

The Effects of Air Vitiation on the Supersonic Turbulent Channel flow using Direct Numerical Simulation

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Temporally evolving supersonic turbulent channel flows are simulated using direct numerical simulation (DNS) approach at Mach number 2.56, Reynolds number 7000 with water vapor (H₂O) mass fraction from 0.00 to 0.161 to study the air vitiation effects. Then, the turbulent statistical characteristics and velocity-temperature correlations have been studied based on the DNS database. It is found that in fully developed turbulent channel flow, many of turbulent statistical characteristics used to express supersonic turbulent channel flow of pure air also hold for the H₂O considered. The difference between fluctuating and turbulent Mach number points to a significant non zero velocity-temperature correlations. After a nondimensional static temperature parameters introduced, the mean velocity-temperature correlations collapses between current DNS results. The results of strong Reynolds analogy decrease with H₂O mass fraction increasing, and modified strong Reynolds analogy show a better agreement than original strong Reynolds analogy. In addition, the correlation $R_{u,T}$ isn't remained the same between the different H₂O mass fraction cases.

Nomenclature

ρ = density

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p	=	pressure
T	=	temperature
E	=	total energy
h	=	mixture enthalpy
cc	=	sound speed
t	=	time
x_i, x_j	=	position vector ($i, j = 1, 3$)
δ_{ij}	=	Kronecker delta
u_i, u_j	=	velocity vector
σ_{ij}	=	shear stress tensor
S_{ij}, S_{kk}	=	strain rate tensor ($k = 1, 3$)
μ	=	mixture viscosity
Pr	=	Prandtl number
Re	=	Reynolds number
Ma	=	Mach number
R	=	universal gas constant
M_s	=	component molecular weight ($s = 1, 3$)
Y_s	=	component mass fraction
w	=	wall conditions
c	=	channel centerline
ref	=	reference conditions
*	=	dimensional flow variable
+	=	scaling with inner or wall values.
s	=	specie variable
$\{\cdot\}$	=	Favre average
'	=	turbulent fluctuations

I. Introduction

GROUND test experiment is crucial approach for supersonic flow study, which is the core topic for scramjet development. The combustion heating facility is widely used in scramjet ground test experiment to provide enough high enthalpy. However, a significant problem is that the high enthalpy air are seriously vitiated by several species, for example, H_2O , CO_2 , CO , H , OH , O , and NO , which are not of representative or very few in actual atmosphere, so-called air vitiation relative to pure air [1]. The flow field in such air vitiation can be influenced by chemical and physical effects due to the different species from actual atmosphere. Therefore, the effect of air vitiation is one important study to the development of scramjet technologies.

Edelman *et al.* (1969) presents an analytical study of the effects of vitiation heating including equilibrium, vibrational and chemical relaxation, finite rate condensation, combustion, mixing, and over all test engine performance. The study is considered to be the starting study of air vitiation effects. Over the years, several more experimental studies have been reported in the literature to help understand air vitiation effects [3-8]. Pellett *et al.* (2002) offers a detailed review and analysis on the physics and chemistry of scramjet ignition and flame holding combustion processes, and the known effects of air vitiation on these processes. With the development of computational fluids dynamics (CFD), numerical simulations are widely used in the community. Recently, Ingenito (2015) have performed a CFD simulation of the combustor configuration to provide useful information in terms of efficiency at various vitiation percentages. Theoretical laws and remedies have been proposed for the ground to flight data extrapolation. Although many air vitiation effects have been studied, most of the works focus on the performance comparative analysis, and few works to investigate their influence on the flow field. However, the performance is mainly dependent on the flow field, so it's necessary to study the mean and instantaneous flow field affected by the air vitiation effects.

Due to direct numerical simulation (DNS) solves the Navier-Stokes equations directly and do not contains any modeling errors, it is become a powerful tool to study the flow mechanism. DNS of supersonic turbulent channel flows have been performed at Mach 1.5 and 3 by Coleman *et al.* (1995) and Huang *et al.* (1995). In order to deeply understand the supersonic turbulence flow, the effect of wall temperature [13-16], Mach number [17], and high enthalpy [18-19] have been detailed discussed. The results indicate that those parameters not only influence the average flow and instantaneous flow, but also turbulent structures and Reynolds analogy. The strong Reynolds analogy (SRA) is one of important factors in the supersonic turbulent flow, which is called the relationships between

velocity and temperature fluctuations and can be used to instead of energy (temperature) equation in engineering application. The SRA suggested by Morkovin [20] is based on the assumption that the fluctuation in total temperature is nearly zero. In further developments that are based on considering the influence of the heat flux on the wall or eliminating the influence of the wall temperature, Cebeci *et al.* [21] employed a similarity relation between velocity and temperature to derive an extended form of SRA (ESRA). The check validity of classic and modified SRA for supersonic turbulent flow has also been performed by several researchers [15-18], while the air vitiation effects on the supersonic turbulent channel flow have not been understood clearly.

Chen *et al.* [22] performed a DNS of temporally evolving supersonic turbulent channel flow with H₂O at Mach number 2.56 and Reynolds number 2.8×10^5 . Based on this, a series DNS of supersonic turbulent channel flows are carried out under various H₂O mass fractions to investigate the air vitiation effects. Then, the characteristics of the time averaged and fluctuating flow field and instantaneous flow field are assessed. Finally, detailed velocity-temperature correlations under various H₂O mass fractions are studied.

II. Governing Equations and Numerical Approach

The governing equations are the time dependent three dimensional Navier-Stokes equations for a compressible fluid in nondimensional form.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \quad (1)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho u_i u_j + p \delta_{ij} - \frac{1}{\text{Re}_{ref}} \sigma_{ij} \right) = 0 \quad (2)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left((E + p) u_j - \frac{1}{\text{Re}_{ref}} \left(u_i \sigma_{ij} + \frac{\mu C_p}{\text{Pr}} \frac{\partial T}{\partial x_j} \right) \right) = 0 \quad (3)$$

where the total energy and the shear stress tensor are given by:

$$E = \rho h - p + \frac{1}{2} \rho u_i u_i \quad (4)$$

$$\sigma_{ij} = 2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk}, \quad S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (5)$$

In this paper, semiempirical formulas or curve fits will be used to simplify the solving method of thermodynamic and transport properties. The species thermodynamic properties, including specific heat and enthalpy, are computed

by NASA Glenn [23], while the species transport properties (viscosity) is taken from the work of CFD-ACE [24], which can be described as follows:

$$Cp_s = \frac{T_{ref}^*}{U_{ref}^{*2}} \frac{R^*}{M_s^*} (a_1 T^{*-2} + a_2 T^{*-1} + a_3 + a_4 T^* + a_5 T^{*2} + a_6 T^{*3} + a_7 T^{*4}) \quad (6)$$

$$h_s = \frac{1}{U_{ref}^{*2}} \frac{R^* T^*}{M_s^*} (-a_1 T^{*-2} + a_2 \ln T^*/T^* + a_3 + a_4 T^*/2 + a_5 T^{*2}/3 + a_6 T^{*3}/4 + a_7 T^{*4}/6 + b_1/T^*) \quad (7)$$

$$\mu_s = \frac{1}{\mu_{ref}^*} \frac{AT^{*3/2}}{B + T^*} \quad (8)$$

Table 1 Nondimensional parameters for the supersonic turbulent channel flow

ρ_{ref}^* , kgm ⁻³	U_{ref}^* , ms ⁻¹	T_{ref}^* , K	Ma _{ref}	Re _{ref}
0.208	1551.0	887.0	2.56	7000.0

Then, a common mixture rule for specific heat and enthalpy is JANAF rule [25], and mixture viscosity is calculated using Wilke's rule [26]. Table 1 gives the nondimensional parameters for the various H₂O mass fractions, which include bulk velocity, wall density and temperature. The table also gives the Mach number Ma_{ref} (based on the bulk velocity and sound speed at the walls) and Reynolds number Re_{ref} (defined in terms of bulk velocity and channel half width, density and viscosity at the walls). Initial conditions are given by superimposing random velocity fluctuations upon a laminar parabolic velocity profile ($\{u_1\} = 1.5(1 - y^2)$, $\{u_2\} = \{u_3\} = 0$) and uniform density and temperature fields ($\{\rho\} = 0.9567$, $\{T\} = 1.0451$). The convection terms in the compressible Navier-Stokes equations are discretized by the 7th order WENO scheme [27]. The viscous terms are approximated with an 8th order central difference. A 3th order Runge Kutta method is used for the time integration.

Table 2 Mass fraction, grid resolution and domain size for the supersonic turbulent channel flow

Cases	Y _{O2} :Y _{N2} :Y _{H2O}	$L_1 \times L_2 \times L_3$	$n_1 \times n_2 \times n_3$	$\Delta x_1^+ \times \Delta x_{2w}^+ \times \Delta x_3^+$	Re _τ
Case 1	0.306×0.694×0.000			17.23×0.31089×8.62	537.85
Case 2	0.298×0.675×0.027			17.24×0.31107×8.62	538.16
Case 3	0.290×0.656×0.054			17.03×0.30720×8.51	531.45
Case 4	0.282×0.637×0.081	2π×2×π	196×512×196	17.08×0.30818×8.54	533.15
Case 5	0.274×0.618×0.108			16.99×0.30647×8.49	530.20
Case 6	0.266×0.599×0.135			17.55×0.31664×8.78	547.79
Case 7	0.257×0.582×0.161			17.57×0.31697×8.79	548.37

The mixture gas is composed by the oxygen (O_2), nitrogen (N_2) and water vapor (H_2O). We used a series DNS of supersonic turbulent channel flows with H_2O mass fractions (Y_{H_2O}) ranging from 0.000 to 0.161. To isolate the effect of varying H_2O mass fraction, the ratio O_2 mass fraction (Y_{O_2}) to N_2 mass fraction (Y_{N_2}) is kept constant, which can be seen from table 2. The domain size ($L_1 \times L_2 \times L_3$), the grid size ($\Delta x_1 \times \Delta x_2 \times \Delta x_3$), the number of grid points ($n_1 \times n_2 \times n_3$) and wall Reynolds number (Re_τ) are also given in Table 2, respectively. In order to increase computational efficiency, a well-designed block-structured grid containing about 19.7M computational cells is applied. Uniform grids are used in the streamwise and spanwise directions, while geometrically stretched grids are used in the wall normal direction. Periodic boundary conditions have been used in the streamwise and spanwise directions. On the wall boundaries, nonslip conditions are used for three velocity components, and wall temperature is kept isothermal.

III. Velocity and Temperature Statistics

In order to study H_2O mass fraction effects, the mean flow quantities need to be analyzed. Figure 1 plots some of mean flow parameters in wall normal direction, including streamwise velocity, static temperature and specific heat, respectively. It is can be seen that the mean static temperature and specific heat increase and mean streamwise velocity decrease away from the wall. The reason may be that shock waves and large kinetic dissipation make the kinetic energy transform to internal energy. It is indicated that the mean streamwise velocity collapse in wall normal direction, while the mean static temperature and specific heat decrease with H_2O mass fraction increasing. In addition, the mean specific heat few smaller than its initial value, which relative deviates are all about 2.3%.

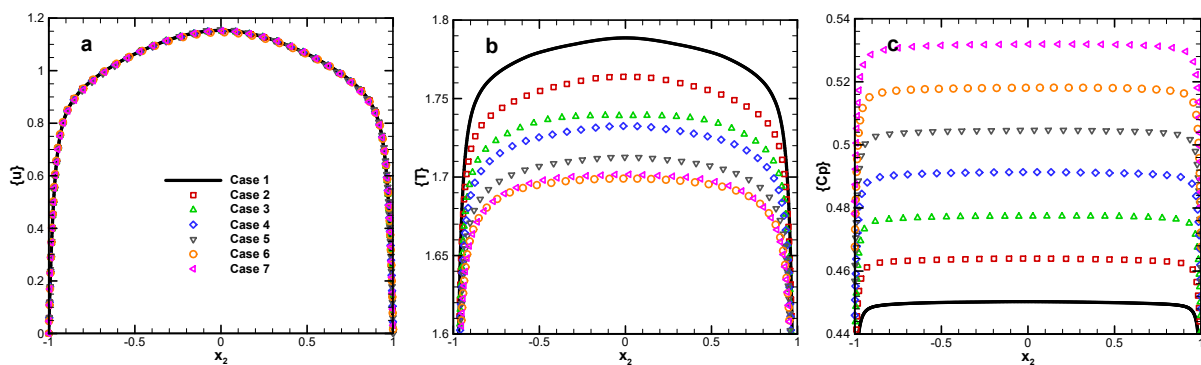


Fig.1 Distribution of the mean *a)* streamwise velocity, *b)* static temperature and *c)* specific heat.

The RMS (room mean square) fluctuation could response the importance of properly accounting for the turbulent intensity. RMS fluctuation of the streamwise velocity and static temperature are plotted in Fig.2. RMS fluctuation of

streamwise velocity defined as $u'_{rms} = \sqrt{u'^2}$ (similar to T'_{rms}). When normalized by conventional wall variables (defined in terms of the mean density, viscosity and shear stress at the wall), it is found that the differences are small. The relative large deviation occurs at the region of $0.96 \leq |y| \leq 0.70$, and the maximum deviation is less than 7.5%. A small region in Fig.2 (a) is chosen and enlarged to display in Fig.2 (b), which show the deviations more clearly. Fairly large RMS fluctuation of static temperature is found, especially near the walls, where the maximum value is about 8%. However, RMS fluctuation of static temperature is not collapsed the profiles for different H₂O mass fraction cases.

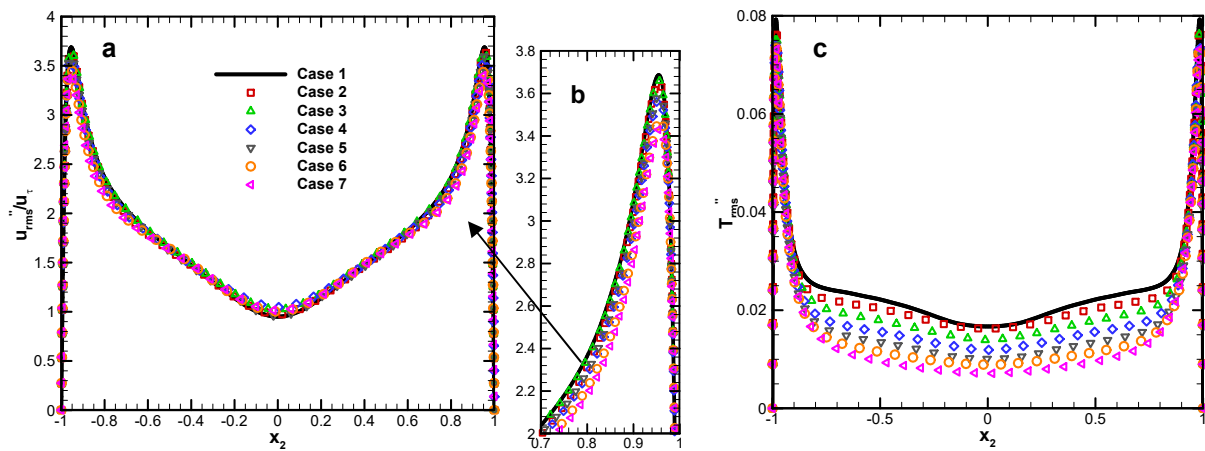


Fig.2 RMS fluctuation of the *a-b*) streamwise velocity and *c*) static temperature.

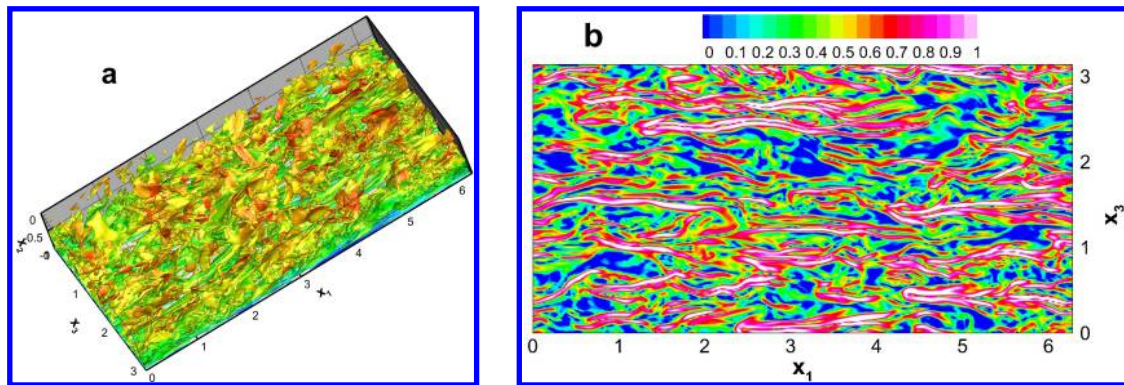


Fig. 3 *a*) Iso-surfaces of the total temperature gradient magnitude ($\log_{10} |\nabla T_t| = 0.5$) colored using local static temperature at the same instant for the case 1, *b*) Instantaneous total temperature gradient magnitude flow field at the section of $|x_2| = 0.9$ for the case 1.

The total temperature, defined as $T_t = T(1 + (\gamma - 1)Ma^2/2)$, is also one of important parameters for supersonic flow field. To explore the total temperature formation and characteristics, the total temperature gradient magnitude

$(\log_{10} |\nabla T_t|)$ exceed prespecified cutoff value are determined. The instantaneous snapshot of case 1 is plotted in fig.3 (a). It is shown that the peak value $((\log_{10} |\nabla T_t|)_{\max})$ is 1.528, and the larger values of $\log_{10} |\nabla T_t|$ are mainly appeared near the wall. However, when move away from the wall, its value will be reduced gradually. Figure 3 (b) represents the instantaneous snapshots of total temperature gradient magnitude at the section of x - z . Similar to the streamwise velocity, several streaks are existed in the spanwise direction, while the mean spanwise spacing of near wall streaks is much smaller. Moreover, the larger value regions of $\log_{10} |\nabla T_t|$ often appear in pairs. Furthermore, Fig. 4 plots the mean and fluctuating total temperature for different H_2O mass fraction cases. Like the static temperature distribution, the mean and fluctuating total temperature decrease with H_2O mass fraction increasing.

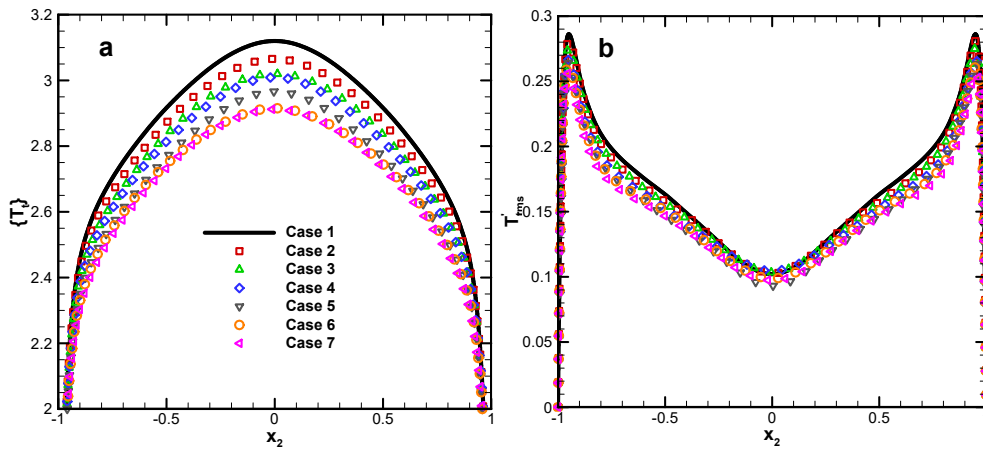


Fig.4 Distribution of the a) mean total temperature and b) RMS fluctuation of total temperature.

IV. Velocity-Temperature Correlations

Figure 5 plots mean-, fluctuating- and turbulent Mach number profiles. The mean Mach number, defined by $\{Ma\} = \sqrt{u_j^2} / \{cc\}$ (cc is the sound speed), increases to 1 quickly away from the wall, which reveals the main flow is supersonic flow. The turbulent Mach number, defined by $Ma_t = \sqrt{u_j^2} / \{cc\}$, is an indicator for the significance of compressibility effects. There is excited some regions where Ma_t larger than 0.3, particularly near the wall. A more significant increase is observed for the fluctuating Mach number, Ma'_{rms} , which is the RMS fluctuation of Mach number. An analogical profile exists between the fluctuating and turbulent Mach number, but the former value is smaller than that for the latter among the wall normal direction.

Due to the channel width is very small, so the boundary layer may fill the entire flow region or its position difficult to confirm. In this paper, the mean streamwise velocity and static temperature at the centerline will be chose to replace that for the boundary layer edge. Figure 6 plots the exact ratios for the DNS data. It can be seen that some deviates are existed as shown in fig.6 (a), which indicate H₂O mass fraction influence the mean velocity-temperature correlations. To remove the explicit dependence, a new nondimensional parameter $((\{T\} - \{T_w\}) / (\{T_c\} - \{T_w\}))$ is introduced. Figure 6 (b) shows that there is excellent agreement for all H₂O mass fraction cases.

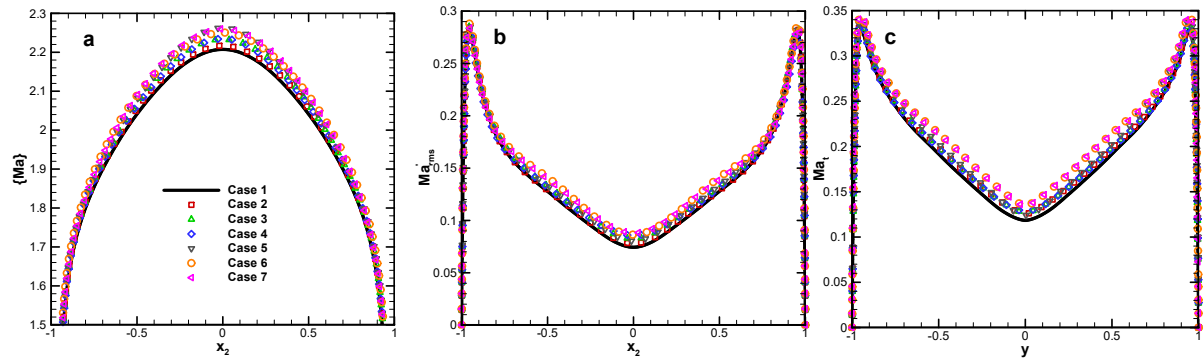


Fig.5 Distribution of the *a)* mean Mach number, *b)* fluctuating Mach number and *c)* turbulent Mach number.

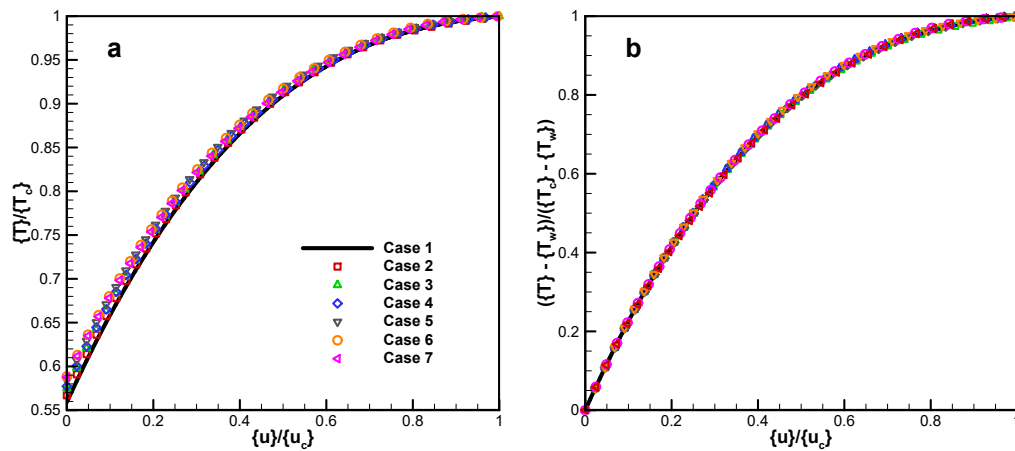


Fig.6 The relationship between velocity $\{u\}/u_c$ and temperature *a)* $\{T\}/T_c$ and *b)* $((\{T\} - T_w) / (T_c - T_w))$.

Morkovin [20] proposed strong Reynolds analogy (SRA) relations, two of which are listed below:

$$\frac{T'_{rms} / \{T\}}{(\gamma - 1) Ma^2 (u'_{rms} / \{u\})} \approx 1 \quad (9)$$

$$R_{uT} \approx -1 \quad (10)$$

Figure 7 (a) plots the relationship between fluctuating streamwise velocity and static temperature, as expressed by (9), for supersonic turbulent channel flows. It is shown that the agreement is not perfect with all H₂O mass fraction cases. Similar results have been reported by Morinishi *et al.* [16]. They explained that not only the total temperature fluctuation can't be negligible compared to the static temperature fluctuation, but also the condition of $\langle T'^2 \rangle / \{T\}^2 \ll (\langle T_i'^2 \rangle - 2\langle T'T_i' \rangle) / \{T\}^2$ is not satisfied. Figure 7 (b) shows that better agreement is achieved between current DNS results except for $1.0 < |y| < 0.6$, and the modified strong Reynolds analogy (ESRA) of Cebeci *et al.* [21], which is given by:

$$\frac{T'_{rms} / \{T\}}{(\gamma - 1) Ma^2 (u'_{rms} / \{u\})} \approx \left[1 + Cp \frac{\{T_w\} - \{T_{t,c}\}}{\{u\} \{u_c\}} \right] \quad (11)$$

As shown in Fig.7 (c), the correlation $R_{u'T'}$ is negative through the channel, which indicates that u' and T' have a negative correlation. Moreover, the above correlations near to -1 in the near wall, and such dependent value quickly degrade in the largest region that is far away from the wall. It is shown that $R_{u'T'}$ is a strong function of H₂O mass fraction, particularly in the flow field. The correlation dependent value will be enhanced with H₂O mass fraction increasing.

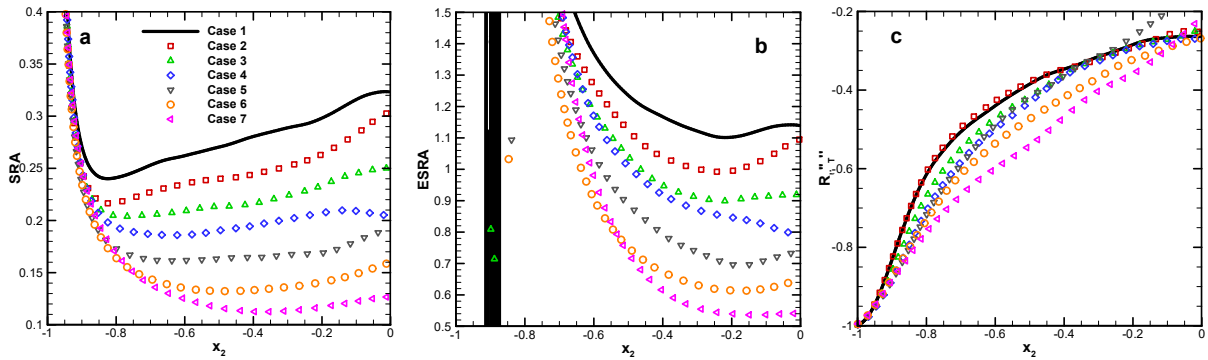


Fig.7 Distribution of the a) SRA, b) ESRA and c) $R_{u'T'}$.

V. Conclusion

In this paper, using 7th order WENO scheme combined with 8th order central scheme, we have performed DNS of supersonic turbulent channel flows. Mach number, based on the bulk velocity and sound speed at the walls, of 2.56 is considered; Reynolds number, defined in terms of the bulk velocity and channel half width, are of the order of 7000; water vapor (H₂O) mass fraction are from 0.000 to 0.161. The velocity and temperature statistical

characteristics and velocity-temperature correlations have been analyzed, and some conclusions can be drawn as follows:

It is shown that many of turbulent statistical characteristics used to express supersonic turbulent channel flow of pure air also hold for the H₂O considered. In particular, when H₂O mass fraction is increased, the mean and fluctuating streamwise velocity are few changing, while the specific heat, static temperature and total temperature are decreased. Simultaneously, the turbulence Mach number (turbulent Mach number, fluctuating Mach number) are increased dramatically.

It is found that H₂O mass fraction influence the mean velocity-temperature correlations. A nondimensional parameter, which is a relative static temperature ratio formula, can be used to connect the mean static temperature with streamwise velocity. In terms of strong Reynolds analogy (SRA), the original SRA relation breaks down for all cases. The Cebeci's version of the modified SRA provides better agreement. In addition, the correlation R_{u-T} isn't remained the same between the different H₂O mass fraction cases.

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