Working Fluid modeling Based on Air Turbine Rocket Engine and Propellant Comparative Analysis

Shangchun Wang[2, a], Yang Liu[1, b, *], Yue Wu[2, c] and Zheng Ni[2, d]

[1] Xi'an Yuan Hang Vacuum Brazing Technology Co., Ltd, Xi'an 710299, China;

[2] Shaanxi Province Aerospace and Astronautics Propulsion Research Institute Co., Ltd, Xi'an 710003, China.

[a] shangchunwang12@163.com, [b] liuyang802@nwpu.edu.cn, [c] realwuyue@163.com, [d]nizheng2017f@163.com

* Corresponding Author

Abstract. The propellant of the Air Turbo Rocket (ATR) engine is burned in the gas generator to produce primary gas. This paper uses the established ATR engine working fluid calculation model to calculate the physical parameters and components of the primary gas produced by the combustion of four propellants at a given pressure and temperature, and compares and analyzes them according to the propellant selection requirements, Choose the appropriate propellant for the ATR engine.

Keywords: Propellant, Primary gas, Molar mass, Specific heat ratio.

1. Introduction

As a combined cycle engine, ATR engine organically combines rocket engine and aero-engine [1, 2]. The primary gas generated by propellant combustion in its gas generator determines the driving characteristics of the turbine, and the combustion products in the combustion chamber determine the overall performance of the engine. Therefore, the selection of propellant suitable for ATR engine is one of the key factors to determine its performance.

2. Working Fluid Modeling

The structure of ATR engine is shown in Fig. 1. The reaction process of propellant combustion in gas generator is complex. When the gas generator pressure and oxygen-fuel ratio change, the thermal parameters of gas will also change greatly, which will affect the calculation of engine working state. In order to simulate the combustion process more accurately, this paper uses the minimum Gibbs free energy method to solve the physical parameters and components of the propellant combustion products.

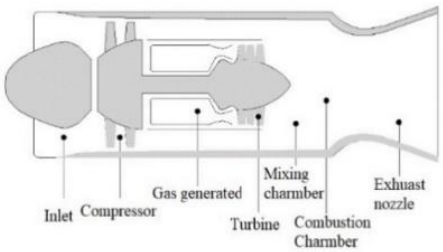


Fig. 1 Structural diagram of ATR engine

2.1 Working Fluid property

There are three kinds of working fluids in ATR engine: the air in the compressor flow path, the rich gas in turbine flow path, and the gas in combustion chamber flow path. The physical properties and components of working fluids in each flow path are very different, so it is necessary to model the physical properties of working fluids in each flow path.

Assuming that there are n components in the working medium, in which the first N1 is gaseous component and the last N2 is condensed phase component, there is N = N1 + N2. For component i, the specific heat and enthalpy at constant pressure are only determined by temperature:

$$\frac{C_{p,i}}{R}=a_1T^{-2}+a_2T^{-1}+a_3+a_4T+a_5T^2+a_6T^3+a_7T^4 \tag{1}$$

$$\frac{H_i}{RT}=-a_1T^{-2}+a_2T^{-1}\ln T+a_3+a_4\frac{T}{2}+a_5\frac{T^2}{3}+a_6\frac{T^3}{4}+a_7\frac{T^4}{5}+\frac{a_8}{T} \tag{2}$$

Under standard pressure, the standard entropy of each component can also be calculated from the fitting relationship with temperature:

$$\frac{s_i^o}{R}=-a_1\frac{T^{-2}}{2}-a_2T^{-1}+a_3\ln T+a_4T+a_5\frac{T^2}{2}+a_6\frac{T^3}{3}+a_7\frac{T^4}{4}+a_9 \tag{3}$$

The fitting coefficients a_1-a_9 can be obtained from literature [3]. For the condensed phase component, under non-standard pressure, its entropy is always equal to its standard entropy:

$$s_i=s_i^o \tag{4}$$

For gaseous components, the entropy is also affected by pressure and molar composition:

$$s_i=s_i^o-R\ln\frac{n_i}{n}-R\ln P \tag{5}$$

In the formula, n_i is the mole fraction of the i-th component in the mixture, n is the total moles of gaseous products:

$$n=\sum_{i=1}^{N1}n_i \tag{6}$$

Then the enthalpy and entropy of the mixture are:

$$h=\sum_{i=1}^{N}n_iH_i \tag{7}$$

$$s=\sum_{i=1}^{N}n_iS_i \tag{8}$$

2.2 Combustion calculation

Assuming that the combustion products of the gas generator and the combustion chamber are in a state of chemical equilibrium, and there are a total of L kinds of elements in the product, the Gibbs free energy of the product is:

$$g=\sum_{i=1}^{N}x_i\mu_i \tag{9}$$

μ_i is the chemical potential, that is, the Gibbs free energy contained in component *i*. For the condensed phase component, its chemical potential is always equal to its chemical potential at standard pressure:

$$\mu_i=\mu_i^o \tag{10}$$

For gaseous products, the chemical potential is also affected by pressure and molar composition:

$$\mu_i=\mu_i^o+RT\ln\frac{n_i}{n}+RT\ln p \tag{11}$$

For the j-th element, there is mass conservation:

$$\sum_{i=1}^{N}n_i\,a_{ij}-b_j=0 \tag{12}$$

In the formula, a_{ij} is the chemical equivalence coefficient, which is the number of moles of element j in unit mole component i; b_j is the number of moles of element j in the reactant. The condition of chemical equilibrium is to minimize the Gibbs free energy of combustion products on the premise of meeting the mass conservation of elements, so the combustion problem is transformed into a constrained optimization problem, which can be solved by Lagrange multiplier method [4] Order:

$$G = g + \sum_{j=1}^{L} \lambda_j \left(\sum_{i=1}^{N} n_i a_{ij} - b_j \right) \tag{13}$$

λ_j is the Lagrange multiplier. Then it should have:

$$\delta G = \sum_{i=1}^{N} (\mu_i + \sum_{j=1}^{L} \lambda_j a_{ij}) \delta n_i + \sum_{j=1}^{L} \left(\sum_{i=1}^{N} n_i a_{ij} - b_j \right) \delta \lambda_j = 0 \tag{14}$$

Regarding δ_{ni} and $\delta_{\lambda j}$ as independent variables, then:

$$\mu_i + \sum_{j=1}^{L} \lambda_j a_{ij} = 0 \tag{15}$$

If the temperature and pressure of the combustion products are known, then the formulas (6), (12) and (15) form an equation group containing N+L+1 equations, and the variables are n, n_i, λ_j, a total of N+L+1, so the equations are closed and can be solved to obtain the combustion product composition.

However, in most calculations of combustion reactions, the product temperature is not known. In order to solve the product temperature, an additional equation needs to be introduced. In this model, since the enthalpy of each component already includes the standard enthalpy of formation, the total enthalpy of the material before and after combustion remains unchanged, and there is an energy conservation equation:

$$h = h_o \tag{16}$$

In the formula, h is the total enthalpy of the product, and ho is the total enthalpy of the reactants. In this case, equations (6), (12), (15) and (16) form a closed equation system of order N+L+2. However, it is quite difficult to solve the equations directly. To solve this problem, it is necessary to linearize it and introduce the Newton-Raphson iterative method to solve it iteratively. For this reason, $\Delta \ln n_i$ (for gaseous products), Δn_i (for condensed phase products), $\Delta \ln n$, $\Delta \ln T$, $\pi_j = -\lambda_j / RT$ are used as correction variables, and the formula (12), (15) and (16) perform Taylor expansion, and omit higher-order terms, there are:

$$\Delta \ln n_i - \sum_{j=1}^{L} a_{ij} \pi_j - \Delta \ln n - \frac{H_i}{RT} \Delta \ln T = -\frac{\mu_i}{RT} \quad (i=1,..N1) \tag{17}$$

$$-\sum_{j=1}^{L} a_{ij} \pi_j - \frac{H_i}{RT} \Delta \ln T = -\frac{\mu_i}{RT} (i=1,..N2) \tag{18}$$

$$\sum_{i=1}^{N1} a_{ij} n_i \Delta \ln n_i + \sum_{i=1}^{N2} a_{ij} \Delta n_i = \sum_{i=1}^{N} n_i a_{ij} - b_j (j=1,...L) \tag{19}$$

$$\sum_{i=1}^{N1} n_i \Delta \ln n_i - n \Delta \ln n = n - \sum_{i=1}^{N1} n_i \tag{20}$$

$$\sum_{i=1}^{N1} \frac{n_i H_i}{RT} \Delta \ln n_i + \sum_{i=1}^{N2} \frac{H_i}{RT} \Delta n_i + \left(\sum_{i=1}^{N} \frac{n_i C_{p,i}}{R} \right) \Delta \ln T = \frac{h_o - h}{RT} \tag{21}$$

The direct solution of equations (17) to (21) still requires a large amount of calculation, and the order of the equations can be reduced to simplify the solution process. Using equation (17) to eliminate $\Delta \ln ni$ in the equations, we get:

$$\sum_{j=1}^{L} \sum_{i=1}^{N1} a_{ik} a_{ij} n_i \pi_i + \sum_{i=1}^{N1} a_{ik} \Delta n_i + \left(\sum_{i=1}^{N1} a_{ik} n_i \right) \Delta \ln n + \left(\sum_{i=1}^{N1} \frac{a_{ik} n_i H_i}{RT} \right) \Delta \ln T = \sum_{i=1}^{N} n_i a_{ik} - b_k + \sum_{i=1}^{N1} \frac{a_{ik} n_i \mu_i}{RT} (k=1,...L) \tag{22}$$

$$\sum_{j=1}^{L} a_{ij} \pi_j + \frac{H_j}{RT} \Delta \ln T = \frac{\mu_i}{RT} (i=1,..N2) \tag{23}$$

$$\sum_{j=1}^{L} \sum_{i=1}^{N1} a_{ij} n_i \pi_j + \left(\sum_{i=1}^{N1} n_i - n \right) \Delta \ln n + \left(\sum_{i=1}^{N1} \frac{n_i H_i}{RT} \right) \Delta \ln T = n - \sum_{i=1}^{N} n_i + \sum_{i=1}^{N1} \frac{n_i \mu_i}{RT} \tag{24}$$

$$\sum_{j=1}^{L} \left(\sum_{i=1}^{N1} \frac{a_{ik} n_i H_i}{RT} \right) \pi_j + \sum_{i=1}^{N2} \frac{H_i}{RT} \Delta n_i + \left(\sum_{i=1}^{N1} \frac{n_i H_i}{RT} \right) \Delta \ln n + \left[\sum_{i=1}^{N1} \frac{n_i C_{p,i}}{R} + \sum_{i=1}^{N1} \frac{n_i H_i^2}{R^2 T^2} \right] \Delta \ln T = \frac{h_o - h}{RT} + \sum_{i=1}^{N1} \frac{n_i H_i \mu_i}{R^2 T^2} \tag{25}$$

Equations (22) to (25) form a linear equation system of order L+N2+2, in which the variables to be determined are π_j, Δn_i, $\Delta \ln n$, and $\Delta \ln T$, and the variables are introduced into equation (17) to get the $\Delta \ln n_i$ of each gaseous component. After solving, use the following iterative format to update the calculation results:

$$ln\, n_i^{(k+1)} = ln\, n_i^{(k)} + \alpha^{(k)} (\Delta\, ln\, n_i)^{(k)} (i=1,..N1) \tag{26}$$

$$n_i^{(k+1)} = n_i^{(k)} + \alpha^{(k)} (\Delta n_i)^{(k)} (i=1,..N2) \tag{27}$$

$$ln\, n^{(k+1)} = ln\, n^{(k)} + \alpha^{(k)} (\Delta\, ln\, n)^{(k)} \tag{28}$$

$$ln\, T^{(k+1)} = ln\, T^{(k)} + \alpha^{(k)} (\Delta\, ln\, T)^{(k)} \tag{29}$$

In the formula, k represents the k-th iteration, and α is the iteration step size correction factor, which is used to prevent the iteration process from diverging due to too large a step size. The convergence conditions set in this article are:

$$\frac{n_i |\Delta\, ln\, n_i|}{\sum_{i=1}^{N} n_i} \leq 1\times10^{-6} (i=1,..N1) \tag{30}$$

$$\frac{|\Delta n_i|}{\sum_{i=1}^{N} n_i} \leq 1\times10^{-6} (i=1,..N2) \tag{31}$$

$$\frac{n |\Delta\, ln\, n|}{\sum_{i=1}^{N} n_i} \leq 1\times10^{-6} \tag{32}$$

$$|\Delta\, ln\, T| \leq 1\times10^{-6} \tag{33}$$

When the calculation result satisfies formulas (30) to (33), the iterative process stops. At this time, if the calculated mole fraction of condensed phase component is negative, it will be excluded from the calculation of this combustion product. List the components and restart the iteration until a reasonable result is obtained and the combustion calculation is completed.

3. Model validation

In order to verify the rationality of the calculation results of the working fluid model, calculate the temperature and composition of the combustion products of methane and oxygen reaction under different oxygen-fuel ratio [5], and compare the calculation results with the CEA program developed by NASA for calculating the equilibrium products of complex chemical reaction, in which the combustion pressure is set to 1.5MPa and the reactant temperature is 300K.

A. When the oxygen-fuel ratio of methane/oxygen is 0.3, the calculation results of physical parameters and components of combustion products are shown in the table:

Table 1. Comparison of physical parameters and product components

Physical parameters and components Mass fraction calculation results	Calculation results of this model	CEA calculation results
T (k)	922.4362	922.54
h (kJ/kg)	-3572.5738	-3573.48
S (kJ/Kg/K)	13.9025	13.9017
G (kJ/kg)	-16403.2539	-16403.3
CH_4	0.48855321	0.48845
CO	0.03621658	0.03619
CO_2	0.05182165	0.05177
C_2H_6	0.00098958	0.00010
H_2	0.04881259	0.04882
H_2O	0.19420105	0.19418
C (gr)	0.18510121	0.18409

B. When the oxygen-fuel ratio of methane / oxygen is 1.2, the calculation results of physical properties and components of combustion products are shown in the table:

Table 2. Comparison of physical parameters and product components

Physical parameters and components Mass fraction calculation results	Calculation results of this model	CEA calculation results
T (k)	1317.8542	1317.14
h (kJ/kg)	-2111.1738	-2110.91
S (kJ/kg/K)	15.8025	15.7094
G (kJ/kg)	-22800.4258	-22802.3
CH_4	0.0159532	0.01685
CO	0.7181658	0.72186
CO_2	0.06582165	0.06654
C_2H_6	0.00098958	0.00010
H_2	0.09881259	0.09932
H_2O	0.09420105	0.09543

It can be seen from the data in the above two tables that the calculation results of this model are approximately consistent with those of CEA. It is reasonable and feasible to use this model to calculate the physical properties of ATR engine working fluid.

4. Requirements for propellant selection

The thermodynamic properties of the primary gas produced by propellant combustion have an important impact on the secondary combustion in the combustion chamber. Combined domestic and foreign related research on the characteristics of ATR engine propellants [6, 9], This paper mainly makes the following four requirements for the propellant, as shown in Table 3.

Table 3. ATR engine propellant requirements

requirements	reasons
The primary gas must have a lower molar mass and specific heat ratio	The lower the molar mass and specific heat ratio of the gas, the more beneficial it is to increase the specific power of the turbine.
The primary gas must have a suitable gas temperature	The higher the turbine inlet temperature, the higher the requirements on the turbine blade design, turbine materials, etc. and the reliability of the turbine operation is reduced.
The working fluid driving the turbine must have good energy characteristics	The primary gas with higher energy is beneficial to the secondary combustion of the combustion chamber and improve engine performance.
The gas must be clean and free of particles	Solid particles and corrosive gases can damage the turbine blades, affect the aerodynamic characteristics of the turbine blades and the reliability of the rotating parts.

5. Comparative analysis of results

In this paper, methane/oxygen, ethanol/oxygen, propane/oxygen and kerosene/oxygen are selected as the spare propellant of ATR engine gas generator. Using the calculation model established in this paper, the propellant is analyzed and selected according to the requirements of ATR engine.

5.1 Gas molar and specific heat ratio

The molar mass and specific heat ratio of combustion products in the temperature range of 1000-1500k are calculated; The change of molar mass of fuel gas with temperature is shown in Fig. 2: it can be seen from the figure that the molar mass of primary fuel gas produced by the same propellant decreases gradually with the increase of temperature, and then increases slowly after a certain

temperature. Comparing the four propellants, the molar mass of primary gas produced by methane/oxygen combustion at the same temperature is the smallest, which is better than the other three propellant combinations.

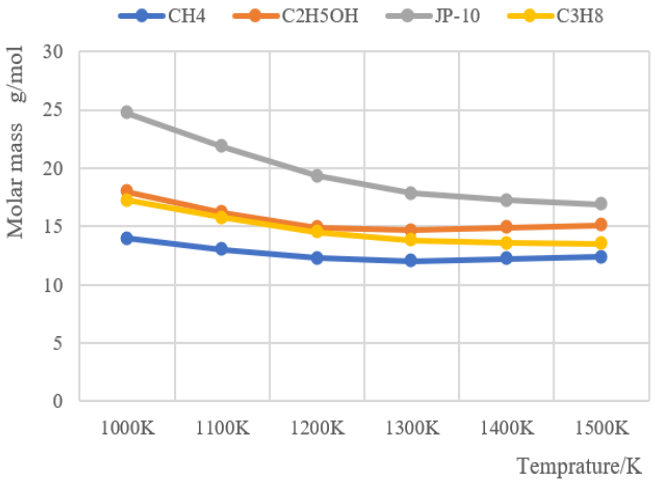


Fig. 2 Molar mass of gas

The change of specific heat ratio of fuel gas with temperature is shown in Fig. 3. It can be seen from the figure that the specific heat ratio of primary fuel gas produced by kerosene/oxygen combustion is the smallest at the same temperature.

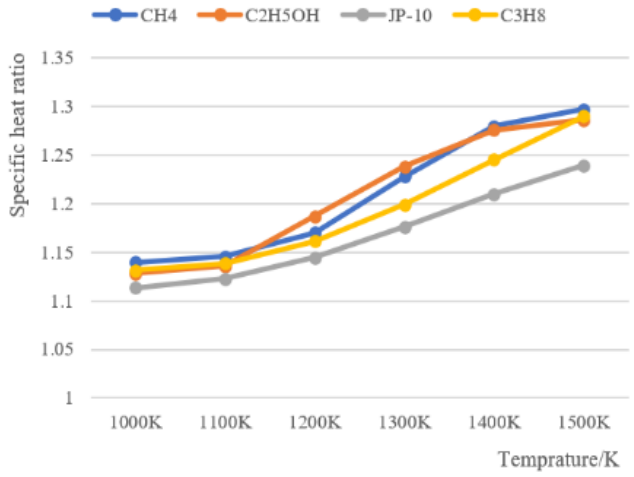


Fig. 3 Gas specific heat ratio

5.2 The gas composition

The mass fractions of the combustion products of the four propellants obtained by using the ATR engine working fluid calculation model are shown in Fig. 4-Fig. 7. It can be seen from the figure that when the primary fuel gas temperature of the combustion of methane/oxygen and ethanol/oxygen propellant reaches 1000K-1200K, 1.2%~19.8% of solid C (gr) particles are generated.When the temperature is higher than 1200k, neither of these two propellants will generate solid C (gr) particles. Therefore, in terms of the cleanliness of primary gas, methane/oxygen propellant is the best, followed by ethanol/oxygen, Finally, kerosene/oxygen.

In order to facilitate the secondary ignition and efficient combustion of combustion chamber, the more combustible gaseous components, the better. It can be seen from the figure that when the temperature is higher than 1200k, more than 80% of the combustible components in the primary gas produced by methane/oxygen propellant can be used for secondary combustion, and ethanol/oxygen can also produce more than 70% of combustible gas components. Therefore, the performance of methane/oxygen propellant combination is obviously better than other propellant combinations.

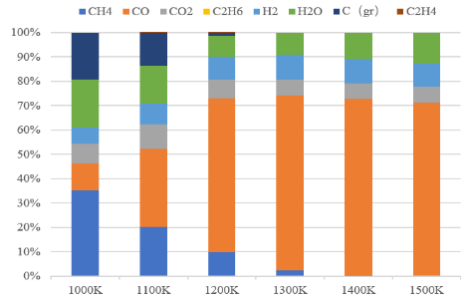


Fig. 4 CH_4 / O_2 combustion products

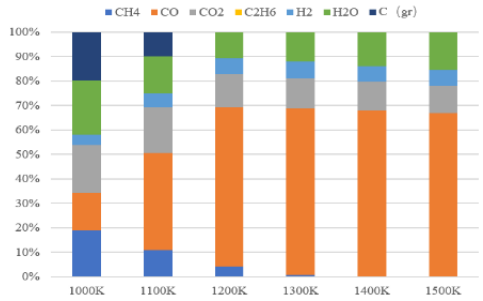


Fig. 5 C_2H_5OH/ O_2 combustion products

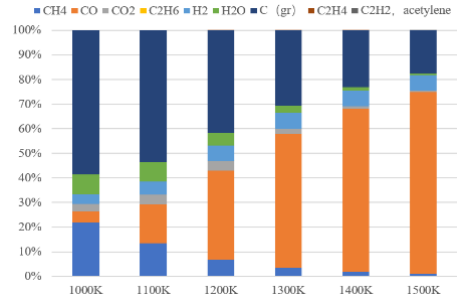


Fig. 6 C_3H_8 / O_2 combustion products

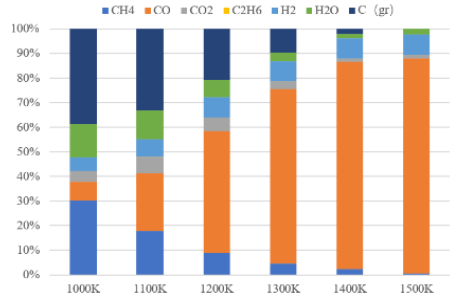


Fig. 7 JP-10/O_2 combustion products

Considering the overall design of the ATR engine, The specific impulse and specific thrust of the ATR engine using methane and ethanol two propellants are not much different, but the density of the two propellants is quite different. In terms of density, ethanol used by ATR engines is better than methane, and ethanol as a normal temperature fuel does not have the problem of low-temperature liquefaction storage [10].

6. Conclusion

According to the ATR engine propellant selection requirements in Table 3 and comprehensive consideration of the impact of the propellant on the overall performance of the ATR engine and the difference in propellant density and storage conditions, ethanol/oxygen propellant was finally selected as the ATR engine propellant.

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