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Chemical non-equilibrium flow analysis of H_2 fueled scramjet nozzle

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ABSTRACT

A numerical analysis of the chemical non-equilibrium phenomena in a scramjet nozzle has been performed using CHEMKIN software. Different operating conditions of the Hy-shot scramjet nozzle were simulated and analyzed. Three chemical status, frozen flow, equilibrium flow, and non-equilibrium flow, were tested and compared to demonstrate the chemical reaction effect on nozzle flow field. The real non-equilibrium flow simulation result is between those of the two limiting cases: frozen flow and equilibrium flow, and is closer to that of frozen flow. With complete combustion condition at nozzle inlet, the radical recombination reaction releases tremendous amount of heat and this heat is mainly used to increases gas temperature and has only slight increasing effect on thrust. With incomplete combustion condition at nozzle inlet, both combustion reaction and radical recombination occur in the nozzle, the effect of reaction heat release on thrust depends on the degree of combustion completeness at nozzle inlet, it could increase thrust tremendously compared to frozen flow.

1. Introduction

Scramjet propulsion is a promising technology capable of reaching hypersonic speed. Nozzle is an important component of Scramjet engine, which is responsible for producing a major part of the thrust [1]. Chemical reaction inside a nozzle comes from two sources: 1, the unburned fuel in combustion chamber (if there is any) will continue their combustion reaction; 2, the dissociated species of combustion product, i.e., radicals, will recombine due to the rapid temperature drop inside the nozzle. Both reactions are with finite chemical reaction rate. However, due to large computational cost associated with finite rate reaction (especially for heavy hydrocarbon fuels), the simplified approaches without reaction rate calculation are usually used: 1, chemically frozen flow: the gas composition in the nozzle is chemically frozen, i.e. there is no reaction and heat release inside the nozzle; 2, chemical equilibrium flow: the gas adjusts its composition according to local temperature and pressure instantly. The chemically frozen and chemical equilibrium flows correspond to the lower and upper limits of reaction where reaction rate is zero and infinite respectively; they do not require the slow and complicated finite rate chemical reaction calculation. Non-equilibrium flow is the real condition inside the nozzle and it is between the two limits.

The non-equilibrium nozzle flow requires three-dimensional simulation with finite rate reaction; this method is prohibitive because of the huge computational resource requirement, thus simple one-dimensional simulation is often used for

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nozzle non-equilibrium flow simulation. One-dimensional nozzle simulations with finite rate chemistry have been performed by Stalker et al. [1], Sangiovanni et al. [2], Ha [3], and Thomas et al. [4], to evaluate the role of non-equilibrium chemistry on the performance of hypersonic nozzle. Different from the previous researches, this paper focuses on two new aspects: 1, the quantitative relationship among non-equilibrium flow, frozen flow, and equilibrium flow; 2, the influence of combustion incompleteness on the nozzle flow field.

2. Numerical method

The PLUG code of CHEMKIN is used to simulate the expansion process in hypersonic nozzle. The PLUG code solves the one-dimensional ordinary differential equations for an internal flow with variable cross section area. In the axial direction, the PLUG code only considers convection and ignores the axial diffusion; due to high flow speed, the axial convection is much more than the axial diffusion, this treatment is consistent with the real physics of the hypersonic nozzle flow.

$$\rho u\frac{dA}{dx} + \rho A\frac{du}{dx} + uA\frac{d\rho}{dx} = 0 \tag{1}$$

$$A\frac{dP}{dx} + \rho uA\frac{du}{dx} = 0 \tag{2}$$

$$\rho uA\frac{dY_k}{dx} = W_k A\dot{\omega}_k \tag{3}$$

$$\rho uA\left(\bar{C}_p\frac{dT}{dx} + u\frac{du}{dx}\right) = -\rho uA\sum_k h_k^o\frac{dY_k}{dx} \tag{4}$$

$$P = \sum_k \rho\frac{Y_k}{W_k}RT \tag{5}$$

where ρ is the density; u is the axial velocity of the gas; A is the cross-section area of the nozzle; P is the pressure; R is the universal gas constant; T is the gas temperature; $\bar{C}_p$ is the mean specific heat capacity; W_k, Y_k, and h_k^o are the molecular weight, the mass fraction, and the enthalpy of formation of species k respectively; $\dot{\omega}_k$ is the reaction rate of species k. The 12 species and 21 steps H_2/air UCSD mechanism [5] is used for the non-equilibrium flow simulation. The reaction rates of all reactions are multiplied by 10^8 for the equilibrium flow simulation (normally, the local equilibrium condition is calculated with equilibrium constant, no chemical reaction calculation is needed; the calculation with infinitely fast chemistry will also give out equilibrium result). The reaction rates of all reactions are 0 for the frozen flow simulation.

The fuel (H_2) and oxidizer (air) mixing, shock wave compression, and turbulent combustion are coupled in combustion chamber of scramjet engine; therefore, it is hard to know the exact nozzle inlet condition. In this study, the actual coupling process before the nozzle inlet is divided into an assumed serial process: fuel and air are uniformly mixed after H_2 is injected into the combustion chamber, the uniform premixture (equivalent ratio is Φ) is gradually pressurized and heated to P_{in} and T_1 through shock waves, then the temperature of mixture rises to T_{in} by constant pressure combustion (complete or incomplete combustion). When H_2/air mixture is completely combusted at nozzle inlet, the equilibrium composition Y_{in} and temperature T_{in} of combustion product are calculated using the EQUIL package of CHEMKIN with the initial temperature of T_1, pressure of P_{in}, and equivalent ratio Φ. When H_2/air mixture is incompletely combusted at nozzle inlet, the transient homogeneous combustion history of the mixture needs to be known and is calculated with the SENKIN package of CHEMKIN. From the results of SENKIN, we can define the degree of combustion completeness based on the temperature history, $\alpha_T=(T-T_{initial})/(T_{equil}-T_{initial})$. The subscript "initial" denotes the initial state, i.e., the state at $t=0$; subscript "equil" denotes the final state of complete combustion, i.e., the final equilibrium state. If α_T is specified, the corresponding gas temperature and composition molar fraction can be obtained from the SENKIN simulation result and then are used in the PLUG simulation as the inlet condition. For quantitative description of the level of non-equilibrium status, a degree of equilibrium is defined as $\Gamma_\varphi=(\varphi_{non\text{-}equil}\text{-}\varphi_{frozen})/(\varphi_{equil}\text{-}\varphi_{frozen})$, where φ is the flow variable such as temperature, pressure, velocity, or molar fraction of species. Since frozen flow are often used to calculate nozzle performance, an augmentation percentage is also defined here $\varepsilon_\varphi=(\varphi_{non\text{-}equil}-\varphi_{frozen})/\varphi_{frozen}$ to reflect the nozzle performance gain compared to frozen flow.

Hyshot scramjet nozzle is chosen as the object [6], whose geometry is shown in Fig. 1.