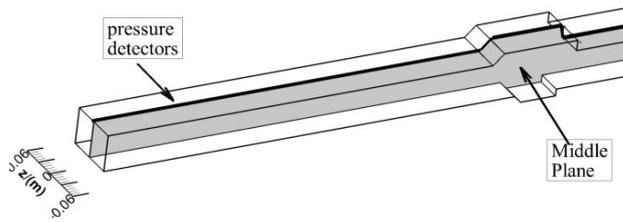


Figure 1: Geometry of chamber

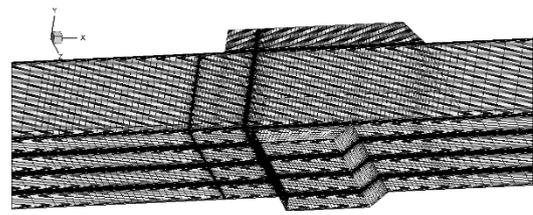


Figure 2: Mesh of chamber

3.2 Boundary conditions

The inlet of the combustion chamber is consistent with the experimental conditions: the air flow rate is 2kg/s, the oxygen mass fraction is 23%, the total temperature is 1300K, the total pressure is 1.84MPa, and the Mach number is 2.64. The exit is supersonic, which is given by first order extrapolation. Walls are adiabatic non-slip. Injection conditions: considering the secondary breakup process of the droplet, the K-H/R-T model (Pattersonm, 1987) is chosen, the initial drop diameter is taken as 0.1mm, and the gravity is taken into account, 9.8m/s^2 . Turbulent model is Smagorinsky LES model.

4. Results and analysis

Figure 3 shows the structure of the flame, which has the effect of spatial superposition. Figure 4 is the simulation of the temperature contour. Compared with the two, it can be seen that the flame is mainly distributed in the cavity and the downstream of the cavity, while the brightest region is located in the cavities, and the simulation results are consistent with the experimental results.

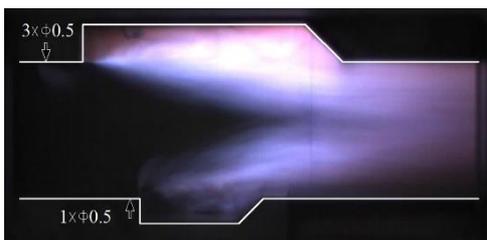


Figure 3: Flame structure near cavity area

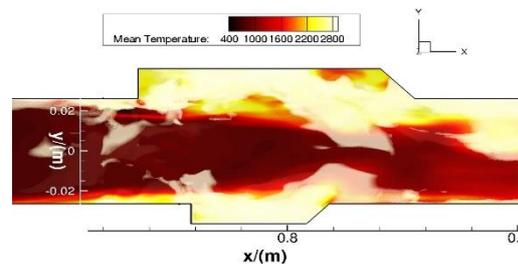


Figure 4: Temperature iso-surfaces

Figure 5 gives an experimental and simulated schlieren image. The dark region of schlieren images reflect the fuel distribution, it can be seen that the fuel is taken to the downstream by the transverse flow, and entrained into the cavities. The fuel distribution in cavities and pre-combustion shock waves upstream of injection from simulation are consistent with those of experiment.

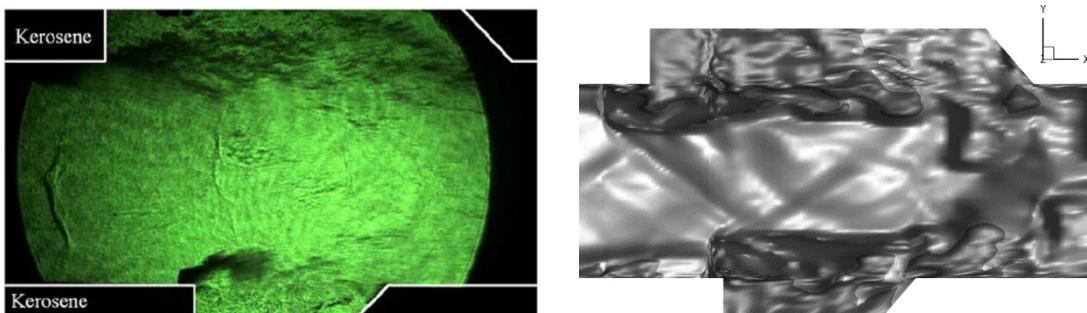


Figure 5: Contrast of schlieren in intermediate section (left is experimental result, right is simulation result)

Figure 6 is the pressure distribution at the center of the wall, it can be seen that the overall simulation results agree with test data, the rising segment is behind the pressure test, indicating the location of the shock train is

behind the test results. The range of 0.15m on the downstream cavity of simulation has a higher pressure than the experimental values, the reason is that the shock waves hit this region, and make a pressure peak, where the pressure measuring point is not set. The trend of the cavity pressure curve is agreed with the experiment. Figure 7 shows the mass fraction of kerosene. Figure 7 (a) is the middle section of the image, the gray sphere shown in the figure are droplets displayed with droplet relative size. It can be seen that liquid kerosene breaks up secondarily with aerodynamic force, producing smaller droplets; due to the static temperature higher than the boiling point of kerosene (370K), kerosene evaporate completely in a short distance; some gaseous kerosene mix with air in the mainstream area, the other part is rolled into the cavities in the recirculation zone. Figure 7 (b) shows the distribution of kerosene concentration along the flow direction. It can be seen that there is a small amount of kerosene vapour in the recirculation zone. Figure 7 (c) shows that the concentration of the iso-surface of the fuel is mainly distributed in the cavities, and close to the mainstream. The fuel is gradually consumed by combustion.

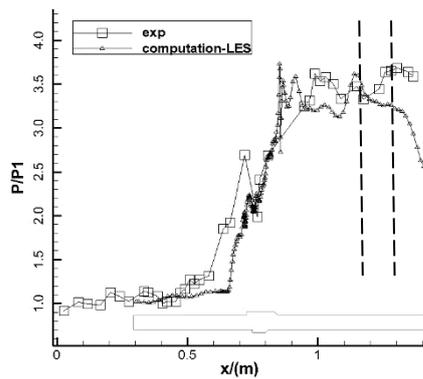


Figure 6: Contrast of pressure distribution on wall centreline

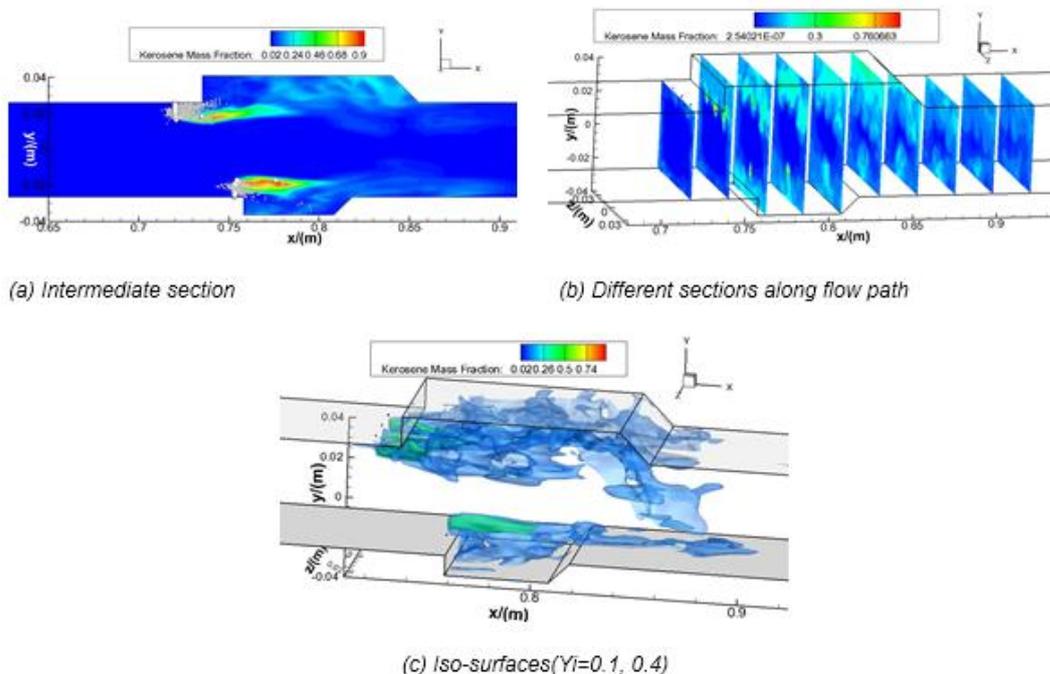


Figure 7: Mass fraction distribution of kerosene

The number of grids is about 2 million for this scramjet, and the reaction mechanism is composed of 17 components, 30-step reaction, besides the secondary breakup and evaporation of the two phases are considered. For the finite rate model by solving the multi component N-S equation, it can only be realized with the help of massively parallel computing (Le,2010). The simulation was performed on a personal PC with quad

core and 5G memory usage, within 100 machine hours. Therefore, from the point of view of computational efficiency and hardware requirements, the laminar flamelet model has obvious advantages.

5. Conclusion

Numerical investigation was conducted to explore the computational accuracy and efficiency of steady laminar flamelet model used in two-phase supersonic combustion flow field. The combustion flow field of a double-cavity scramjet was simulated, liquid phase was described by DPM considering secondary break-up process. The reaction mechanism uses NASA Lanley center's 30 reactions with 17 components. The results show that: (1) the flamelet model decouples chemical reaction calculation and flow, so the chemical mechanism can be more detailed with less computational resource; (2) the flame structure, the schlieren images and the wall pressure distribution of calculation results are in good agreement with the experimental measured; (3) get the details of the flow field with the help of high accuracy simulation.

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