The simulation of endothermic fuel flow in cooling channels of Scramjet

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Abstracts: To quantitatively understand the flow characteristics and physio-chemical properties of the kerosene in cooling channels of scramjet, one numerical method is adopted. Firstly, the boundary conditions of combustion gas side wall are derived using a parallel CFD tool. Secondly, the temperatures on walls of cooling channels are given using a quasi-3D thermal evaluation tool and the derived boundary conditions. Lastly, one axisymmetric CFD code is used to calculate the heated low-speed flow of kerosene under supercritical pressure inside cooling channels. The modeling of physio-chemical properties of aviation kerosene is described in detail.

Key words: regenerative cooling; aviation kerosene; supercritical flow

0 Introduction

The fuel (kerosene at M<=8) of Scramjet serves at least two functions. The first one is its conventional role as a source of heat through combustion. The second role is that the kerosene is used as a “heat sink” to remove waste heat from the engine flow path, which is called regenerative cooling, analogous to rocket thrust chamber cooling[1].

From the point view of regenerative cooling, whether the thermal structure of engine is effective or not should be carefully investigated via heat transfer analysis and tests. The heat sink capacity and the physio-chemical properties of kerosene must be well determined before conducting heat transfer analysis. This is driven by the fact that the basic properties of the supercritical fuel (such as density) are significantly different from the subcritical (liquid) fuel, which includes the behaviors of heat transfer, injection/combustion, and thermal/catalytic cracking (pyrolysis) of the hydrocarbon.

Figure 1. Heat sink required as a function of Mach number (Lander and Nixon, 1971).

Using the classical Lander–Nixon plot (Figure 1), a Mach 8 Scramjet engine could require fuel heat-sink levels of 3500 kJ/kg[2]. This heat-sink level is partially due to sensible heating and partially due to endothermic (heat-absorbing) reactions of the fuel. This endothermic reactions process is a complex combination of thermal and catalytic cracking, with the effect of process variables (fluid velocity/residence time, surface/volume ratio, etc.) still under investigation in China Aerodynamics Research and Development Center (CARDC).

For the purpose of understanding the flowing characteristics of the fuel under supercritical
pressure, one numerical strategy is adopted. The numerical process includes three steps, which will be introduced after describing the modeling of physio-chemical properties of aviation kerosene.

1 The modeling of physio-chemical properties of aviation kerosene

Kerosene is a mixture which includes more than 100 species. One way to determine the physio-chemical properties of kerosene is to have the knowledge of its species. For the significance to heat transfer analysis, the design of thermal structure of Scramjet, and the injection to combustor, the components of one aviation kerosene at normal temperature were measured by two universities in China. One measurement was conducted using mass spectrograph, and the other using the method of single vacuum ultraviolet photon ionization combining the mass spectrum of molecular beam.

According to the two measurements, nearly 100 species were detected, mainly C8-C13, among which the most abundant component had a molar concentration of 10.6%. Considering the convenience of calculation, one surrogate model for aviation kerosene should be found complying with at least the following two principles. Firstly, the surrogate should have only a few components, less than 5 for example. Secondly, the surrogate should have nearly the same physical properties as the original kerosene. In principle, the surrogate should also have similar chemical behaviors as the original kerosene. This is not considered in search of the surrogate model, and will be further explained later.

Figure 2. Density vs. temperature and pressure

Figure 3. Specific heat vs. temperature and pressure

Figure 4. Viscosity vs. temperature and pressure

Figure 5. Thermal conductivity vs. temperature and pressure
Using one computer program for predicting the thermophysical properties of hydrocarbon mixtures, the thermophysical properties of the original aviation kerosene and its surrogate were calculated and compared with each other, as shown in Figures 2-5. The program can deal with the mixture having 150 hydrocarbon components at most.

In Fig.2-5, the solid lines are the thermophysical properties of the surrogate, and the dash lines are those of the original aviation kerosene based on one species measurement. The surrogate is consisted of 79% of n-decane, 13% of 1,1,2-trimethylcyclohexane, and 8% of n-hexylbenzene, and its critical point is $T_c=622.5$K, $p_c=2.198$MPa. One can see that the surrogate has nearly the same physical properties as the original aviation kerosene.

At temperature above 750K, the fuel may begin to crack into smaller hydrocarbons which are easier to combust. For a precise flow calculation, one should consider the change of thermophysical properties of the supercritical fluid when the components are changed. To encompass the difficulty of numerosness of components and the complexity of the deposition of kerosene, Ward\[3\] gave a PPD (proportional production distribution) model at low cracking degree.

Due to lack of cracking data of aviation kerosene, another method was chosen here. As a commonly used method the author adopted the global cracking rate data. For the supercritical fluid when the components are changed, it was assumed that the thermophysical properties of the mixture still behave the same way as those of the original aviation kerosene.

The global catalytic cracking rate data of n-Decane given by ward\[3\] were used in present work and are listed in Table 1. The rate has an expression of

$$Rate = \nu \exp\left(-\frac{E_a}{RT}\right) \times \text{[fuel]}$$  \hspace{1cm} (1)

In which, the pre-exponential term $\nu$ has the dimension of s$^{-1}$, the activation energy $E_a$ has the dimension of J/mol, the gas constant $R=8.314$J/mol·K, and the temperature of fuel $T$ is in K and the concentration of the uncracked fuel $p_{\text{fuel}}$ is in mol/m$^3$. The chemical heat sink of the kerosene was assumed to be 0.93MJ/kg.

### Table 1  Catalytic cracking rate data for n-Decane\[3\]

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Catalytic pyrolysis rate</th>
<th>$n$(s$^{-1}$)</th>
<th>$E_a/R$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-Decane</td>
<td></td>
<td>2.1E15</td>
<td>31704.6</td>
</tr>
</tbody>
</table>

2 The CFD computation of internal combustion flow in Scramjet

The CFD group of Airbreathing Hypersonic Laboratory (AHL) of CARDC, CARDC-AHL, has been carrying on the CFD research of internal combustion flow in scramjet from 1997. The group began to develop a parallel three dimensional CFD platform which is now called AHL3D at 2001, concerning of the complex configuration, different fuels(mainly H$_2$ and hydrocarbons), chemically reacting flows, and computational efficiency.

At present, the CFD platform AHL3D is parallelized using MPI for multi-processor machines, and can be used to solve the Reynolds-averaged conservation equations (in 2-D, axisymmetric, 3-D, or PNS form) with a cell-center finite volume method. AHL3d can be used for calorically perfect gas flows, flows of an arbitrary mixture of thermally perfect gases undergoing non-equilibrium chemical reactions, two phases flows, steady and unsteady flows, laminar and turbulent flows. The platform
can use multiblock, patched multiblock, or overset grids. The solutions are advanced in time with a LU-SGS scheme. A dual-time step scheme is used for unsteady flows. Now the group has made new progresses on the unstructured grid method and parabolized NS equation solver.

AHL3d has been validated for many kinds of flows. The present paper adopted AHL3D to compute the internal flow in tested scramjet. 10 species and 12 chemical reactions are included. To resolve the dependence on free-stream values of turbulence, the turbulence model of k-ωTNT is used. The scramjet model has a 32mm-height inlet (330mm in length) and a 300mm-length nozzle. The total length is 1360mm. The parameters of the CFD computation for this study are $M_\infty=6$, total pressure $p_0=6$Mpa, total temperature $T_0=1650K$, equivalent fuel/air ratio $\Phi=1.1$. The results are parts of inputs for the quasi three-dimensional thermal evaluation tool, which will be discussed in next part.

3 Quasi three-dimensional thermal evaluation tool

One group of CARDC-AHL has been carrying on the study of the regenerative cooling for scramjet from 2003. Two rounds of tests have been made, of which the coolants were respectively water and aviation kerosene. Good agreements between calculations and tests were derived, which indicated that the thermal evaluation tool and the model of thermophysical properties for aviation kerosene can be used extensively in thermal structure designs and analysis of tests.

The quasi three-dimensional thermal evaluation tool uses a two dimensional steady state heat transfer analysis and steps down the length of the cooling channels. Heat transfer and friction losses are calculated for each interval using empirical correlations. It is assumed that the heat going into the channel wall is completely absorbed by the coolant and at each interval the coolant property is homogeneous. For brevity, the detail of the heat transfer calculation method will not be described here. The detailed methods and its validation can be found in Ref.7.

In calculation, the size of the cooling channel is 2mm×3mm, the thickness of the liner is 1mm, the thickness of the outer layer is 2mm, and the width of rib is 2mm. The model was made of stainless steel (1Cr18Ni9Ti), inside which wall it was assumed there were 100 cooling channels, and the fuel mass flow rate was chosen as 1g/s for each channel. The fuel inlet conditions were $T=293$K and $p=65$atm. A one dimensional method was used to determine the fuel flow inside the channel. The resulted wall temperatures of cooling channels are inputs for the axisymmetric calculation of the low-speed heating flow of the fuel inside the cooling channel, which will be discussed in next part.

4 The axisymmetric calculation of the fuel flow inside the cooling channel

The axisymmetric calculation of the low-speed endothermic flow of the fuel inside the cooling channel is based upon compressible SIMPLE method. This CFD tool can calculate steady laminar or turbulent (k-ε equations plus wall function) flows which are two dimensional or axisymmetric. The modeling of physio-chemical properties of aviation kerosene which was described in part 1 has been incorporated in it, and the global pyrolysis model can be included so that the low-speed heating flow of the fuel inside the cooling channel under supercritical pressure can be simulated.

Concerning the heating effects of four walls along one cooling channel and the difference of the wall temperatures at one station is small, the turbulent flow was assumed axisymmetric instead of two dimensional. The thickness of wall was chosen as 1mm, and the outer wall temperatures of
cooling channels which are inputs of this tool were the mean values of the results described in part 3. The total length of the channel is 0.89m and its inner area is 6mm$^2$ which were the same as the original. The fuel inlet conditions were also the same as described in part 3. Only one channel flow results will be given here.

Figure 6. Axial velocity along the channel

Figure 7. Density of kerosene along the channel

Figure 8. Temperature of kerosene along the channel

Figure 9. The mass fraction of uncracked kerosene along the channel
The results are shown in Fig. 6-9. According to the results, at the exit the fuel temperature is 970K. The fuel begins to crack at the place of 0.7m from the entrance where its temperature is about 870K, and at the exit about 54% of the fuel has been cracked. The fuel speeds at the entrance and the exit are respectively 0.23m/s and 1.48m/s. The fuel density has decreased from 750kg/m³ at the entrance to 125kg/m³ at the exit. The difference of fuel pressure between the entrance and the exit is not large. One can also see there are differences along the radial direction, which is larger near the entrance.

In the process of part 3, a one dimensional method was used to determine the fuel flow inside the channel. The difference of coolant temperature at the exit is only about 20K between the one dimensional method and the axisymmetric calculation, of which the former gave a larger value. Even so, the one dimensional method cannot give the differences along the radial direction, and is difficult to account the wall surface effects. So it is necessary to develop 2D and 3D method.

5 Concluding remarks

For the purpose of quantitatively understanding the flow characteristics and physio-chemical properties of the kerosene in cooling channels of scramjet, one numerical method was adopted. The modeling of physio-chemical properties of aviation kerosene was described in detail.

Firstly, the boundary conditions of combustion gas side wall were derived using a parallel CFD tool developed in CARDC. Secondly, the temperatures on walls of cooling channels were acquired using a quasi-3D thermal evaluation tool and the derived boundary conditions. Lastly, one CFD code based upon SIMPLE method was used to calculate the low-speed heating flow of the endothermic fuel under supercritical pressure inside the cooling channel.

The agreement of coolant temperature at the exit between the one dimensional method and the axisymmetric calculation indicates that the developed CFD code based upon SIMPLE method can be used in future work. The 3D method to account for the asymmetric heating will be developed, and the surface catalytic effect will be considered in the near future.

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References