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# Effects of Chemical Reactions on Turbulent Channel flow

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## Abstract

Effect of finite-rate chemical reactions on turbulence has important implications in the design of hypersonic vehicles, which is a very challenging problem. Several experimental and theoretical/numerical works have been conducted to explore the physics of this type of flows in literature. However, the physical mechanism of the flow behaviours is still poorly understood. In this paper, temporally evolving high-temperature turbulent channel flows (at $Ma_\infty$=6 and 10, and $Re_\infty$=12000) are simulated using the direct numerical simulation (DNS) approach. The medium is assumed to be calorically perfect gas and chemically reacting gas in non-equilibrium. The numerical method is based on the 7th-order WENO scheme for spatial discretization and 3th-order Runge-Kutta method for time integration. The results from DNS show that many important scaling relations formulated can be generalized for channel flow with finite-rate chemical reactions, including the mean quantities, the instantaneous flow features and the Morkovin scaling for RMS (Root Mean Square) quantity fluctuations. Furthermore, turbulent kinetic energy (TKE) budget and vortex structures have been studied from the DNS results.

## Introduction

Effect of finite-rate chemical reactions on turbulence has important implications on the design of hypersonic vehicles, which is a very challenging problem. These flows are significantly different with turbulent combustion flows which have been studied extensively. In hypersonic flows, the expression "(finite-rate) chemical reactions" is commonly used as a synonym for "chemical non-equilibrium" or "real-gas effects" [1].

Study of the turbulence-chemistry interaction has mostly been based on theories or experiments [2]. Theoretical research has a huge help to understand turbulence. However, because of the wide space and time scales and the strong nonlinear, turbulent theoretical researches are extremely difficult. At the same time, turbulent experimental measurements have been one of the important means. Experimental results are convincing, but they also have some shortcomings, such as: high cost, long cycle. There are very few tests described in the open literature, and these tests generally provide limited turbulence data with large uncertainties.

With the development of computational fluids dynamics, numerical simulations are widely applied. In a turbulent flow simulation, compared with large-eddy simulation (LES) and Reynolds Average Navier-Stokes (RANS), direct numerical simulation (DNS) solves the Navier-Stokes equations directly and do not contains any modeling errors, and is a powerful tool to study the mechanism of turbulent flows. Most previous DNS studies have been carried out at non-reacting conditions, i.e. if we have a calorically perfect gas. DNS of non-reacting turbulent channel flows have been performed previously, such as Coleman et al [3] and Huang et al. [4] at Mach 1.5 and 3, Foysi et al. [5] at Mach 0.3, 1.5, 3.0 and 3.5, Li et al. [6] at Mach 0.8, 1.5 and 3.0, Chen et al. [7] at Mach 6 and 10.

The reports of DNS for turbulent flows with chemical reactions in high Mach number are relatively few. Martin et al. [8-9] used simplified single dissociation/recombination reaction mechanism and constant species heat capacities to study the nonlinear interaction between turbulence and finite-rate chemical reactions in the presence of predominantly exothermic or endothermic reactions in isotropic turbulence and turbulent boundary layers. Duan et al. [10] performed DNS of flat- plate hypersonic turbulent boundary layers at high- and low-enthalpy conditions on air to study the effects of enthalpy conditions on boundary layer flow. Based on the assumption of local thermal equilibrium and chemical non-equilibrium, Chen et al. [11] performed direct numerical simulations of hypersonic and high-temperature turbulent channel flows, in which the inflow Mach number is 6 and 10. Simultaneously, Marxen et al. [12] have done some research, for example, using different gas-modes to analysis the problem of hypersonic boundary layer stability.

Although the effect of finite-rate chemical reactions on turbulence has been studied in hypersonic boundary layers, equivalent information is not yet known for inlet channel environments. Furthermore, the effect of finite-rate chemical reactions on turbulent vortexes has not yet been studied. In this paper, DNS study of high speed and temperature turbulent channel flow have been performed to investigate the effect of chemical reactions on turbulent statistics and vortexes by comparing DNS results assumed to be calorically perfect gas and finite-rate chemical reaction in air.

## Governing equations and simulation details

The governing equations are the time-dependent three dimensional Navier-Stokes equations for a compressible fluid in non-dimensional form. For a calorically perfect gas, the mass conservation equations only need to keep the total mass equation because the gas composition does not change [7]. The specific heat is constant and the internal energy is only a function of temperature. However, considering finite-rate chemical reactions, these equations are formulated for a mixture of thermally perfect gases in local thermal equilibrium, where chemical reactions are assumed to take place with a finite reaction rate, but vibrational relaxation occurs infinitely fast [11]. Non-dimensionalization is based on the free-steam conditions.

Chemically reacting gas in non-equilibrium model often corresponds to a particular physical problem, such as the flight height and velocity. In this paper, the simulated flight height is 20km, flight speed includes two situations (inflow Mach number $Ma_\infty$ equals 6 and 10, respectively). The specific value can be reference to the earth standard atmosphere table, where the subscript ($_\infty$) indicates parameters, as shown in Table 1. In order to study easily, direct numerical simulations of calorically perfect gas are also performed.

| | |
|---|---|
| Density $\rho^*_\infty$(kg/m$^3$) | 8.891e-02 |
| Temperature $T^*_\infty$(K) | 216.65 |
| Speed of sound $c^*_\infty$(m/s) | 295.07 |
| Wall temperature $T_w$(K) | 1300 |
| Reynolds number $Re_\infty$ | 12000 |
| Mach number $Ma_\infty$ | 6(M11), 10(M21) Chemically reacting gas<br>6(M12), 10(M22) Calorically perfect gas |

Table 1. Free-stream and wall parameters for the compressible turbulent channel flow.

Periodic boundary conditions have been used in the stream-wise and span-wise directions for computational efficiency. On the wall boundary, non-slip conditions are used for the three velocity components. The wall temperature is prescribed according to different conditions and is kept isothermal as indicated in Table 1. In addition, species boundary conditions need to be given for chemical reactions cases. The fully catalytic wall assumes infinitely fast atom recombination at the wall.

The compressible Navier-Stokes equations are solved by using the Van-Leer flux vector splitting and the 7rd order WENO [13] scheme to discrete convection terms. The viscous terms are approximated with an 8th-order central difference. A 3rd order Runge-Kutta method is used for the time integration.

We take the stream-wise, span-wise and wall-normal directions to be $x$, $y$, and $z$, respectively. Uniform grids are used in the stream-wise and span-wise as $\Delta x^+$ and $\Delta z^+$, where the superscript ($^+$) indicates scaling with inner. However, geometrically stretched grids are used in the wall-normal direction, whose minimum value is $\Delta y_w^+$. The domain size ($L_x \times L_y \times L_z$), the grid size ($\Delta x \times \Delta y \times \Delta z$) and the number of grid points ($n_x \times n_y \times n_z$) are given in Table 2, respectively.

| Cases | $L_x$ | $L_y$ | $L_z$ | $\Delta x^+$ | $\Delta y_w^+$ | $\Delta z^+$ | $n_x$ | $n_y$ | $n_z$ |
|---|---|---|---|---|---|---|---|---|---|
| M11 | 4π | 2 | 4π/3 | 22.4 | 0.43 | 7.47 | 161 | 201 | 161 |
| M21 | | | | 24.2 | 0.45 | 8.01 | 201 | 261 | 201 |
| M12 | | | | 24.4 | 0.47 | 8.10 | 161 | 201 | 161 |
| M22 | | | | 28.5 | 0.51 | 9.50 | 201 | 261 | 201 |

Table 2. Grid resolution and domain size for the DNS data.

## DNS results

### Mean flow

Figure 1 plots the distribution of average density, velocity, pressure and temperature, respectively. The chemical reactions do not change average density and velocity largely from Fig. 1(a). In the near wall region, the density values are smaller; while away from the wall, its values are larger. However, in general, chemical reactions have an effect on the pressure and temperature, especially temperature. The average pressure is almost unchanged in the normal wall direction; but chemical reactions will bring the pressure value decreases. In hypersonic flight, shock waves and large kinetic dissipation make the temperature extremely high. The excited vibrational energy and finite-rate chemical reactions need to absorb energy, thereby reducing the average temperature. As can be seen from Figure 1, the higher the Mach number, the greater effects.

The maximum flow temperatures are above 3000K, and chemical reactions exist significantly. The specific heat ratio is one of the important parameters used to evaluate real-gas effects, which defined as follows:

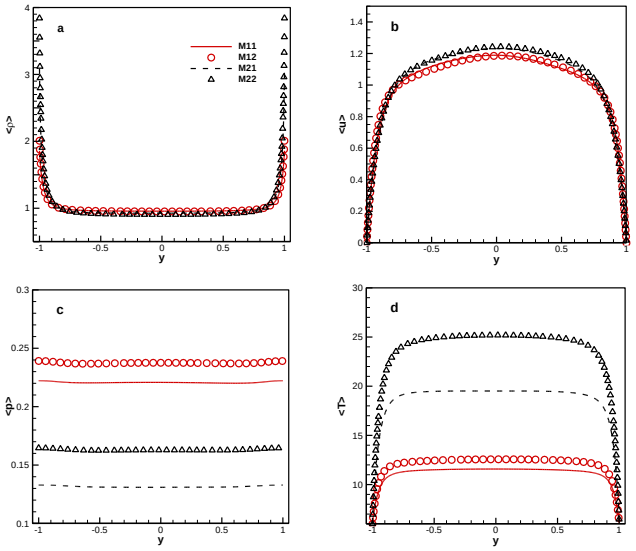


Figure 1. Distribution of average parameters for (a) density, (b) velocity, (c) pressure, and (d) temperature.

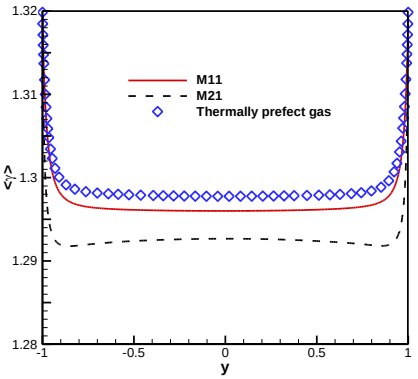


Figure 2. Distribution of Specific heat ratio.

$$\langle \gamma \rangle = \frac{\langle C_p \rangle}{\langle C_v \rangle} \tag{1}$$

$$\langle C_v \rangle = \left\langle \sum_{s=1}^{ns} Y_s C_{v,s} \right\rangle \Big/ \left\langle \sum_{s=1}^{ns} \frac{Y_s}{M_s} \right\rangle \tag{2}$$

$$\langle C_p \rangle = \langle C_v \rangle + R \tag{3}$$

$$R = R^* \sum_{s=1}^{ns} \langle f_s \rangle \Big/ M_s \tag{4}$$

where $R^*$ is the universal gas constant (8.314 J mol$^{-1}$ K$^{-1}$). Figure 2 shows that the specific heat ratio deviates significantly from the calorically perfect gas value of 1.4 throughout the wall-normal direction. From Figure 2, it is seen that the specific heat ratio of the thermally perfect gas is smaller than that of the calorically perfect gas, while it is still a little larger than that of the chemical non-equilibrium gas.

### Turbulence quantities

An indicator for the significance of compressibility effects is the turbulent Mach number, defined by:

$$M_t = \frac{\sqrt{< u_i' u_i' >}}{< c >} \tag{5}$$

Figure 3 (a) plots the distribution of turbulent Mach number of four cases, which shown that turbulent Mach numbers having similarity. The magnitude of turbulent Mach number is larger than the critical value of 0.3; moreover, that magnitude of Mach number $Ma_\infty$=10 is larger than the critical value in a very long area. Based on the Morkovin hypothesis, compressibility effects can't be ignored. To some extent, chemical reactions have effect on turbulent Mach number. Especially when chemical reactions are remarkable, the turbulent Mach number changes significantly, such as the maximum value.

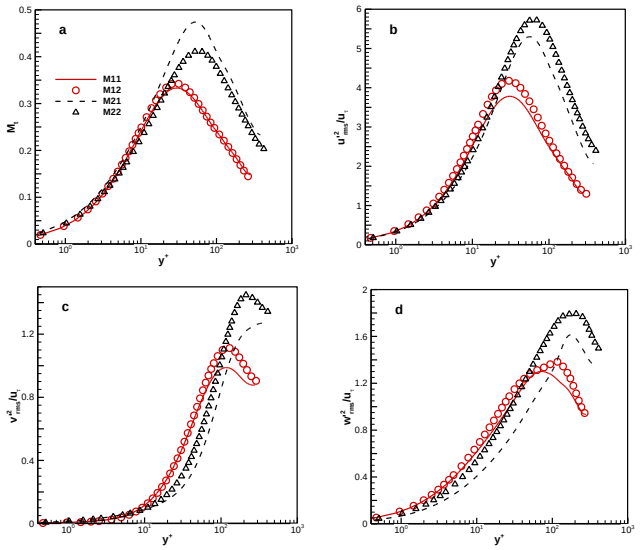


Figure 3. Distribution of turbulent fluctuations: (a) turbulent Mach number, (b-d) RMS velocity fluctuations of stream-wise, wall-normal and span-wise directions.

The importance of properly accounting for the mean property variations can be seen in Figure 3 (b-d). When normalized by conventional wall variables (defined in terms of the average density, viscosity and shear stress at the wall), RMS velocity profiles have little to do with inflow Mach number near the wall; however, they increase with inflow Mach number away from the wall. Chemical reactions do not affect the RMS velocity, especially in the near wall region.

## Structure analysis

In this section, we investigate the effects of chemical reactions on turbulent structure. Figure 4 gives the instantaneous stream-wise velocity at y+=5. Several long regions at a low speed u with deep dark are identified. It is shown that streaks occur in all cases, and the superficial similarity between the calorically perfect gas and the chemically reacting gas in non-equilibrium is apparent.

Vortex identification and visualization are often used in the study of turbulent. Over the past twenty-five years several criteria for identification of vertical structures have been introduced in many literatures. Hunt et al define eddy regions as "strong swirling zones with vorticity." They pointed out that in turbulent flows, these eddies will be stretched by irrotational straining but that for a swirling zone to qualify as an eddy it should satisfy two criteria. They quantify this using the second invariant of the velocity gradient tensor which is given by:

$$Q = -\frac{1}{2}\left(S_{ij}S_{ij} - W_{ij}W_{ij}\right) \tag{6}$$

where

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad W_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

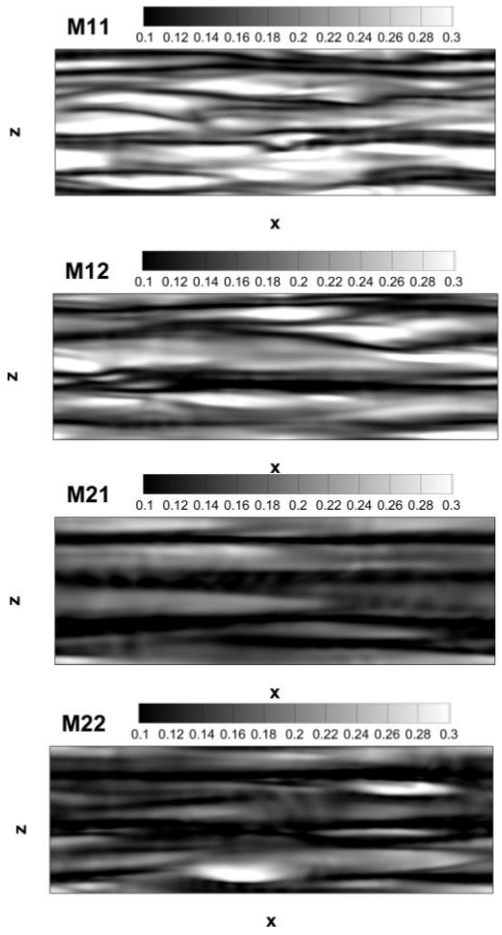


Figure 4. Instantaneous flow field at y+=5 to visualize near-wall streaks for (a) M11, (b) M12, (c) M21, and (d) M22.

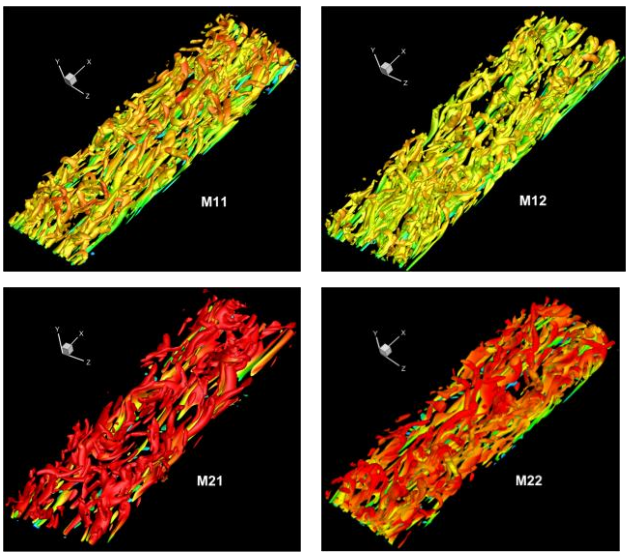


Figure 5. (Color) Iso-surfaces of the second invariant of the velocity gradient tensor Q=0.1 colord using average Mach number at the same instant for (a) M11, (b) M12, (c) M21, and (d) M22.

Figure 5 plots the instantaneous of Q=0.1, where Q is the second invariant of the velocity gradient tensor. It can be seen that the coherence vortices are arranged to be smoother and stream-wised, and the hair-pin vortices occasionally occur in the chemically reacting gas in non-equilibrium condition. Thus, it is helpful to maintain the vortices structure in the stream-wise direction when the chemical reactions considered.

## Conclusions

In summary, based on the DNS results of assumption of calorically perfect gas and finite-rate chemical reactions, we study the effect of finite-rate chemical reactions on turbulent channel flow at the inflow Mach number at 6 and 10. The value of specific heat ratio are between 1.400 (perfect-gas) and 1.286 (vibrational excited completely), which proved that the finite-rate chemical reactions begin to emerge and become more and more important. The chemical reactions do not affect the average density and velocity largely, but the average pressure and temperature significantly. It is also shown that the turbulent Mach number and RMS velocity fluctuations have little to do with chemical reactions, especially in the near wall region. In terms of turbulent structure, streaks occur in two gas models. Considering finite-rate chemical reactions can increase the stream-wise coherency of near-wall streaks, which is much larger than the calorically perfect gas, and helpful to maintain the vortices structure in the stream-wise direction.

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