УДК 533; 532.517.4; 536.46:533.6; 534.222.2

Ye. Belyayev[1], A. Kaltayev[2], A. Naimanova[3], Harsha K. Chelliah[4]
[1 2]*Al-Farabi Kazakh National University, Almaty, Kazakhstan*
[1]*e-mail: yerzhan.belyayev@gmail.com*
[2]*e-mail: aidarkhan.kaltayev@kaznu.kz*
[3]*Institute of Mathematics, Ministry of Education and Science, Almaty, Kazakhstan*
[3]*e-mail: ked@math.kz*
[4]*University of Virginia School of Engineering and Applied Science, Mechanical and Aerospace Engineering, Charlottesville VA, USA*
[4]*e-mail: harsha@virginia.edu*

# Numerical Investigation of Combustion in Supersonic Flow at the Transverse Injection of Hydrogen[1]

A computational fluid dynamics code for multispecies, Favre-Averaged Naveir-Stokes equations is developed to simulate the turbulent supersonic two-dimensional reacting flow. The explicit ENO scheme of third-order in accuracy has is used to solve the system of equations, together with the algebraic Baldwin-Lomax's turbulence model to calculate the eddy viscosity coefficient. For the description of reaction pathways of hydrogen, a seven species chemical reaction model by Jachimowski is adopted. Computer code is validated by comparison of the predicted solution with previous simulations of the two-dimensional chemically reacting supersonic hydrogen-air flow, where the fuel is injected in transverse direction to the main air flow via slots located on the wall. Influence of boundary conditions for the temperature on the walls on turbulent mixture is reported.
*Keywords*: supersonic flow, hydrogen combustion, ENO-scheme, seven chemical reactions mechanism.

Е.К. Беляев, А. Қалтаев, А. Ж. Найманова, Харша К. Чэллая

## Дыбыс жылдамдығынан жоғары ағындағы көлденең бағытта инжекцияланатын сутектің жануын сандық түрде зерттеу

Екі өлшемді дыбыс жылдамдығынан жоғары турбулентті ағынды модельдеу үшін Фавр бойынша орташаланған көп компонентті Навье-Стокс теңдеулер жүйесіне есептеу гидродинамикасының бағдарламалық коды жасалынған. Берілген теңдеулер жүйесін шешу үшін айқындалған ENO схема (үшінші ретті дәлдікпен) қолданылған және турбулентті тұтқырлықты табу үшін алгебралық Болдуин-Ломакс моделі колданылған. Сутектің реакцияға түсуін сипаттау үшін Спарктың жеті реакциялық механизмін аламыз. Жасалынған бағдарламалық код екі өлшемді химиялық реакцияға түсетін дыбыс жылдамдығынан жоғары сутекті-ауа ағынының байланысы, оның ішінде басты ауа ағыны жазық каналға кіріп, перпендикулярлы бағытта шекаралық қабырғалардан үрленетін сутекпен байланысын сипаттайтын есеппен тексерілген. Қабырғалардағы температураның шекаралық шартының турбулентті араласу процесіне әсері зерттелінген.

[1]Работа выполнена при поддержке грантового финансирования научно-технических программ и проектов Комитетом науки МОН РК, грант № 0716/ГФ, 2012г.-2014г.

Е.К. Беляев, А. Калтаев, А. Ж. Найманова, Харша К. Чэллая

## Численное исследование горения в сверхзвуковом потоке с поперечной инжекцией водорода

В данной работе был разработан вычислительный программный код для многокомпонентного осредненного по Фавру уравнения Навье-Стокса, который позволяет моделировать двумерные турбулентные сверхзвуковые реагирующие течения. Для численного решения системы уравнений была использована ENO схема третьего порядка точности, для вычисления турбулентной вязкости использована модель Болдуина-Ломакса. Для описания процессов реакции водорода был использован механизм семи химических реакций Спарка. Построенный компьютерный код был проверен решением двумерной химически реагирующей сверхзвуковой водородно-воздушной смеси, где основной воздушный поток входит в плоский канал и водород вдувается перпендикулярно из стенок канала. Было исследовано влияние граничных условий для температуры на стенке на турбулентное смешение.

**Introduction.** Interaction of finite-rate chemical reaction of hydrogen with turbulent mixing of supersonic air and fuel flow is observed in many problems of modeling SCRAM jet engines used in modern rocket and space technology. It is very difficult to ignite and maintain combustion process in supersonic ramjet (scramjet) engines and it continues to be a very challenging and time consuming problem. Since the airflow is supersonic, fuel in the combustion chamber is associated with a very short residence time (about 1 ms). During this short period of time, the fuel must mix with air at the molecular level and the chemical reaction should be completed prior to leaving the engine for realization of the full thrust.

The layer of mixing and combustion length is an important factor in the design of supersonic ramjet engines. The flow field in such devices is very complex. It is well known that the level of complexities are determined by processes controlling turbulent fuel-air mixing, chemical reaction, shock waves, separation region ahead of the jet and behind of it. Consequently, the investigation of the turbulent reactive flows is of great importance in supersonic combustion. Some of aspects of the supersonic flows with transverse injection of fuel jets, with and without chemical reaction have been considered in the past [1-3]. The angle of inclination of the shock waves formed and the length of the separation-region were found to be a function of the jet's pressure ratio. The enhancement of mixing have been investigated in [4] by using TVD scheme. Thus, further developed computational fluid dynamic codes for solution of reacting Navier-Stokes equations for supersonic multi-species flow is an important task and is the focus of this work.

The two-dimensional supersonic turbulent flow of multi-component gas, in the presence of cross injection hydrogen from the bottom and top walls of the channel, has been considered previously. For convenience of calculation, in this work we consider only the injection of the fuel stream from the bottom wall, as show in Fig. 1.

### 1. Mathematical Model

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

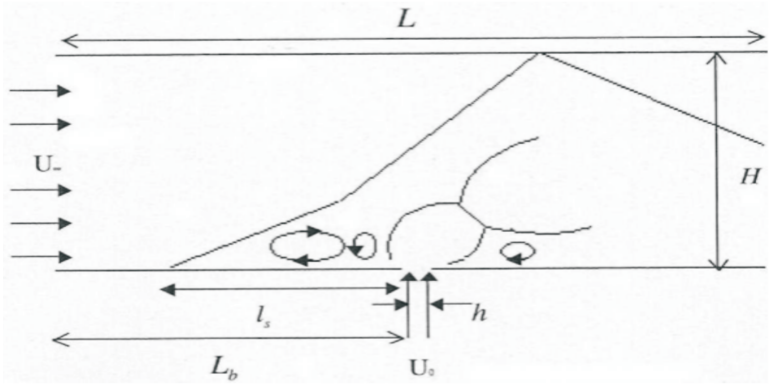


Figure 1: An illustration of the flow configuration.

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

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

$$\vec{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho w \\ E_t \\ \rho Y_k \end{pmatrix}, \quad \vec{E} = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u w \\ (E_t + P)\, u \\ \rho u Y_k \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} \rho w \\ \rho u w \\ \rho w^2 + P \\ (E_t + P)\, w \\ \rho w Y_k \end{pmatrix},$$

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

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

$$\tau_{xx} = \frac{\mu}{Re}(2u_x - \frac{2}{3}(u_x + w_z)), \tau_{zz} = \frac{\mu}{Re}(2w_z - \frac{2}{3}(u_x + w_z)), \tau_{xz} = \tau_{zx} = \frac{\mu}{Re}(u_z + w_x),$$

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

$$J_{kx} = -\frac{\mu}{ScRe}\frac{\partial Y_k}{\partial x}, J_{kz} = -\frac{\mu}{ScRe}\frac{\partial Y_k}{\partial z},$$

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

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

where $W_k$ is the molecular weight of the species.

The equation for a total energy is given by

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

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:

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

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 [5].

The system of the equations (1) is written in the conservative, dimensionless form. The flow parameters are $\rho_\infty, u_\infty, w_\infty, T_\infty, h_\infty, W_\infty, R_\infty$, jet parameters are $\rho_0, u_0, w_0, T_0, h_0, W_0, R_0$. The governing parameters are the entrance 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 by the slot width $l$.

The coefficient of viscosity is represented in the form of the sum of $\mu_l$ - molecular viscosity and $\mu_t$ - turbulent viscosity: $\mu = \mu_l + \mu_t$, where $\mu_t$ is defined according to Baldwin-Lomax's algebraic model. 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 [5]. This model includes the following seven species: ($H_2, O_2, H_2O, OH, H, O, N_2$).

The boundary conditions at the entrance plane is given as:

$$p = p_\infty, T = T_\infty, u = M_\infty \sqrt{\frac{\gamma_\infty R_0 T_\infty}{W_\infty}}, w = 0, Y_k = Y_{k\infty}, \quad x = 0, 0 \le z \le H;$$

in the input section the turbulent boundary layer on the wall is given, and the velocity profile approximated by power law.

The boundary conditions in the slot has the following form:

$$p = np_\infty, T = T_0, w = M_0 \sqrt{\frac{\gamma_0 R_0 T_0}{W_0}}, u = 0, Y_k = Y_{k0}, \quad z = 0, L_b \le z \le L_b + h;$$

here, $n = p_0/p_\infty$ is the jet pressure ratio, $p_0$ is the jet pressure, and $p_\infty$ is the flow pressure. On the lower wall the no-slip velocity condition is imposed, for the temperature the adiabatic and

constant wall condition are imposed, while on the upper boundary the condition of symmetry is assumed. At the outflow, the non-reflecting boundary condition is used [1].

## 2. 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 $(\rho, u, w, E_t)$ 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 [1,6-7]. 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 the Beam-Warming method with using matrix sweep. 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

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

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; $T_0 = 293K$ - 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 $(\dot{w_k} = W_k\dot{\omega_k})$ is solved implicitly. These source terms $\dot{W_k}$ are linearized by expansion in a Taylor series,

$$\dot{W_k^{n+1}} = \dot{W_k^n} + \gamma(\frac{\partial \dot{W_k}}{\partial Y_m}\Delta Y_m + \frac{\partial \dot{W_k}}{\partial T}\Delta T + \frac{\partial \dot{W_k}}{\partial \rho}\Delta\rho)$$

The temperature is found by using the Newton-Raphson iteration from the equations [1].

## 3. Numerical Results

The computation was performed on 241×181 space grid with respect to spatial coordinates. In the first case considered, the perpendicular injection of a gas into two-dimensional channel without chemical reactions was considered. The parameters of jet and air flow adopted were [1]: $M_0 = 1, T_0 = 217K, p_0 = 1.24MPa$, width of slot $0.0559cm$; $M_\infty = 2.9, T_\infty = 108K, p_\infty = 0.0663MPa$. The channel height and length were 7.62 and $15cm$, respectively. The slot was located at a distance of $10cm$ from the inflow plane. The results of the numerical experiment were in satisfactory agreement with experimental data and numerical calculations by other authors [1,8-9].

In the next case, the perpendicular injection of jet of hydrogen into planar air flow was numerically tested. Here, the width of slot is $0,0559cm$, jet parameters are $M_0 = 1.1, T_0 = 400K, p_0 = 1MPa$ and air $M_\infty = 3, T_\infty = 1300K, p_\infty = 0.25MPa$, and constant boundary

conditions on the wall was adopted. The height of the channel is 7.62$cm$, and length - 15$cm$. The slot was located on distance of 10$cm$ from the inflow plane.

The mechanism of hydrogen oxidation is a chain reaction, which is a consequence of the production of active centers or species, i.e. radicals, in the mixing region of the jet and the flow. Further dissociation of the molecular components of the mixture, as well as exchange reactions lead to the accumulation of active centers. Since the initiation reactions and chain-propagation reactions are endothermic, this stage of oxidation of hydrogen proceeds without significant heat generation, which indicates the presence of the induction period, characterized by constant temperature of homogeneous mixture. Figure 2 shows the flame propagation in the mixing zone using Jachimowski's seven species reaction model, i.e. $H_2$, $O_2$, $H_2O$, $OH$, $H$, $O$, $N_2$.

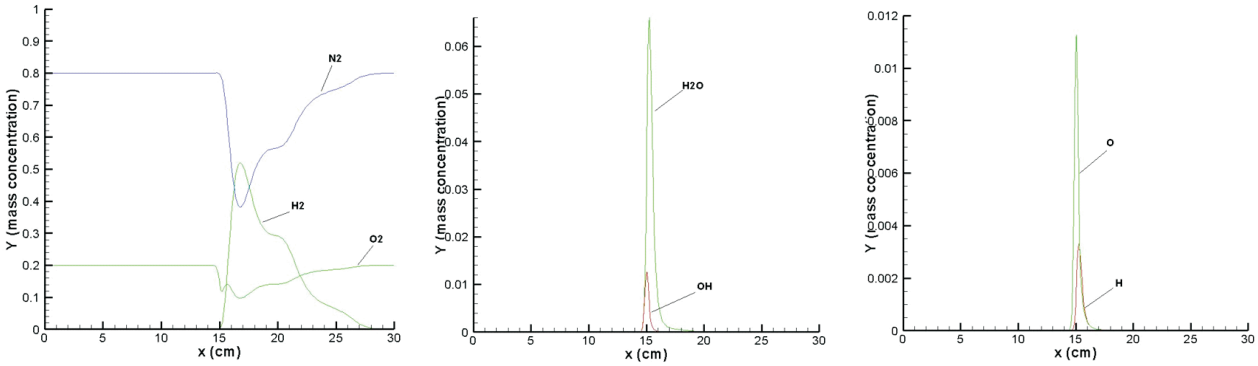


Figure 2 - The flame propagation in the mixing zone longitudinal section

Ignition begins in the mixing region of the jet with the flow at time t = 0.595 mks, where there are significant concentrations of water vapor, hydroxyl radical, hydrogen and oxygen atoms, which indicates the beginning of a chain branching reaction. As the shock waves occurs with sharp change in temperature, these values exceeds initial temperature of jet and flow. Temperature increase by shock waves precedes the oxidation of hydrogen by Arrhenius dependence of reaction rate on temperature. In turn, the hydrogen combustion, due to the intense heat release, leads to an increase in temperature and pressure in the combustion zone. Figure 3 shows that the maximum temperature is concentrated in the mixing zone where ignition of the mixture is occurring. Starting point of increasing the concentration of water vapor, and maximizing its value in the region where shock waves exert a significant influence on the diffusion of hydrogen burning. Shock waves lead to an increase in the temperature and mixing intensity of fuel and oxidizer.

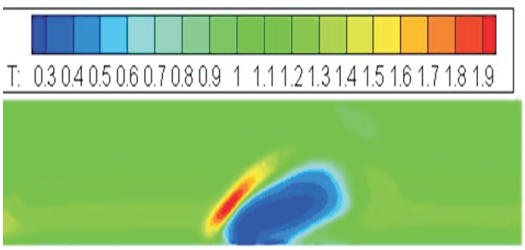


Figure 3 - The temperature field

In Figs.4-8, the contour plots of the distribution of hydrogen ($H_2$), water vapor ($H_2O$), hydroxyl radical ($OH$), hydrogen atom ($H$) and oxygen atom ($O$) concentrations are shown at different times. The present numerical experiments clearly show that the intense combustion zone is concentrated near wall for adiabatic boundary. Thus the constructed computer code for turbulent supersonic reacting flow allows to study influence parameters that control mixing and combustion.

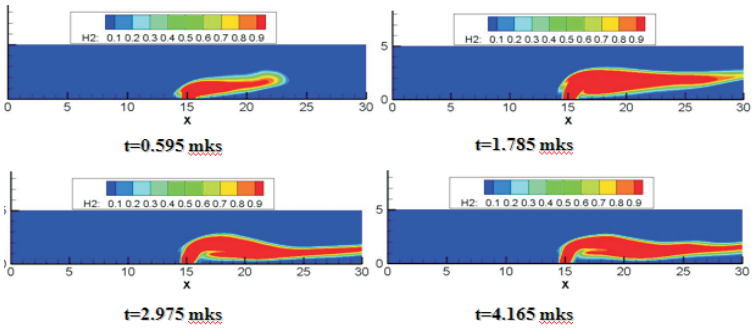


Figure 4 - The distribution of hydrogen concentration at different times

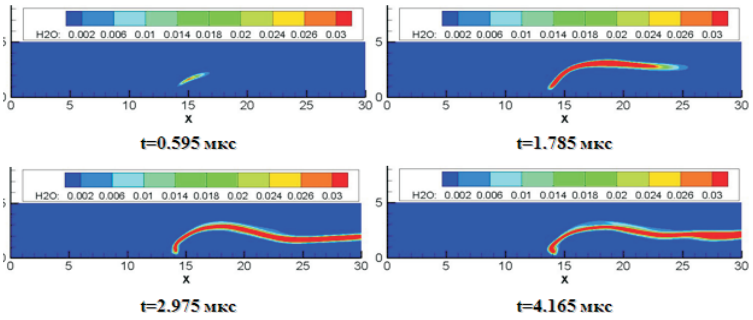


Figure 5 - The distribution of water vapor concentration at different times

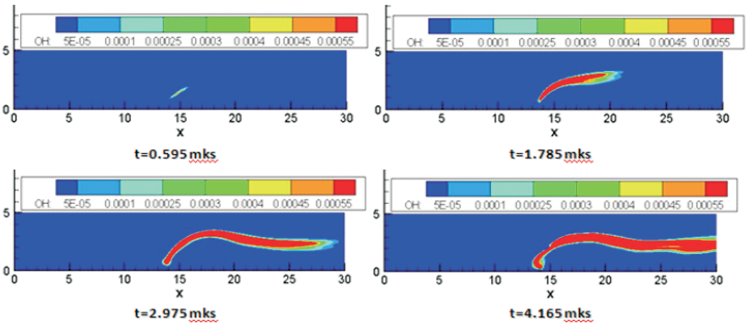


Figure 6 - The distribution of hydroxyl radical concentration at different times

## 4. Conclusion

In the present work, the numerical model and computer code have been developed for turbulent supersonic two-dimensional reacting flow. The numerical method is based on the

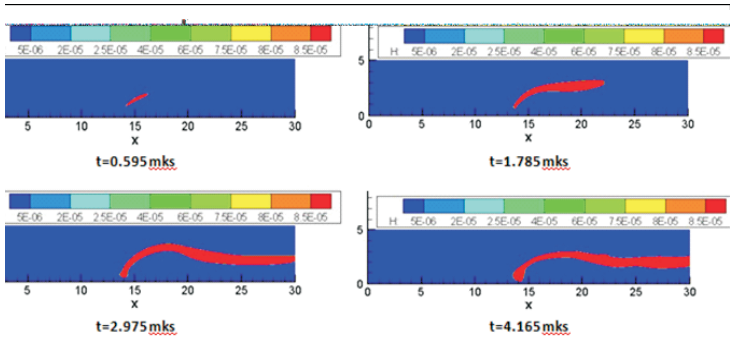


Figure 7 - The distribution of hydrogen atom concentration at different times

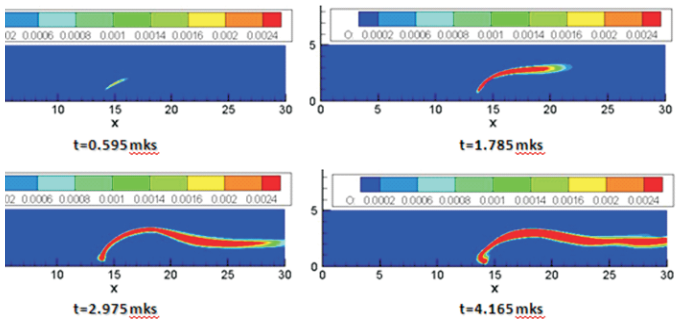


Figure 8 - The distribution of oxygen atom concentration at different times

ENO scheme. Numerical experiments has shown that the zone of combustion is concentrated near wall for adiabatic boundary. The results of combustion of hydrogen-air mixture, based on Jachimowski's seven-species reaction model. Extension to other reaction models will be considered in a future study.

The developed computer code allows to study of mixing fuel and air streams with various injector geometries and subsequent reaction, which is important in the design of supersonic combustion ramjet (scramjet) engines.

## References

1 *Beketaeva A.O., Naimanova A.Zh.* Numerical simulation of a supersonic flow with transverse injection of jets // Journal of Applied Mechanics and Technical physics. - 2004.- Vol. 45, №3, - P. 367-374.

2 *Dean R. Eklund, J. Philip Drummond and H.A. Hassan* Calculation of Supersonic Turbulent Reacting Coaxial Jets // AIAA Journal. -September, 1990. - Vol. 28, №9.

3 *SUN De-chuan, HU Chun-bo, CAI Ti-min* Computation of Supersonic Turbulent Flowfield with Transverse Injection // Applied Mathematics and Mechanics. English Edition - Junuary 2002. - Vol. 23, №1 - P. 107-113.

4 *Muhamed Ali, S. Ahmed, A. K. M. Sadrul Islam* The Two-Dimensional Supersonic Flow and Mixing with a Perpendicular Injection in a Scramjet Combustor // Journal of Thermal Science - 2003. - Vol. 12, №4 - P. 372-380.

5 *Kee R.J., Rupley F.M., Miller J.A.* CHEMKIN-II: a Fortran chemical kinetic package for the analysis of gas-phase chemical kinetics // SANDIA Report SAND89-8009. - 1989.

6 *Harten A., Engquist B., Osher S., Chakravarthy S.R.* Uniformly High Order Accurate Non-oscillatory Schemes, III // Journal of Computational Physics. - 1987. - Vol.71. - P.231-303.

7 *Harten A., Osher S., Engquist B., Chakravarthy S.R.* Some Results on Uniformly High-Order Accurate Essentially Non-oscillatory Schemes // Applied Num. Math. - 1986. - Vol.2. - P.347-377.

8 *E. H. Weidner and J. Ph. Drummond* Numerical study of staged fuel injection // AIAA J. 20. - 1982. - No.10 - P. 1426-1431.

*Поступила в редакцию 12 август 2012 года*