2D-DNS and 2D-RANS Simulations of Supersonic QUASI-2D Turbulent Reacting Shear Flow

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Abstract

Numerical studies of quasi-2D supersonic turbulent hydrogen-air mixing and combustion in free shear layer configuration are performed using 2D-DNS [1] and RANS equations. In order to produce the roll-up and pairing of vortex rings, an unsteady boundary condition is applied at the inlet plane. Frequencies of initial velocity perturbations have been taken in accordance with linear stability theory. The influences of different inflow perturbations on mixing layer structure are presented. At the outflow, the non-reflecting boundary condition is adopted. In the case of RANS simulation two-parameter *k-e* turbulence model is used. Thermal conduction is described by Fourier's law, while diffusion of species by Fick's law. Equation of state for thermally perfect multispecies gas is used. Thermodynamic parameters, such as specific heat, enthalpy, entropy and internal energy are determined by fourth order degree polynomial formula, which has dependence on temperature. Temperature is determined using Newton-Raphson iteration procedure. The Wilke's formula is used to determine the mixture viscosity coefficient. Approximation of convection terms are performed by the ENO-scheme of third-order accuracy and approximation of diffusion terms – by second-order central-difference operators. For the description of reaction pathways of hydrogen, a seven species chemical reaction model by Jachimowski is adopted. Chemical reaction source term implicitly includes in mass fraction transport equations, where linearization is applied using Taylor decomposition. The hydrogen flow parameters are M_0 = 2.0, T_0 = 2000 K, P_0 = 101325 Pa, and air flow parameters are M_∞ = 2.1, T_∞ = 2000 K, p_∞ = 101325 Pa. Convective Mach number is M_c = 0.38, where effect of compressibility is significant.

Introduction

As it is well known, the "real" turbulent flow is three-dimensional with random change of the physical characteristics both in time and space. In nature there are no two-dimensional turbulence, however, at some conditions we can observe quasi-two-dimensional flow. Experimental implementation of such turbulent flow represents certain difficulties [1]. In [1] outlines the basic conditions that allow organizing quasi-2D flow, which has some characteristics of two-dimensional turbulence. According to this work "two-dimensionalization" of turbulent flow depends on the geometric parameters of the problem. As a geometrical parameter considered thin mixing layers, where its thickness (on axis Oy) significantly smaller than sizes of other two spatial coordinates (Ox and Oz). Basically these flows are found in the oceans and atmosphere. Also thin mixing layers can be observed in the jet flow, the boundary layer along the long thin plate, etc. Geometrical size – this is only one possible way to suppress the movement along one of the coordinates, the other options are the stable stratification of the fluid, strong rotation, magnetic fields and the compressibility of the medium.

For the plane turbulent mixing layer, which is described by the system of full Navier-Stokes equations appropriate definition of the physical characteristics of the instantaneous flow can be obtained only in a three-dimensional formulation of the problem, while the average characteristics can be modeled by two-dimensional Navier-Stokes equations [2]. Experimental studies [2-4] showed that the two-dimensional turbulent field accurately predicts the structure of the flow until the transitions (go to the intense turbulence) [3-5]. Even after the appearance the developed mixing layer with intense turbulence

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coherent structures are quasi-two-dimensional and turbulent field can be described by 2D Navier-Stokes [6]. One additional benefit of two-dimensional turbulence is that it provides an excellent opportunity to test different turbulence models (model aspiring to an adequate description of turbulence, must be sensitive to a change in the dimension of space and correctly reflect its properties in the case of two and three dimensions [1]).

In the present paper a numerical simulation of quasi-2D supersonic mixing layer of multispecies reacting gases using 2D-DNS and 2D-RANS approaches are implemented. In this study, suggesting that the integral scale is small and the significant influence of compressibility at turbulent field is considered to be quasi-2D.

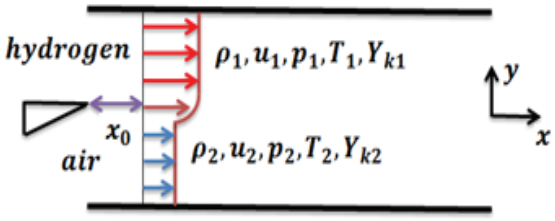

Fig. 1. Shear layer flow configuration.

The inflow physical parameters profile across the non-premixed hydrogen (fuel) and air flow at the splitter plate leading edge is assumed to vary smoothly according to a hyperbolic-tangent function (Fig. 1).

Mathematical Formulation and Numerical Methods

The mathematical model is based on the main conservation laws of mass, momentum, energy and transport of components. The system of Navier-Stokes and Reynolds averaged Navier-Stokes equations for multispecies turbulent chemically reacting gas mixtures are used. The energy fluxes due to thermal conduction and diffusion of species are given by Fourier heat conduction law and Fik's law, respectively. A thermally perfect gas is assumed for each species so that the heats, enthalpy and internal energy are functions of temperature only. The specific heat at constant pressure and enthalpy of each species are approximated using fourth order polynomial formula. Temperature is determined using Newton-Raphson iteration procedure [11-12]. Numerical values of empirical constants taken in accordance with the JANAF thermochemical table [11]. The Wilke formula is used to determine the mixture viscosity coefficient in terms of the mass fractions [11-12]. Turbulent viscosity is calculated using *k-e* model [11]. The chemical reactions of hydrogen H_2 with air are described using Jachimowski's seven species model used in the NASA SPARK code [12]. This model includes the seven species: H_2, O_2, H_2O, OH, H, O, N_2.

For the shear layer configuration at the inflow all physical variables are varied smoothly from hydrogen (fuel) flow to air flow using a hyperbolic-tangent function [9]. The pressure is assumed to be uniform across the shear layer. On the lower, upper boundary and at the outflow the non-reflecting boundary conditions are imposed [11-12]. In order to produce the roll-up and pairing of vortex rings, an unsteady boundary condition is also applied at the inlet plane [9].

The numerical solution of 2D-DNS and 2D-RANS equations are calculated in two steps. The first-step solves for the gas dynamic parameters (ρ, u, w, E_t) and second-step the species (Y_k, k = 1.7) with mass source terms. The approximation of convection terms are performed by the ENO-scheme of third-order accuracy [10-12]. The ENO scheme is constructed on the basis of Godunov method, where piecewise polynomial function is defined by the Newton's formula of the third degree. In approximation of derivatives of diffusion terms, second-order central-difference operators are used. The system of the finite difference equations are solved by using matrix sweep method. Then it is necessary to define Jacobian matrix which in the case of the thermally perfect gas represents difficult task. This problem is connected by explicit representation of pressure through the unknown parameters. Here pressure is determined by using the following formula

$$p = (\bar{\gamma} - 1)\left[E_t - \frac{1}{2}\rho\left(u^2 + w^2\right) - \rho\frac{h_0}{\gamma_\infty M_\infty^2}\right] + \frac{\rho T_0}{M_\infty^2 W} \quad (1)$$

where $\bar{\gamma} = \frac{h_{sm}}{e_{sm}}$ - is an effective adiabatic parameter of the gas mixture $h_{sm} = \sum_{i=1}^{N} Y_i \int_{T_0}^{T} c_{p_i} dT$, $e_{sm} = \sum_{i=1}^{N} Y_i \int_{T_0}^{T} c_{v_i} dT$ - enthalpy and internal energy of the mixture minus the heat and energy of formation; T_0 = 293 K - standard temperature of formation.

The equations for species are solved by the scalar sweep, where in the first-step convection and diffusion terms are included and calculated using ENO scheme. In the second-step, the matrix equation with terms ($\dot{w}_k = W_k \dot{\omega}_k$) is solved implicitly. These source terms $\dot{W}_k$ are linearized by expansion in a Taylor series,

$$\dot{W}_k^{n+1} = \dot{W}_k^n + \gamma\left(\frac{\partial \dot{W}_k}{\partial Y_m}\Delta Y_m + \frac{\partial \dot{W}_k}{\partial T}\Delta T + \frac{\partial \dot{W}_k}{\partial \rho}\Delta\rho\right) \quad (2)$$

2D Mixing and Combustion Simulation

The free shear layer of hydrogen-air flows mixing and combustion are numerically studied. The simulations are performed in a dimensionless rectangular domain of 350 in stream-wise direction and 120 in transverse direction. Initial momentum thickness is 0.0000935 m. At the inflow plane, hydrogen-nitrogen mixture enters from the upper half and air enters from the lower half. A 526 × 201 grid with stretching at the entrance and mixing layer was used. This grid allows taking into account the smallest Kolmogorov scale. The hydrogen flow parameters are M_0 = 2.0, T_0 = 2000 K, p_0 = 101325 Pa, and air flow parameters are M_∞ = 2.1, T_∞ = 2000 K, p_∞ = 101325 Pa. Initial mass fraction of upper flow Y_{H_2} = 0.1, Y_{O_2} = 0, Y_{N_2} = 0.9, while lower flow Y_{H_2} = 0, Y_{O_2} = 0.232, Y_{N_2} = 0.768.

Isolines of hydrogen (H_2) and water vapor (H_2O) fraction without inflow perturbation and using 2D-DNS are presented in Figs. 2 and 3.

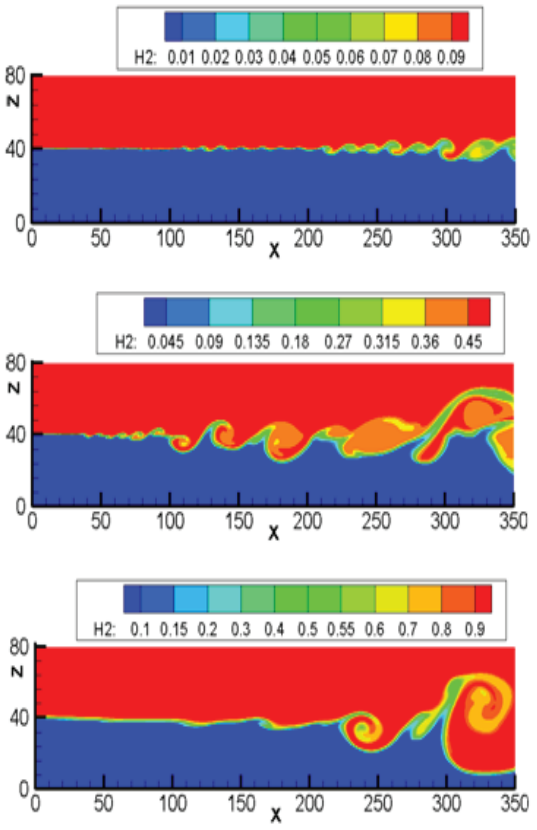

Fig. 2. Isolines of H_2 with variation of initial mass fraction of upper flow hydrogen: (a) Y_{H_2} = 0.1, (b) Y_{H_2} = 0.5, (c) Y_{H_2} = 1.0.

It is seen from these figures that with increasing initial mass fraction of hydrogen in upper flow side the vorticity thickness increases. Formation of combustion product occurs in the lower part of mixing layer, where is more oxidant is placed (Fig. 3). The maximum value of water vapor is observed in the case of Y_{H_2} = 1.0 (Fig. 3 c).

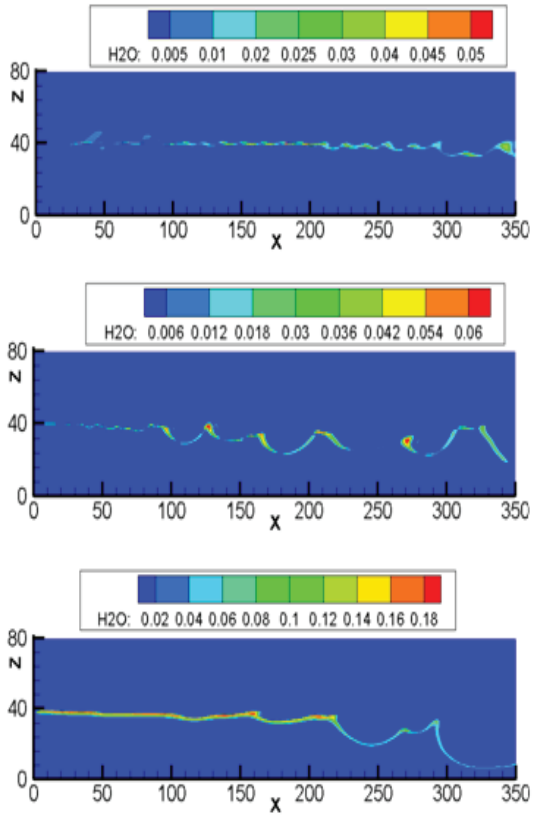

Fig. 3. Isolines of H_2O with variation of initial mass fraction of upper flow hydrogen: (a) Y_{H_2} = 0.1, (b) Y_{H_2} = 0.5, (c) Y_{H_2} = 1.0.

Isolines of hydrogen (H_2) and water vapor (H_2O) fraction for the case of Y_{H_2} = 1.0 with different inflow perturbations obtained from linear stability theory (LST) [13] and using 2D-DNS are presented in Figs. 4 and 5 for the short domain. Initial perturbation allows obtaining (organize) a more realistic turbulent flow. In [13] LST analysis as a base flow was considered laminar flow. In the present study it is assumed that perturbation in [13] allows modeling turbulent flow structure.

From the Figs. 4 and 5 it can be observed that results obtained by perturbation with different frequency predicted from LST [13] and without perturbation quantitatively has no difference, while qualitatively their little differs. It is due to the fact that frequencies predicted using LST is the natural frequencies of vortex shedding, which has no additional perturbation (such as acoustics, etc.).

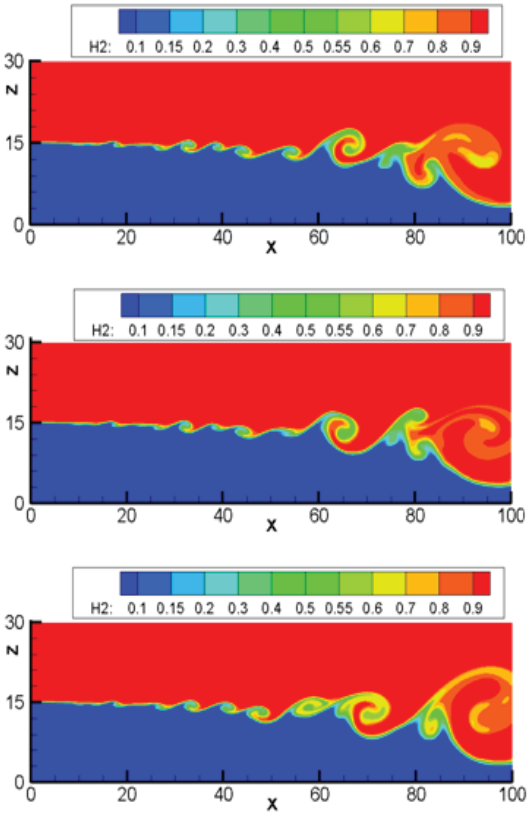

Fig. 4. Isolines of H_2 with various inflow perturbations: (a) – no pert., (b) – one freq. pert., (c) – four freq. pert.

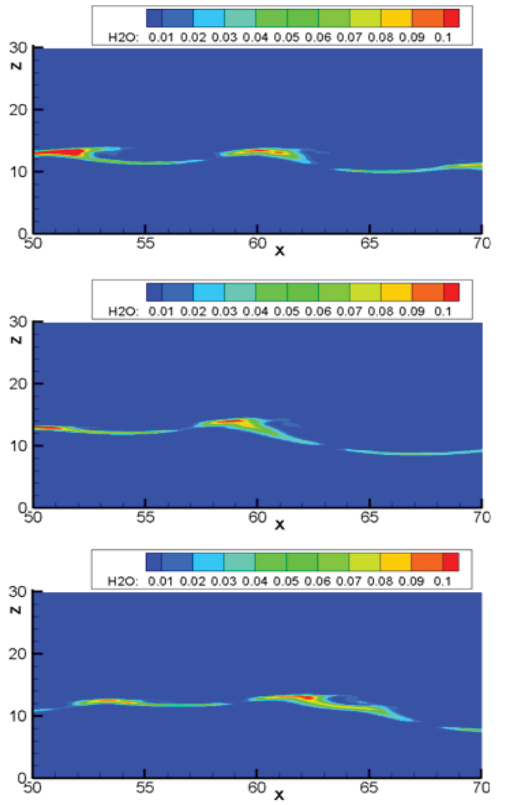

Fig. 5. Isolines of H_2O with various inflow perturbations: (a) – no pert., (b) – one freq. pert., (c) – four freq. pert.

Figure 6 illustrates dependence of mean velocity on transverse coordinate for calculations of [8] and present calculations using 2D-DNS, 2D-RANS.

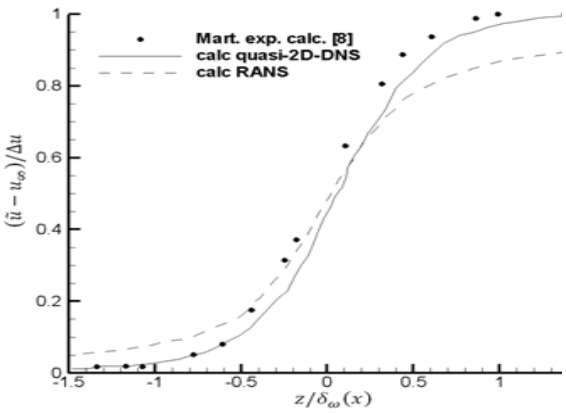

Fig. 6. Mean velocity profile.

It can be observed from Fig. 6 that 2D-DNS is closure to numerical experiment of [8] comparing with 2D-RANS simulation.

Isolines of mass fraction of oxygen (O_2) without inflow perturbation using 2D-RANS and 2D-RANS approaches are presented in Fig. 7.

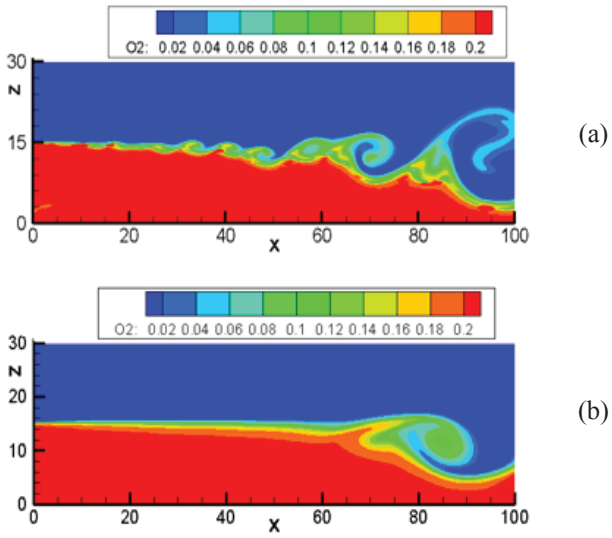

Fig. 7. Isolines of O_2 without perturbation using (a) – quasi-DNS, (b) – RANS approaches.

As it is seen from Fig. 7 in the case of RANS simulation the information about mixing layer structure is lost. At the same time 2D-DNS calculation is more accurate and unsteady mixing layer well observable.

Conclusion

The developed mathematical model based on 2D-DNS and 2D-RANS, as well as computer code allows to study of turbulent mixing and combustion with various flow configuration and subsequent reaction. At the same time detailed information can be pull out by using first method for quasi-2D turbulent problem. Second approach provides inaccurate, smoothed results. So 2D-DNS with certain inflow perturbation for quasi-2D turbulent shear flow can be serving as a recommendation tool.

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