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Numerical study of test gas vitiation effects on hydrogen-fueled scramjet combustion

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Abstract: The effects of major vitiated species (H_2O and CO_2) and minor vitiated species (H , OH and O radicals) produced by combustion air preheater on ignition and combustion of hydrogen-fueled scramjet were numerically investigated. Firstly, kinetic analyses with CHEMKIN SENKIN code were conducted to evaluate the effects of contamination on the ignition delay times of hydrogen fuel over a range of temperature and pressure variations. Then numerical simulation of a three-dimensional reacting flow in hydrogen-fueled scramjet combustor was performed. The two-equation shear stress transport $\kappa\text{-}\omega$ turbulence model was used for modeling turbulence and 33 reactions finite-rate chemistry was used for modeling the H_2 /air kinetics. The results show that: free radical species such as H , O , and OH may significantly promote the ignition process of hydrogen-air at relatively low initial temperature and pressure. However, H_2O and CO_2 have inhibition effects on the ignition process. Under the same conditions, H_2O has more effective inhibition effects than CO_2 . The temperature and pressure rise due to combustion are lower in the air vitiated with H_2O and CO_2 because of their higher heat capacities and more dissociation. Combustion efficiency and thrust calculated for vitiated air case are lower than clean air case. These results indicate the importance of accounting for vitiation effects when extrapolating performance data from ground test to flight demonstration.

Key words: scramjet; contaminant; ignition; supersonic combustion; preheater

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Introduction

The development and refinement of scramjet engine system rely heavily on ground testing. In ground test, the air must be heated to simulate hypersonic flight conditions, for example, the temperature, pressure and Mach number at the entrance to a combustor. Several methods of air heating, including thermal storage heating, arc heating, shock tube heating, and combustion heating, are used to generate the high enthalpy test gas. The combustion air preheating is the most widely used method of obtaining high enthalpy air based on operating cost and ease of operation. However, the combustion major products H_2O or H_2O and CO_2 and minor products H , OH and O radicals cause the air to become vi-

tiated. These vitiated species change the bulk thermodynamic and chemical kinetic properties of the test gas^[1]. This creates uncertainties when extrapolating the ground-test results to flight because of the different properties of the air. It is necessary to understand the effects of these species contaminants on the ignition and combustion in the hydrogen-fueled scramjet combustor.

Many numerical and experimental works have reported the effects of air containing H_2O , CO_2 and radicals on hydrogen-air combustion^[2-5]. Rogers et al. studied the vitiation effects using one-dimensional kinetic (ODK) code^[3]. They reported the radicals, such as H , OH and O , enhance the ignition processes generally under certain conditions. The ignition de-

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lay time can lead to a tenfold reduction at moderately low temperatures near atmospheric pressure. They also reported H_2O and CO_2 increase the ignition delay time significantly at static temperature near 1000 K.

Han and Sung studied the effects of vitiation on ignition in supersonic laminar mixing layer by two-dimensional numerical simulation. It was found that the ignition distance decreases effectively in the transition regime with the addition of H, OH, and O radicals, while it is less effective in the high-pressure regime^[4]. Additional calculation examining the individual effects of O and OH showed the same trend as that of H vitiation. This is different from the Stephen et al. study, where they had shown that the addition of H radical has a much greater decrease in ignition distance than that of the O and OH radicals^[5].

The presence of H_2O and CO_2 in vitiated air will affect the thermodynamic properties of the test gas^[6]. Their higher heat capacities have been shown to lower the maximum temperature and pressure of hydrogen-fueled scramjet combustion. Mitani et al. conducted a set of experimental studies with vitiated air heated by hydrogen-air combustion and with dry air heated using a storage heater^[7-8]. Significant differences in self-ignition and combustion performance between the dry and vitiated air were observed. Unfortunately, in these tests the influence of major and minor vitiation species could not be isolated because the combustion heater produces both contaminants. Recently, experiments at the University of Virginia have shown the combustor pressures decreased when H_2O and CO_2 added to the electrically heated clean air. The H_2O and CO_2 have a significant effect on combustor mode transition also^[9-10].

In general, the experimental studies are difficult and expensive and the results are limited by the experimental facilities and measurement technology. All the numerical studies mentioned above are based on one or two-dimensional flow models and relatively simple flow configuration.

The numerical results are not validated by experiment, and they may not be credible in a true scramjet model. In the present work, we study a true dual-mode scramjet combustion flow field, which is a full complex three-dimensional flow model including supersonic mixing, finite-rate reactions with detailed reaction mechanism. The influence of major and minor contaminants on the ignition and combustion performance are examined and compared with the experimental data. This paper begins with a description of the dual-mode scramjet combustor, together with a description of the computational methodology. The effects of vitiation on the performance of ignition are firstly calculated by using the SENKIN code in the CHEMKIN package^[11]. The effects of H_2O and CO_2 contaminants on the combustion performance are investigated using the commercial software FLUENT.

1 Computational methodology

1.1 Combustor geometry

The dual-mode scramjet combustor considered in the present work is shown in Fig. 1^[9]. It consists of a constant area rectangular isolator, a rectangular combustor including an unswept 10° compression ramp, and an extender section with a 2.9° divergence on the injector-side wall. The ramp height H is 0.64 cm and is used to normalize all dimensions. The inlet of the isolator is $4H \times 6H$. The total pressure and temperature at the inlet of the isolator are 330 kPa and 1200 K respectively. Hydrogen is injected at Mach number 1.7, normal to the ramp base.

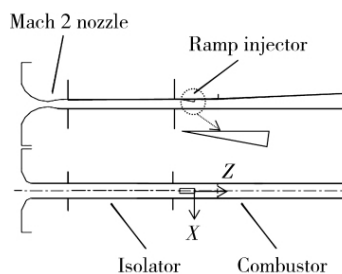


Fig. 1 Schematic of dual-mode scramjet combustor^[9]

1.2 Solution methodology

In the present work, compressible and turbulent Favre-averaged Navier-Stokes equations are solved along with species conservation equations. The calculations have been carried out using two-equation shear stress transport $\kappa\omega$ turbulence model (SST $\kappa\omega$)^[12]. The SST $\kappa\omega$ model is a hybrid of the standard $\kappa\epsilon$ and $\kappa\omega$ models. It uses a $k\omega$ formulation in the inner boundary layer and a $k\epsilon$ formulation in the free stream. This characteristic integrates the near-wall robustness of the $\kappa\omega$ models with the capabilities of the $k\epsilon$ model away from the walls. This SST $\kappa\omega$ models with default model constants ($\alpha_\infty^* = 1$, $\alpha_\infty = 0.52$, $\beta_\infty^* = 0.09$, $R_\beta = 8$, $\xi^* = 1.5$) has been used here.

A detailed reaction mechanism with 10 species (H_2O , H_2 , O_2 , CO_2 , O , H , OH , HO_2 , H_2O_2 , N_2) and 33 reactions is necessary in order to capture the effects of vitiated species^[13]. The third body efficiencies for the recombination reactions have also been taken from the mechanism. The viscosity and c_p of the mixture have been evaluated using ideal-gas mixing laws. For the individual species in the mixture these properties have been evaluated using kinetic theory and fifth order polynomials in temperature respectively. The coupled solver has been used with explicit time stepping. All of the calculations have been carried out using second-order accurate discretization.

1.3 Boundary conditions

At the combustor inlet where the flow is supersonic, the static and stagnation pressure, stagnation temperature and species mass fractions are specified. The O_2 mole fraction in the air is kept at 21% throughout the study. The mass-flow-inlet boundary conditions are used for H_2 inlet. A turbulence intensity and hydraulic diameter setting is used to describe the turbulence condition. The outlet of the combustor where the flow is supersonic, all the flow variables are determined from the interior of the domain by extrapolation. All the walls have been

assumed to be adiabatic and enhanced wall functions have been used. The initial grid was consisted of 580 000 hexahedron cells. This grid was adapted further based on the gradients of reacting species so as to resolve the supersonic combustion phenomenon in the flow field accurately. The final grid with 820 000 cells has been taken for the subsequent calculations. The maximum value of wall y^+ on this grid is below 30.

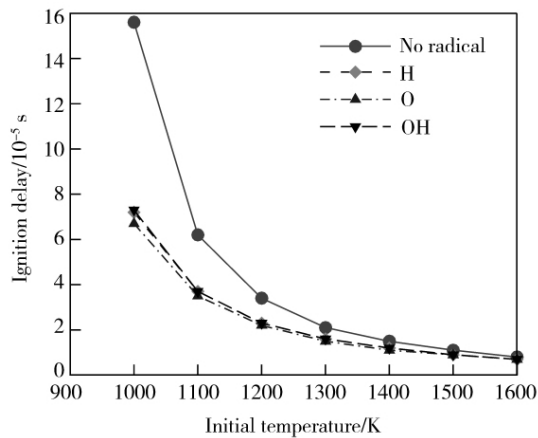
2 Results and discussion

2.1 Effects on the ignition delay

The vitiation effects on the hydrogen-air ignition are firstly investigated by CHEMKIN SENKIN code firstly. The ignition time will be computed at the point where the rate of change of temperature with respect to time is the largest (Temperature Inflection Point criteria).

The system pressure is kept at 0.1 MPa, the radical mole fraction is 0.001%, and the H_2O and CO_2 mole fraction is 10%. Fig. 2(a) shows the ignition delays with and without radicals. It is seen from Fig. 2(a) that the ignition delay time decreases with radicals addition over the temperature range investigated. The ignition enhancement of radicals strongly appeared at low initial temperature. It is less effective in the high temperature regime. The ignition response curves due to the O , H and OH are essentially the same, except that O vitiation exhibits a stronger effect on ignition promotion in low temperature regime. Fig. 2(b) displays the effect of added H_2O and CO_2 on ignition delay time. The presence of H_2O and CO_2 inhibit the ignition at low temperature due to their large third body efficiencies with respect to nitrogen or oxygen in the chain termination reaction $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$. This reaction depletes highly reactive H atoms and produces unreactive species HO_2 , so the chain branching reaction $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$ is retarded, and the ignition delay of the hydrogen oxidation process is lengthened. At static temperature is above 1100 K, the H_2O and CO_2 have progressively less effects on ignition delay because the critical kinetics become substantially

faster than mixing rate. Under the same conditions, the inhibition effect of CO_2 is weaker than for H_2O because the third body efficiency of CO_2 is only about 25% of that H_2O ^[9].



(a) Vitiation with radicals

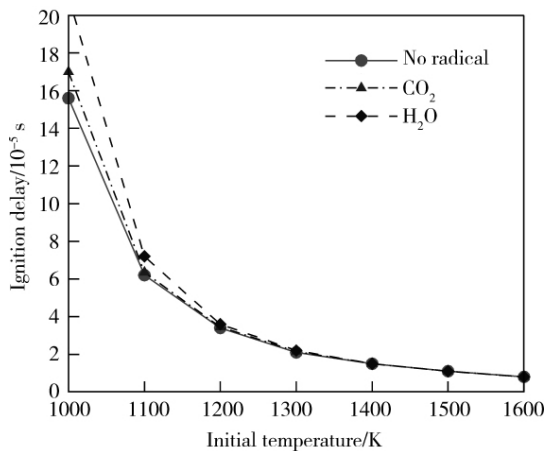
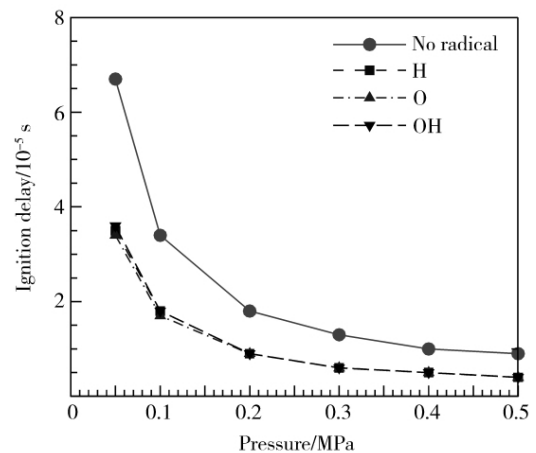
(b) Vitiation with H_2O and CO_2

Fig. 2 Vitiation effects on the ignition delay times at various system temperature

Fig. 3 shows the effects of vitiation on ignition delays over a wide range of ambient pressure. It is seen from Fig. 3(a) that the ignition delay time decreases with radicals addition over the pressure range investigated. The ignition enhancement of radicals is more effective at lower pressure. Fig. 3(b) shows the H_2O and CO_2 have inhibition ignition effects at higher pressure. The retardation effect on ignition does not appear in the low pressure regime, since the chain termination reactions: $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$, $\text{H} + \text{HO}_2 + \text{M} \rightarrow \text{H}_2 + \text{O}_2 + \text{M}$ are termolecular reactions. In addition, for H_2O vitiated case,

Fig. 3(b) demonstrates that the response of ignition delay to the system pressure variation is non-monotonic. The ignition delay time is minimal at pressure about 0.4 MPa. The pressure about 0.4 MPa is called as crossover pressure. This is consistent with the non-monotonic behavior resembling the classical homogeneous explosion limit of the hydrogen-oxygen system^[14]. As the system pressure is on the left side of the crossover pressure, the branching reaction $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$ is the controlling chemistry. As the system pressure is on the right side of the crossover pressure, the pressure-sensitive terminating mechanism $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$ is the controlling chemistry.



(a) Vitiation with radicals

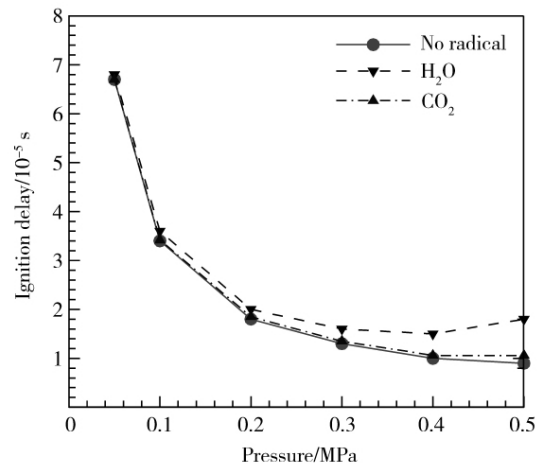
(b) Vitiation with H_2O and CO_2

Fig. 3 Vitiation effects on the ignition delay times at various system pressure

2.2 Effects of the addition of H_2O and CO_2 on combustion performance

In this section, the effects of the addition of H_2O and CO_2 on combustion performance of a dual-mode scramjet combustor are studied for four cases: clean inlet air, air vitiated with 3 mole percent H_2O , air vitiated with 9% H_2O , and air vitiated with 9% CO_2 . The combustion temperature and pressure are compared for various inlet air conditions at a fixed fuel equivalence ratio 0.26.

2.2.1 Effect of H_2O

Large amounts of H_2O are present in hydrogen-fueled combustion heater. And if the hydrocarbon fuel is used, the CO_2 is formed. The vitiation of H_2O and CO_2 can alter the thermodynamic (increasing specific heats and changing the molecular weights) and chemical kinetic properties (react with other species) of the test gas. Fig. 4 shows the specific heats variations of different species over a wide range of temperature. It is clearly demonstrated that the specific heats of H_2O and CO_2 are higher than that of N_2 . The gas with higher specific heat will tend to absorb more enthalpy and thereby suppress the temperature and pressure rise produced by combustion. The mass capture and thrust may be affected by the alteration of the molecular weight.

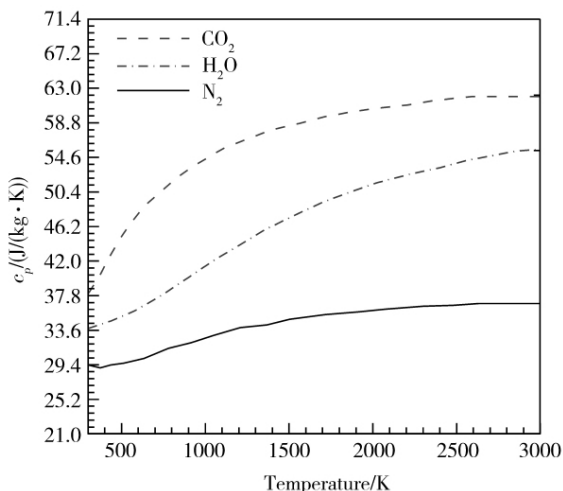


Fig. 4 Specific heat

Fig. 5 shows the contours of Mach number

on the centre plane of the scramjet combustor with clean air and air vitiated with 3% H_2O . For clean air, the heat release of combustion leads to thermally choked along the injection wall. The shock trains are moved upstream of the ramped fuel injector. The boundary layer separation occurred at $Z/H = -20$. The flow upstream the fuel injector is approximately subsonic. Fig. 5 (b) clearly shows the shock trains are moved downstream with 3% H_2O addition. The inflow of the combustor is supersonic clearly. The presence of vitiates may cause mode transition to occur at some given conditions. One of the reasons for the mode transition in the vitiated air case is the higher heat capacities for H_2O .

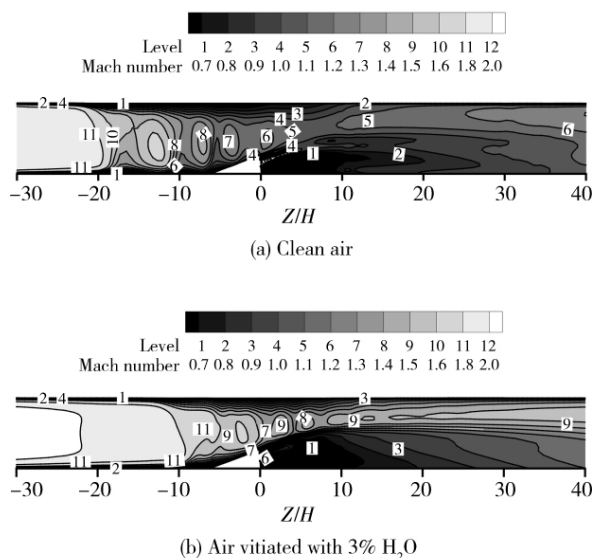


Fig. 5 Mid-plane Mach-number contours

The variation of the mass-weighted static temperature along the entire length of the combustor is shown in Fig. 6. Trends in the static temperature distribution are almost the same for clean air and air vitiated with H_2O . However, there are some substantial differences in the temperature level. The temperature in vitiated air case is lower than the clean air case. The maximum temperature difference is about 100 K. This is because the higher specific heat for H_2O . The air vitiated with H_2O could absorb more heat produced by combustion than that of clean air. On the other hand, the dissociation of some of

the additional H_2O in the vitiated air causes the lower temperature. Fig. 7 shows the axial distribution of the mole concentration of OH radical, the trends in the distribution of H, O radicals are similar. It is seen that more free radicals produced by additional dissociation of H_2O . However, no significant differences in temperature level are noted between the vitiated air with 3% H_2O and vitiated air with 9% H_2O . Therefore, the vitiation effects of H_2O on combustion temperature have nonlinear characteristics. This indicates that mixed mode heating, where a combination of combustion and resistance preheating

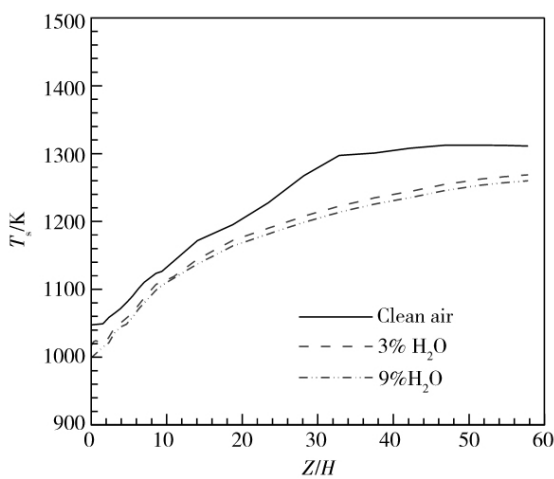


Fig. 6 Combustor axial temperature distribution for various amounts of H_2O

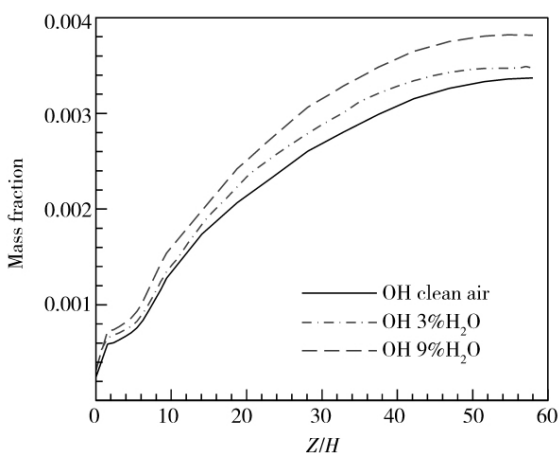


Fig. 7 Combustor axial mole fraction of OH for various amounts of H_2O

is used, may not offer a significant advantage over combustion heating alone.

Fig. 8 shows the variations of the pressure on the bottom wall of the combustor, normalized by the combustor inlet static pressure p_{ref} . The pressure rises significantly upstream of the compression ramp for all cases. There is a significant reduction of pressure for vitiated air cases due to lower static temperature rise. At the same time, the pressure rise location moves downstream from $-20H$ to $-10H$ for vitiated air cases. However, the differences in pressure with 3% H_2O and 9% H_2O are less obvious. The vitiation effects of H_2O on combustion pressure have also nonlinear characteristics^[10].

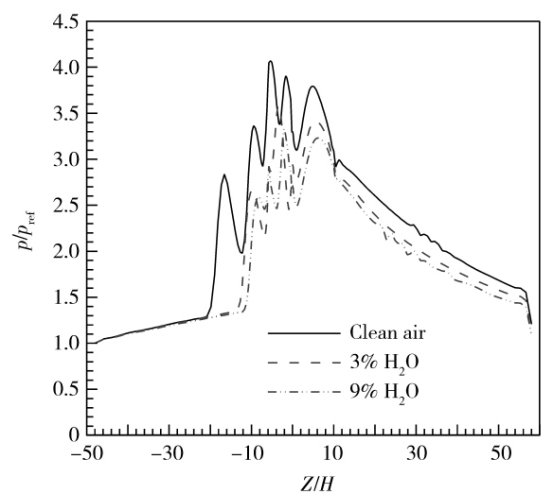


Fig. 8 Combustor axial pressure distribution for various amounts of H_2O

2.2.2 Effect of CO_2

The CO_2 are present in vitiated air when hydrocarbon fuel is used. Fig. 9 compares the wall pressure distribution along the combustor with three cases: clean air, air vitiated with 9% CO_2 and air vitiated with 9% H_2O . It is seen that the addition of CO_2 reduced the wall pressures more than H_2O . The peak value of pressure decrease relative to the clean air case is 21% with 9% CO_2 and 16% with the same amounts of H_2O . This result is in conformity with that of Ref. [10]. It is because the specific heat of CO_2 is larger than that of H_2O ; CO_2 could absorb more heat

released by combustion. The temperature and pressure produced by combustion is lower significantly with addition of CO₂. On the other hand, H₂O accelerate the termolecular reaction, H + O₂ + M → HO₂ + M, which is followed by a series of exothermic reactions that lower the high heat capabilities influence. Therefore, the CO₂ is more effective at reducing the pressure produced by combustion than H₂O under the same conditions.

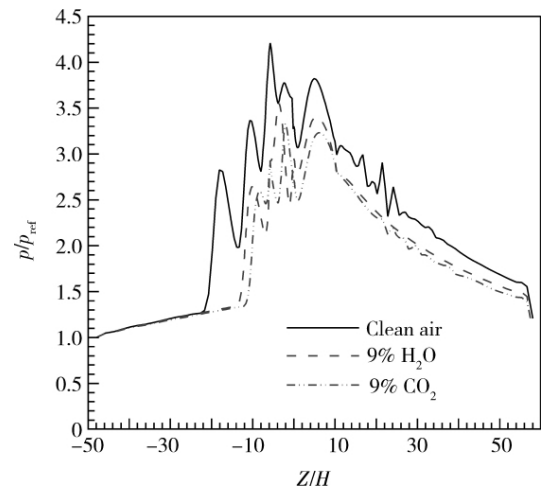


Fig. 9 Combustor axial pressure distribution for 9% H₂O and 9% CO₂

2.2.3 Effect on the overall performance

In this section, two metrics for assessing the overall vitiation effects, namely, the combustion efficiency and thrust are analyzed. In scramjet, the combustion efficiency demonstrates the regions of heat release and completeness of the combustion; it is one of the key performance metrics used to evaluate a scramjet.

The combustion efficiency is calculated and compared with and without contaminants addition. In present work, combustion efficiency is calculated based on the amount of fuel H₂ that is consumed completely. The amount of H₂ consumed is calculated from the amount of H₂O formed because the H₂ can be formed in the intermediate reactions in the multi step chemistry model^[15]. The combustion efficiency on a given constant Z plane is given as

$$\eta_c = \frac{\int_{\text{inlet}}^x \frac{1}{9} \alpha_{\text{H}_2\text{O}} \rho u dA}{\sum_x m_{\text{fuel}, \text{in}}}$$

where, the α is the local mass fraction of water vapor and the multiplicative constant in the numerator accounts for the fact that 1 kmol(18 kg) of H₂O is produced from the combustion of 1 kmol(2 kg) of fuel.

Fig. 10 shows the combustion efficiency for the case of H₂O addition in the vitiated air stream. There is a decrease in the combustion efficiency for the vitiated air cases comparing the clean air case. Since this calculation of combustion efficiency is based on the amount of fuel that has been assumed, the addition of H₂O slows down this process. The addition of CO₂ is very similar in behavior and is not shown. The internal thrust of combustor decrease relative to the clean air case is 3.5% with 3% H₂O, 6.2% with 9% H₂O and 7% with 9% CO₂. Table 1 lists the internal thrust and the exit-plane combustion efficiency for all cases.

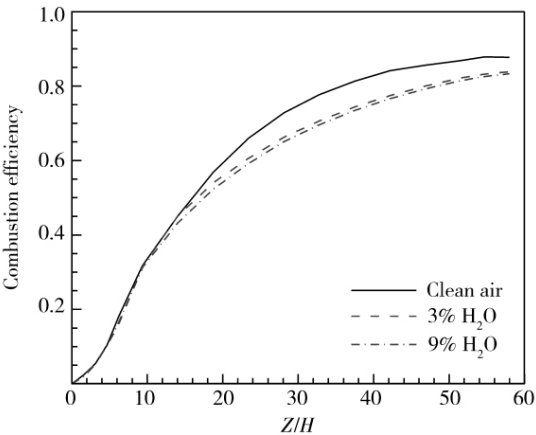


Fig. 10 Axial combustion efficiency for various amounts of H₂O

Table 1 Combustion efficiency and thrust for various amounts of H₂O

Conditions	Thrust/N	Combustion efficiency
Clean air	144	0.88
3% H ₂ O	139	0.84
9% H ₂ O	135	0.83
9% CO ₂	133	0.82

2.3 Comparison with experimental data

The calculated values of dimensional pressure along the centerline at the bottom wall of the combustor are compared with experimental data reported by Ref. [10]. Fig. 11 shows that there are good agreement between tests and computational fluid dynamic (CFD) results, with and without H_2O vitiation. The pressure rise location upstream of the ramp is predicted well, the vitiation effects on the pressure profiles are captured accurately. In summary, it can be said that the numerical calculations are able to predict pressure rise caused by combustion and the vitiation effects. All the calculation results above are credible.

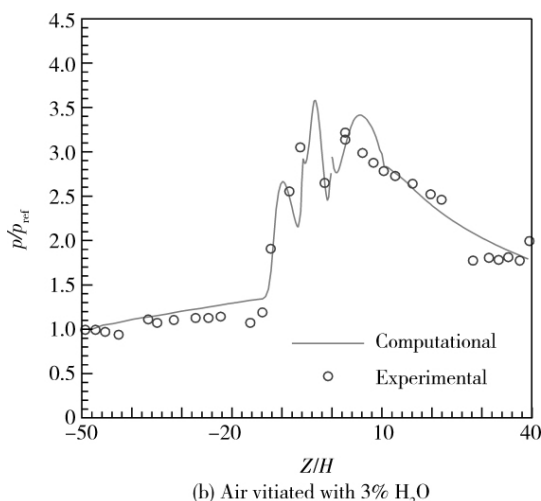
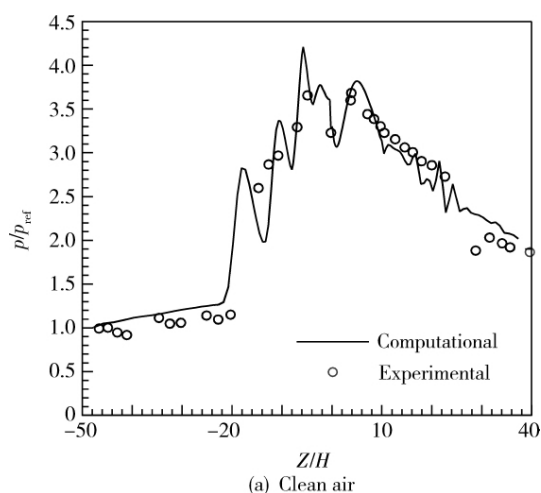


Fig. 11 Experimental and numerical wall-pressure distribution

3 Conclusions

In the present study we have computationally investigated the influence of contaminants introduced by combustion preheater on the ignition and combustion performance of hydrogen-fueled scramjet combustor by a set of calculations. Significant findings from these studies are as follows:

1) Free radical species such as H , O , and OH may significantly promote the ignition process of hydrogen-air, especially at relatively low initial temperature and pressure. The ignition enhancement of radicals is less effective in the high temperature and pressure regime. The addition of O is more effective than the addition of H and OH under the same conditions. However, the H_2O and CO_2 have an inhibition effect on the ignition process. Such an inhibition effect results from the effectiveness of them as a third body in recombination reactions. For the conditions studied, H_2O is more effective at inhibiting the ignition process than CO_2 .

2) Numerical simulation of three-dimensional, supersonic combustion in a dual-model scramjet combustor with the clean and vitiated air has been carried out. It is observed from the results that the difference between the clean air case and vitiated air case appear to be mainly due to the thermodynamic effects. The temperature and pressure in the vitiated air case is lower because of the higher heat capacity and any dissociation of H_2O and CO_2 . The pressure decreases relative to the clean air case is 13% with 3% H_2O , 16% with 9% H_2O and 21% with 9% CO_2 . The H_2O vitiation effects on combustion pressure and temperature have nonlinear characteristics. It is suggests that the mixed mode heating, where a combination of combustion and clean air preheating is used, may not offer a significant advantage over combustion heating alone. In addition, the CO_2 is more effective on reducing the pressure produced by combustion than H_2O under the same conditions. The combustion efficiency and thrust calculated for vitia-

ted air cases are lower than clean air case.

3) In dual-mode scramjet combustor, the presence of vitiation may cause mode transition at critical fuel equivalence ratio. The scramjet works properly in a ground test with combustion heater may result in unstart in clean air flight conditions.

In general, the vitiation has both effects on ignition and combustion performance in scramjet ground testing. The experimental results must be calibrated when extrapolating to flight conditions.

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