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Numerical study of combustion efficiency in supersonic free shear layer*

Numerical study of two-dimensional supersonic hydrogen-air mixing and combustion in free shear layer is performed. The system of Navier-Stokes equations for multispecies reacting flow is solved using ENO scheme of third-order in accuracy. In order to produce the roll-up and pairing of vortex rings, an unsteady boundary condition is applied at the inlet plane. At the outflow, the non-reflecting boundary condition is taken. For the description of reaction pathways of hydrogen, a seven species chemical reaction model by Jachimowski is adopted. The combustion efficiency is reported for different Mach number of flows.
Key words: supersonic shear flow, mixing layer, hydrogen combustion, ENO-scheme, seven chemical reactions mechanism, combustion efficiency.

Е. Беляев

Численное изучение полноты сгорания в сверхзвуковом свободном сдвиговом слое

В работе представлено численное изучение двумерного сверхзвукового смешения и горения водородно-воздушной смеси в свободном сдвиговом слое. Система уравнений Навье-Стокса для многокомпонентного реагирующего газа была решена с использованием ENOсхемы третьего порядка точности. Для того, чтобы получить образование пары закручивающихся вихрей, во входном сечении реализована постановка нестационарных граничных условий. На выходном сечении было использовано граничное условие не отражения. Для моделирования протекания химических реакций была использована семи стадийная модель Джачимовского. Полнота сгорания смеси была представлена для различных чисел Маха потоков.
Ключевые слова: сверхзвуковое сдвиговое течение, слой смешения, горение водорода, ENOсхема, семи стадийный механизм химических реакций, полнота сгорания.

Е. Беляев

Дыбыс жылдамдығынан жоғары еркін жылжымалы қабаттағы толық жануды сандық түрде зерттеу

Осы жұмыста екі өлшемді еркін жылжымалы қабаттағы сутегі-ауа қоспасының дыбыс жылдамдығынан жоғары араласуы мен жануы сандық түрде зерттелінген. Көп компонентті реакцияланатын газ үшін Навье-Стокс теңдеулер жүйесі үшінші ретті дәлдікпен аппроксимацияланатын ENO сұлбасымен шешілген. Қос бұралатын құйындар жұбын алу үшін кірберіс шекарада бейстационарлы шекаралық шарты қойылған. Шығаберіс шекарада шағылыспайтын шекаралық шарты бейімделген. Жеті сатылы Джачимовский химиялық реакция нобайы сутегінің жануын сипаттауға қолданылды. Қоспаның толық жануын зерттеу үшін ағындардың әр түрлі Мах сандары қарастырылды.

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Түйін сөздер: дыбыс жылдамдығынан жоғарыжылжымалы қабат, араласу қабаты, сутегінің жануы, ENO сұлбасы, жеті сатылы химиялық реакциялар механизмі, толық жану.

Introduction

One of the actual challenges of modern aircraft industry is to create a hypersonic vehicles allowing for the short period of time cover the farthest distances in the globe. As a fuel oxidizer in such devices is taken the oxygen in the air from the atmosphere, therefore the ratio of fuel weight to the hypersonic vehicle weight is about the same as in conventional aircrafts. As the fuel it can be used hydrogen or hydrocarbon fuels.

Hydrocarbon fuels such as aviation kerosene, methane or ethylene attracts great attention today. For example, methane, which is simplest hydrocarbon fuel has comparatively high specific impulse as well as the best thermochemical properties. However, hydrogen has been of primary interest as a fuel of the future aerospace vehicles. The specific combustion heat of hydrogen is about 2-2.5 times more than methane and ethylene. As the same time the hydrogen has a limitations such as low density, which results in the need for large fuel tanks.

The mathematical model and numerical method of solution of supersonic combustion in shear layer flow has been performed by many researchers [1-10]. In these works the basic efforts is directed on analysis of influence different effects such as inlet swirl, initial temperature, velocity and pressure ratios on ignition time delay. The detail chemical reaction mechanism during calculation have been adopted in [4, 5-6], while in [1-2, 6] reduced reaction mechanisms. In these investigations with the simulation of reacting shear layer were insufficiently paid attention to the combustion efficiency estimation.

In the present study, the third order essentially non-oscillatory (ENO) finite difference scheme is adopted to solve the system of Navier-Stokes equations with chemical kinetics terms to supersonic planar shear layer. Simulation of the flame propagation with combustion products formation is performed including the seven reaction and seven component Jachimowski's kinetics mechanism. The inflow physical parameters profile across the non-premixed hydrogen (fuel) and air stream at the splitter plate leading edge is assumed to vary smoothly according to a hyperbolic-tangent function (Fig. 1).

Mathematical model

The two-dimensional Favre-averaged Navier-Stokes equations for multi-species flow with chemical reactions is:

$$\frac{\partial \overrightarrow{U}}{\partial t} + \frac{\partial \left(\overrightarrow{E} - \overrightarrow{E}_v\right)}{\partial x} + \frac{\partial \left(\overrightarrow{F} - \overrightarrow{F}_v\right)}{\partial z} = \overrightarrow{W} \tag{1}$$

where the vector of the dependent variables and the vector fluxes are given as

$$\overrightarrow{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho w \\ E_t \\ \rho Y_k \end{pmatrix}, \qquad \overrightarrow{E} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u w \\ (E_t + p)\, u \\ \rho u Y_k \end{pmatrix}, \qquad \overrightarrow{F} = \begin{pmatrix} \rho w \\ \rho u w \\ \rho w^2 + p \\ (E_t + p)\, w \\ \rho w Y_k \end{pmatrix},$$

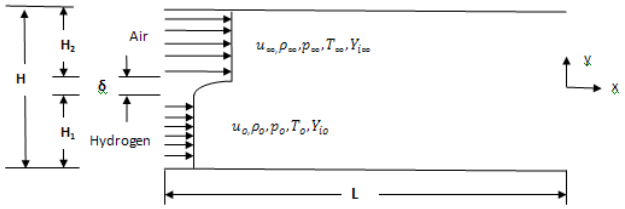

Figure 1. An illustration of the flow configuration

$$\overrightarrow{E}_v = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xz} \\ u\tau_{xx} + u\tau_{xz} - q_x \\ J_{kx} \end{pmatrix}, \quad \overrightarrow{F}_v = \begin{pmatrix} 0 \\ \tau_{xz} \\ \tau_{zz} \\ w\tau_{xz} + w\tau_{zz} - q_z \\ J_{kz} \end{pmatrix}, \quad \overrightarrow{W} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ W_k \cdot \dot{\omega}_k \end{pmatrix}.$$

Here, the viscous stresses, thermal conduction, and diffusion flux of species are:

$$\tau_{xx} = \frac{\mu}{Re}\left(2u_x - \frac{2}{3}(u_x + w_z)\right), \tau_{zz} = \frac{\mu}{Re}\left(2w_z - \frac{2}{3}(u_x + w_z)\right),$$

$$q_x = \left(\frac{\mu}{PrRe}\right)\frac{\partial T}{\partial x} + \frac{1}{\gamma_\infty M_\infty^2}\sum_{k=1}^{N} h_k J_{xk}, \quad q_z = \left(\frac{\mu}{PrRe}\right)\frac{\partial T}{\partial z} + \frac{1}{\gamma_\infty M_\infty^2}\sum_{k=1}^{N} h_k J_{zk},$$

$$J_{kx} = \frac{-\mu}{ScRe}\frac{\partial Y_k}{\partial x}, \quad J_{kz} = \frac{-\mu}{ScRe}\frac{\partial Y_k}{\partial z}, \quad \tau_{xz} = \tau_{zx} = \frac{\mu}{Re}(u_z + w_x),$$

where Y_k is the mass fraction of k^{th} species, $\dot{\omega}_k$ – rate of mass production of species, $k = 1, \ldots, N$, with N – number a components in a gas mixture. The thermal equation for multi-species gas is:

$$p = \frac{\rho T}{\gamma_\infty M_\infty^2 W}, \quad W = \left(\frac{1}{\gamma_\infty M_\infty^2}\frac{Y_k}{W_k}\right)^{-1}, \quad \frac{1}{\gamma_\infty M_\infty^2} Y_k = 1, \tag{2}$$

where W_k is the molecular weight of the species.

The equation for a total energy is given by

$$E_t = \frac{\rho h}{\gamma_\infty M_\infty^2} - p + \frac{1}{2}\rho\left(u^2 + W^2\right). \tag{3}$$

The enthalpy of the gas mixture is calculated according to $h = \sum_{k=1}^{N} Y_k h_k$, with specific enthalpy of k^{th} species evaluated suing $h_k = h_k^0 + \int_{T_0}^{T} c_{pk} dT$.

The specific heat at constant pressure for each component c_{pk} is:

$$c_{pk} = C_{pk}/W, \quad C_{pk} = \sum_{i=1}^{5} \overline{a}_{ki} T^{(i-1)}, \quad \overline{a}_{jk} = a_{jk} T_\infty^{j-1},$$

where the molar specific heat C_{pk} is given in terms of the fourth degree polynomial with respect to temperature, consistent with the JANAF Thermochemical Tables [11].

The system of the equations (1) is written in the conservative, dimensionless form. The air flow parameters are ρ_∞, u_∞, w_∞, T_∞, h_∞, W_∞, R_∞, hydrogen jet parameters are ρ_0, u_0, w_0, T_0, h_0, W_0, R_0. The governing parameters are the air flow parameters, the pressure and total energy are normalized by $\rho_\infty u_\infty^2$, the enthalpy by $R_0 T_\infty / W_\infty$, the molar specific heat by R_0 and the spatial distances for case I by the slot width l, for case II by the initial thickness of the vorticity layer δ.

The mixture averaged molecular viscosity is evaluated using from Wilke's formula.

The chemical reactions of hydrogen H_2 with air are described using Jachimowski's seven species model used in the NASA SPARK code [11]. This model includes the following seven species: H_2, O_2, H_2O, OH, H, O, N_2.

Initial and boundary conditions

At the entrance:

$$u_1 = M_0\sqrt{\frac{\gamma_0 R_0 T_0}{W_0}}, \quad w_1 = 0, \quad p_1 = p_0, \quad T_1 = T_0, \quad Y_{k1} = Y_{k0}, \quad k = k_0, \quad \varepsilon = \varepsilon_0$$

$$\text{at} \quad x = 0, \quad 0 \le z < H_1;$$

$$u_2 = M_\infty\sqrt{\frac{\gamma_\infty R_0 T_\infty}{W_\infty}}, \; w_2 = 0, p_2 = p_\infty, \; T_2 = T_\infty, Y_{k2} = Y_{k\infty}, \; k = k_\infty, \; \varepsilon = \varepsilon_\infty$$

$$\text{at} \quad x = 0, \; H_1 + \delta \le z < H_2.$$

In the region of $H_1 \le z \le H_1 + \delta$ all physical variables are varied smoothly from hydrogen (fuel) flow to air flow using a hyperbolic-tangent function of any variable φ, so the inflow profiles are defined by

$$\varphi(z) = 0.5(\varphi_2 + \varphi_1) + 0.5(\varphi_2 - \varphi_1)\tanh(0.5z/\theta) \quad \text{at} x = 0, 0 \le z \le H,$$

where $\varphi = (u, v, p, T, Y_k, k, \varepsilon)$, θ – is the momentum thickness. The pressure is assumed to be uniform across the shear layer. On the lower and upper boundary the condition of symmetry are imposed. At the outflow, the non-reflecting boundary condition is used [12]. In order to produce the roll-up and pairing of vortex rings, an unsteady boundary condition is also applied at the inlet plane [13].

Method of solution

The numerical solution of the system of equations (1) is 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 is performed by the ENO-scheme of third-order accuracy [14-18]. 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

$$p = (\overline{\gamma} - 1)\left[E_t - \frac{1}{2}\rho\left(u^2 + W^2\right) - \rho\frac{h_0}{\gamma_\infty M_\infty^2}\right] + \frac{\rho T_0}{M_\infty^2 W}, \tag{4}$$

where $\overline{\gamma} = \dfrac{h_{sm}}{e_{sm}}$ – is an effective adiabatic parameter of the gas mixture $h_{sm} = \sum\limits_{i=1}^{N} Y_i \int\limits_{T_0}^{T} c_{p_i} dT$, $e_{sm} = \sum\limits_{i=1}^{N} Y_i \int\limits_{T_0}^{T} c_{v_i} dT$ – enthalpy and internal energy of the mixture minus the heat and energy of formation; $T_0 = 293K$ – 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 $\left(\dot{w}_k^{n+1} = W_k\dot{\omega}_k\right)$ is solved implicitly. These source terms $\dot{W}_k$ are linearized by expansion in a Taylor series,

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

The temperature is found by using the Newton-Raphson iteration from the equations [16-18].

Results and discussion

Table 1 – Jachimowski's reaction mechanism

Reaction number	Reaction	A_k $(m^3/mole \cdot s)$	β_k	E_k/R
1	$H_2 + O_2 = OH + OH$	0.170E +14	0.0	24233
2	$H + O_2 = OH + O$	0.142E +15	0.0	8254
3	$OH + H_2 = H_2O + H$	0.316E +08	1.8	1525
4	$O + H_2 = OH + H$	0.207E +15	0.0	6920
5	$OH + OH = H_2O + O$	0.550E +14	0.0	3523
6	$H + OH + M = H_2O + M$	0.221E +23	-2.0	0
7	$H + H + M = H_2 + M$	0.653E +18	-1.0	0

The free shear layer of hydrogen-air flows mixing and combustion are numerically studied. The simulations are performed in a rectangular domain of $4cm$ in stream-wise direction and

1.5cm in transverse direction. The splitter plate thickness is 0.1cm, and at the trailing edge is 0.0045cm. At the inflow plane, hydrogen enters from the lower half and air enters from the upper half. A 401×151 grid with stretching at the entrance and mixing layer was used. The hydrogen flow parameters are $M_0 = 1.4$ ($M_0 = 1.1$), $T_0 = 400$K, $P_0 = 101320$Pa, and air flow parameters are $M_\infty = 1.8$ ($M_\infty = 1.5$), $T_\infty = 1300$K, $P_\infty = 101320$Pa.

To modeling of hydrogen-air combustion a Jachimowski's model is adopted (Table 1). It includes the seven species and seven elementary reactions.

For example, in the case of elementary reaction $OH + H_2 = H_2O + H$ due to molecular motion in gas phase hydroxyl radicals (OH) can impact with hydrogen molecule (H_2). In the case of nonreacting inert collision molecules just collide and repulse, in the case of reacting collision the H_2O and H are formed.

The isolines of the formation of water vapor (H_2O) concentrations contours at various times are presented in Figures 2.

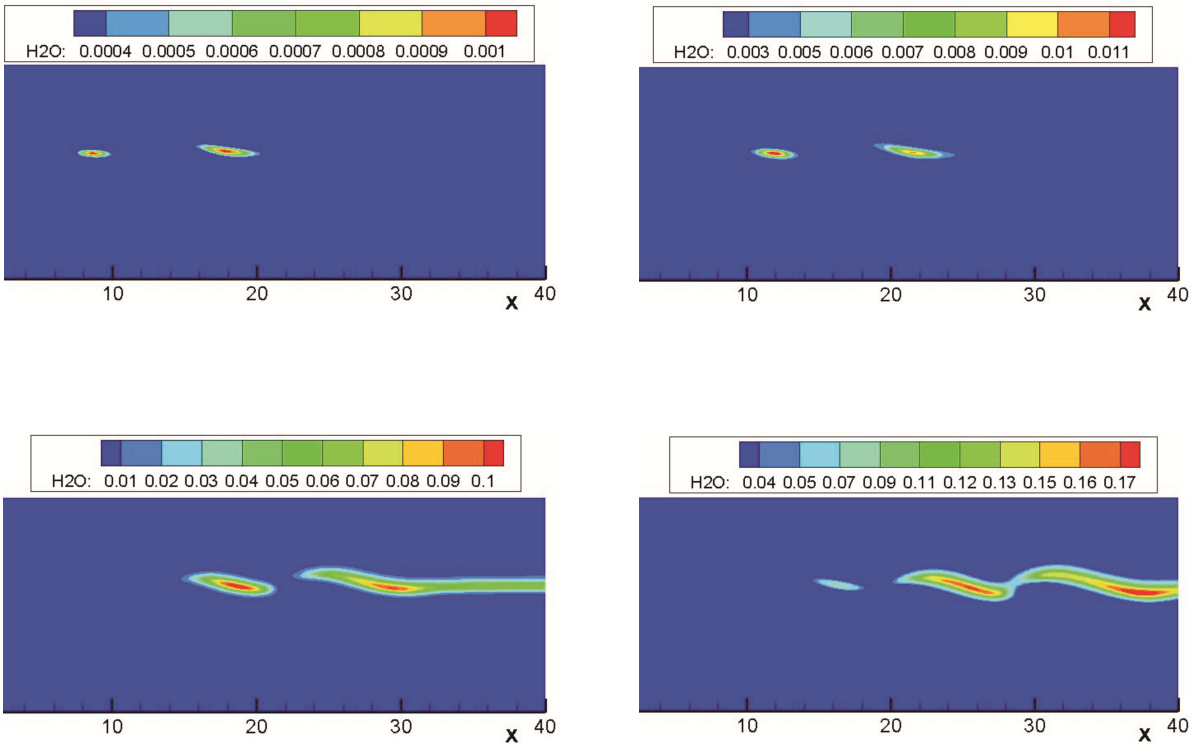

Figure 2. The dynamic of water vapor concentration formation at four times a) $t = 5.35$, b) $t = 6.4$, c) $t = 8.5$, d) $t = 10.6$ mks

It is visible (Figure 2-a), initially combustion product H_2O is concentrated in the thin mixing layer at the moment $t = 5.35$ mks. In this time the maximum of water vapor is of the order 10^{-4}, Figure 2-a. From the period of time $t = 5.35$ up to $t = 6.4$ mks (Figure 2-b) this value growth up to 10^{-3}. Obviously, it is the induction period which is period of accumulation of radicals and active centers, where there is also growth reaction rate.

The combustion efficiency can be estimated from the overall chemical reaction (5) of hydrogen oxidation. It appears from this reaction that for the 0.004 $kg/mole$ hydrogen

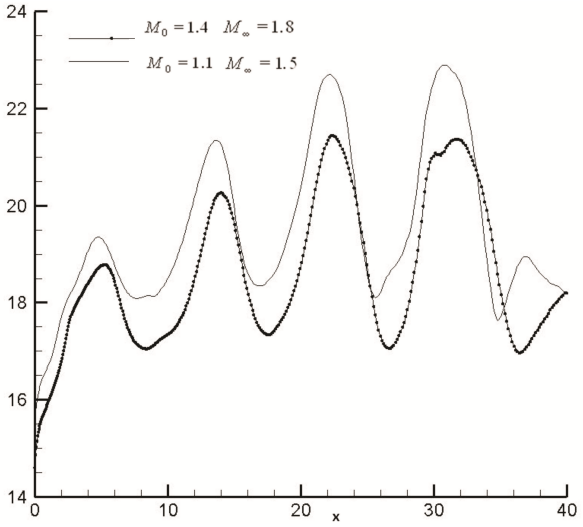

Figure 3. An illustration of combustion efficiency along the longitudinal coordinate

completely oxidation it is need 0.032 $kg/mole$ oxygen. As a parameter characterized complete combustion it is taken the relation of the mass flow rates Q_{O_2}/Q_{H_2}, where $Q_{O_2} = \int \rho_{O_2} u_\infty dz$ and $Q_{H_2} = \int \rho_{H_2} u_0 dz$. Figure 3 shows the dependence of Q_{O_2}/Q_{H_2} on longitudinal coordinate for two cases. This relation should be $Q_{O_2}/Q_{H_2} \geq 8$ to complete hydrogen combustion.

Numerical experiment revealed that at the exit plane $x = 40$ this relation is equal to 18.07 for both Mach number cases, which is pointing out that the hydrogen completely oxidize. The initial mass flow rates ratio at the entrance for M_0 =1.4, $M_\infty = 1.8$ is $Q_{O_2}/Q_{H_2} = 14.8$, which indicate on the poor mixture. For Mach numbers M_0 =1.1, $M_\infty = 1.5$ the initial mass flow rates ratio $Q_{O_2}/Q_{H_2} = 15.6$. Maximum value of Q_{O_2}/Q_{H_2} for higher Mach number case is 21.44, while for lower case is 22.9. The value lowering of this parameter is due to the formation of combustion products.

This comparison has been confirmed that subsonic zones have not strong affect on increasing the total residence time of fuel (hydrogen) in the combustion chamber. So the presence of isolated vortices and their growth downstream provides a better mixing of fuel, air and hot combustion products, which greatly stabilizes the combustion process.

Conclusion

The flowfield structures of supersonic planar shear layer and combustion computed by calculation of the system of two-dimensional Navier-Stokes equations. The numerical method is based on the third order ENO finite-difference scheme. The numerical results of hydrogen-air mixture combustion based on Jachimowski's seven-species seven reaction model.

The calculation reacting shear layer revealed distribution and enhancement of hydrogen-air mixing and combustion is strongly depend on vortices formation, a namely their intensity and growing. The present numerical experiments show that for the given geometrical and physical parameters the hydrogen reaches the combustion efficiency.

Thus the constructed algorithm based on the high order scheme and computer code for turbulent supersonic reacting flow allows to study influence parameters that control mixing and combustion, which is important in the design of supersonic combustion ramjet (scramjet)

engines.

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