DIRECT NUMERICAL SIMULATION OF HYPERSONIC BOUNDARY LAYERS IN CHEMICAL NON-EQUILIBRIUM

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Summary The influence of high-temperature effects on compressible wall-bounded turbulence is investigated by means of a direct numerical simulation of a hypersonic, chemically out-of-equilibrium, turbulent boundary layer. The analysis aims at assessing the effects of chemical reactions on turbulence, also by comparing the results with those of a frozen flow. We will present a detailed analysis of the turbulent statistics and near-wall dynamics; the validity of some classical scalings and Reynolds analogy will also be discussed.

The investigation of turbulent hypersonic flows is a major subject for a wide range of applications, including reentry vehicles, spatial tourism or trans-atmospheric flights. The high temperatures reached in these regimes can cause chemical reactions (with characteristic times similar to those of the fluid motion), giving rise to a nonequilibrium chemical state. Such high-temperature effects have a strong impact on aerodynamic performance and heat transfer rates, but may also affect transition and turbulence dynamics [1].

In this work, we investigate the influence of finite-rate chemistry on compressible wall-bounded turbulence. More specifically, we carry out the direct numerical simulation of a hypersonic, chemically out-of-equilibrium, turbulent boundary layer, encompassing the laminar-to-turbulent transition, triggered by means of a suction-and-blowing forcing at the wall. The analysis aims at assessing the effects of chemical reactions on turbulence, also by comparing the results with those of a frozen flow (i.e. a flow with chemical reaction times much longer than the flow scales).

Flows under investigation are governed by the compressible Navier–Stokes equations for multicomponent chemically-reacting gases. Concerning the chemical modeling, the five-species (N_2, O_2, NO, O, N) model of Park [2] is considered. Thermodynamic quantities are determined using the contributions of the translational, rotational and vibrational modes of each species, whereas transport properties are computed by means of Blottner's model and Eucken's formula [3]. Finally, mass diffusion pheomenon is modeled following Hirschfelder's approximation [4].

The simulations are carried out by means of an in-house CFD code. The code is equipped with high-order finite-difference schemes (tenth order for convective fluxes and fourth order for viscous ones) and selective standard filters, supplemented with the Localized Artificial Diffusivity (LAD) method for shock capturing [5]; this technique consists in adding artificial transport properties to the physical ones, in order to smooth out discontinuities and/or strong unresolved dynamic, thermal and mass gradients. The time integration is carried out by means of a low-storage, explicit third-order Runge–Kutta algorithm. The direct numerical simulation strategy has been preliminary validated against literature results for two single-species boundary layer configurations at $M_\infty = 6$ [6] and $M_\infty = 2.25$ [7], whereas the chemical non-equilibrium model has been assessed against the configurations described in [8], [9] and [10].

The proposed work is carried out in the free-stream conditions of [10], representing a reference state widely used for stability studies; specifically, $M_\infty=10$, $T_\infty=350$ K, $p_\infty=3596$ Pa and $T_w \approx 5400$ K. A computational grid of $\approx 3.2 \times 10^8$ points is considered, which ensures a good spatial resolution in all directions, i.e. $\Delta x^+ = 3$, $\Delta y_w^+ = 0.6$ and $\Delta z^+ = 2$, being x, y and z the streamwise, wall-normal and spanwise directions respectively. An instantaneous visualization of the chemically out-of-equilibrium simulation is shown in figure 1; the oxygen mass fraction varies of one order of magnitude, from the wall (where the temperature is the highest and the oxygen is highly dissociated) to the edge of the boundary layer, where it reaches the free-stream conditions.

Some quantitative results are reported in figure 2. The trend of the skin friction coefficient $C_f = 2\tau_w/(\rho_e U_e^2)$ is shown in figure 2(a): finite-reate chemistry little affects the skin friction distribution in the laminar and fully turbulent regions. Significant discrepancies are observed in the transition region, albeit the qualitative trends are close-by. This result is mainly due to the varying mixture composition in the chemically-reacting case. The root mean square values of the temperature are shown in figure 2(b). The results for the chemically-reacting simulation present lower values of temperature fluctuations; this is due to the endothermic nature of the reactions, which subtract energy from the system. Figure 2(c) presents the root mean square values of the mass fractions, for the chemically-reacting simulation. The strongest chemical activity is concentrated at the wall, where the temperature is the highest; however, the peaks of the fluctuations are shifted away from the wall and their position corresponds to the largest temperature fluctuations. The curves are plotted with respect to $y^+ = y\rho_w u_\tau/\mu_w$, at $Re_\tau = 180$.

In the final study, we will present a detailed analysis of first- and second- order statistics and near-wall dynamics. The validity of classical Reynolds analogy will be assessed and a skin friction decomposition will also be discussed.

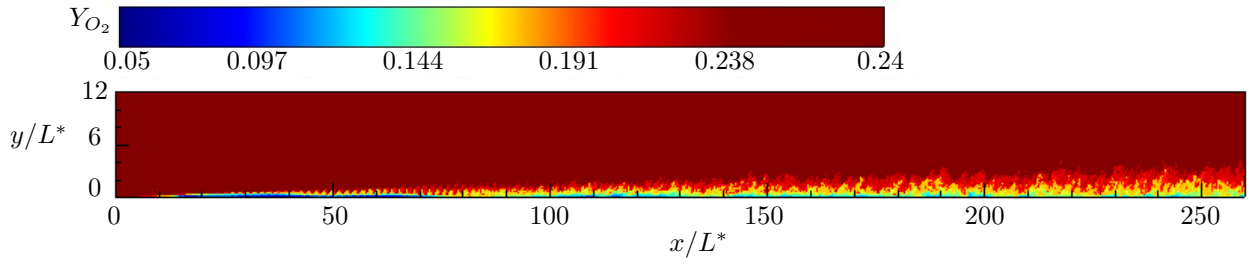*Corresponding author. E-mail: donatella.passiatore@poliba.it.

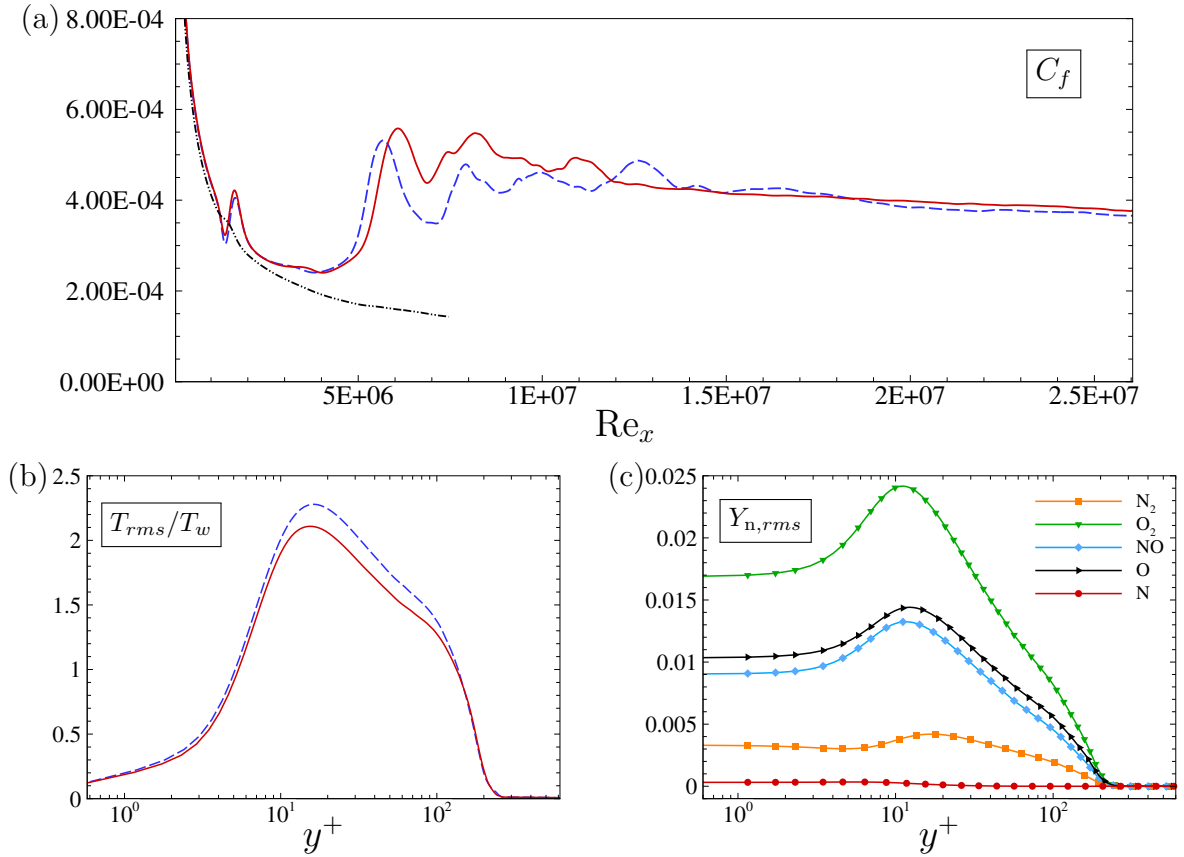Figure 1: Isocontours of oxygen mass fraction Y_{O_2} in a (x,y) plane, with aspect ratio $x/y = 0.5$.

Figure 2: Skin friction coefficient (a), rms values of the temperature, normalized with wall temperature (b) and rms values of the mass fractions, for the chemically-reacting simulation (c). (- - - -) frozen simulation; (——) chemically-reacting simulation.

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