Numerical simulation of particle transport in supersonic mixing layer

Altyn Makasheva, Altynshash Naimanova

Abstract—Direct numerical simulations of the flowfield structures and the properties of the particle dispersion in the quasi-2D turbulent mixing layer (hydrogen-air) are performed by solving the time-dependent, compressible Euler equations. The 3D numerical code using the high-order essentially non-oscillatory (ENO) scheme is developed. The dispersion of the particles is studied by following their trajectories in the mixing layer with the Lagrangian method. In detail, the effect of the initial mass fraction of hydrogen and the number of particles on the growth of vortices and their thickness are studied. The simulation reveals that the capturing of the particles by the vortices essentially depend on the density of particles.

Keywords—supersonic shear flow, mixing layer, particle dispersion, multi-species flow , ENO-scheme.

I. Introduction

In many practical problems gas flows containing particles are involved. Particle-laden flows play an important role in high-speed technologies such as solid rocket propulsion systems and high-speed fuel combustors. The flow physics in such devices is very complex due to shock dynamics, turbulence and particle dispersion in mixing layers.

Understanding the dynamic behavior of particles in vortex system is important. Free mixing layers have been extensively studied over the past decades. Direct numerical simulation (DNS) is a reliable tool and has been successfully used for compressibility effects in the turbulent shear layer [1], spatial mixing layers [2], single-phase and two-phase flows [3]. The particle dispersions in the mixing layers for the different Stokes numbers have been obtained in [4]. In that study it has been shown that DNS is capable to reveal detailed mechanisms of vortex structure formulation in mixing layer. In spite of that there are a few investigations of a compressible multispecies shear layer flow with the dispersion of particles.

This work is our first stage of the simulation in a comprehensive study of the flow-particle interactions in a three-dimensional multispecies turbulent medium.

The purpose of this paper is particle – multi-species flow on the basis Eulerian-Lagrangian of representation are numerically simulated. The third order essentially non-oscillatory (ENO) scheme is adopted to solve the system of Euler equations for the supersonic planar mixing layer. A Lagrangian approach is used to trace the particles which move in gas flow.

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II. Problem Description

The inflow physical parameters profile across the non-premixed hydrogen (fuel) and air stream at the leading edge of the splitter plate is assumed to vary smoothly according to a hyperbolic-tangent function (Fig. 1). Particles enter at the splitter plate, i.e. particles distribution is in the mixing layer. The effect of the particle on the fluid and the particle-particle interaction are neglected (one-way coupled).

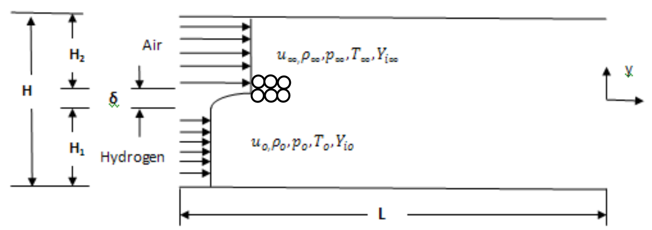

Fig. 1 an illustration the flow configuration

III. The Mathematical Model and Governing Equations

A. Euler Equation For Multi-Species Gas

The two-dimensional system of Favre-averaged Navier-Stokes equations for multi-species flow is

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial\left(\vec{E} - \vec{E}_V\right)}{\partial x} + \frac{\partial\left(\vec{F} - \vec{F}_V\right)}{\partial z} = 0, \tag{1}$$

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

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

$$\vec{E}_V = (0, \tau_{xx}, \tau_{xz}, u\tau_{xx} + w\tau_{xz} - q_x, J_{kx})^T,$$

$$\vec{F}_V = (0, \tau_{xz}, \tau_{zz}, u\tau_{xz} + w\tau_{zz} - q_z, J_{kz})^T,$$

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

1

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

$$\tau_{xz} = \tau_{zx} = \frac{\mu}{Re}(u_z + w_x);$$

$$q_x = \frac{1}{Pr\,Re}\left(\mu_l + \frac{\mu_t}{\sigma_k}\right)\frac{\partial T}{\partial x}; \quad q_z = \frac{1}{Pr\,Re}\left(\mu_l + \frac{\mu_t}{\sigma_k}\right)\frac{\partial T}{\partial z};$$

where Y_k is the mass fraction of k th species, $k = 1...N$, where N is the number of components in a gas mixture. τ, q and J_k are the viscous stress tensor, the heat flux and the diffusion flux, respectively.

Pressure, total energy and specific entalphy of the k^{th} species are defined by

$$p = \frac{\rho T}{\gamma_\infty M_\infty^2}\left(\sum_{k=1}^{N}\frac{Y_k}{W_k}\right), \quad E_t = \frac{\rho h}{\gamma_\infty M_\infty^2} - p + \frac{1}{2}\rho\left(u^2 + w^2\right),$$

$$h = \sum_{k=1}^{N} Y_k h_k, \quad h_k = h_k^0 + \int_{T_0}^{T} c_{pk}\, dT$$

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

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

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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 air flow parameters are $\rho_\infty, u_\infty, w_\infty, T_\infty, h_\infty, W_\infty, R_\infty$, hydrogen jet parameters are $\rho_0, u_0, w_0, T_0, h_0, W_0, R_0$. In terms of dimensionless variables, $\rho_\infty u_\infty^2$ is the scale, $R_0 T_\infty / W_\infty$ is the enthalpy scale, R_0 is the molar specific heat scale and δ (the thickness of the splitter plate) is the spatial distance.

B. Particle Equation in the Lagrangian Frame

The following assumptions are made for the dispersed phase:

- all particles are rigid spheres;
- particle-particle interactions are neglected;
- the effect of particles on the fluid is negligible.

With these assumptions the Lagrangian transport of the particles through a continuous carrier gas flow is characterized by the following governing equations after applying the Favre filter. The particles are tracked individually in a Lagrangian manner. The Lagrangian particle equations for the position and the velocity are given by:

$$\frac{\partial}{\partial t}\vec{x}_p = \vec{u}_p, \quad \frac{\partial}{\partial t}\vec{u}_p = D_p\left(\vec{u} + \vec{u}' - \vec{u}_p\right) \tag{2}$$

where $\vec{x}_p$ and $\vec{u}_p$ are respectively the position and velocity vectors for a particle represented by the subscript p; $\vec{u}'$ is the turbulent fluctuating component and D_p is the drag force with the particle radius r_p is given by

$$D_p = \frac{3}{8}\frac{\rho}{\rho_p}\frac{\left|\vec{u} + \vec{u}' - \vec{u}_p\right|}{r_p}C_D\left(Re_p\right)$$

The drag coefficient C_D is taken in accordance with the solid sphere drag correlation [6]:

$$C_D = \begin{cases} \dfrac{24}{Re_p}\left(1 + \dfrac{1}{6}Re_p^{2/3}\right), & Re_p \le 1000 \\ 0{,}424, & Re_p > 1000 \end{cases}$$

and $Re_p = \dfrac{2\rho\left|\vec{u} + \vec{u}' - \vec{u}_p\right|}{\mu}$ is the particle Reynolds number, μ is the gas viscosity.

The equation for the particle energy is described by following

$$m_p C_p \frac{dT_p}{dt} = 2\pi r_p K_{conv}\left(T - T_p\right)Nu_p + g$$

where $\vec{g}$ is the gravity force acting on the particle, m_p is the particle mass, $\rho_p = m_p \Big/ \left(\frac{4}{3}\pi r_p^3\right)$ is the density of the solid particles, $K_{conv} = \left(\mu c_p\right)/\Pr_p$ is the convective heat transfer coefficient between the gas and the particle.

IV. Initial and Boundary Conditions

At the entrance:

- for multi-species gas:

$u_1 = M_0\sqrt{\dfrac{\gamma_0 R_0 T_0}{W_0}}$, $w_1 = 0$, $p_1 = p_0$, $T_1 = T_0$, $Y_{k1} = Y_{k0}$ at $x = 0$, $0 \le z < H_1$.

$u_2 = M_\infty\sqrt{\dfrac{\gamma_\infty R_0 T_\infty}{W_\infty}}$, $w_2 = 0$, $p_2 = p_\infty$, $T_2 = T_\infty$, $Y_{k2} = Y_{k\infty}$ at $x = 0$, $H_1 + \delta \le z \le H_2$.

- for particles:

$\rho_p = \rho_{p0}$, $T_p = T_{p0}$ at $x = 0$, $z = H_1 - 5\delta$ and $z = H_1 + 5\delta$.

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

$$\phi(z) = 0.5(\phi_2 + \phi_1) + 0.5(\phi_2 - \phi_1)\tanh(0.5z/\theta) \text{ at } x = 0,\ 0 \le z \le H.$$

where $\phi = (u, v, p, T, Y_k)$, θ is the momentum thickness. The pressure is assumed to be uniform across the mixing layer. On the lower and upper boundaries the condition of symmetry is imposed. At the outflow, the non-reflecting boundary condition is used [7].

In order to produce the roll-up and pairing of vortex rings, an unsteady boundary condition for velocity field is used at the inlet plane [2], i.e.

$$u = \Delta U \cdot Gaussian \cdot \sum_{m=0}^{3} A \cdot \cos(\omega \cdot t + \phi_m),$$

$$w = \Delta w_{factor} \cdot \Delta U \cdot Gaussian \cdot \sum_{m=0}^{3} A \cdot \sin(\omega \cdot t + \phi_m)$$

$$Gaussian(z) = \exp(-z^2/2\sigma^2),$$

The random phase equation had the following form

$$\phi = \phi + sign(\Delta\phi, random), \quad -1 \le random \le 1,$$

where $\Delta U = (u_\infty - u_0)$ is the difference of the two stream velocities which measures the strength of shearing. $Gaussian(z)$ is a Gaussian function which has a peak value of the unity at z=0 and the $\pm 2\sigma$ width is matched to the vorticity layer thickness at the entrance. Coefficient $A = 0.001$ is the forcing amplitude. The Δw_{factor} is taken as [7]. The

$$\omega = 2\pi\left(\frac{\left(\sqrt{\dfrac{\gamma_0 R_0 T_0}{W_0}} + \sqrt{\dfrac{\gamma_\infty R_\infty T_\infty}{W_\infty}}\right)/2}{2\delta_w}\right)$$

is the frequency of perturbation. $\delta_w = \dfrac{(u_\infty - u_0)}{(\partial u/\partial z)_{\max}}$ is the vorticity thickness.

V. Method of Solution

The numerical solution of the equations system (1) is calculated in two steps. The gas dynamic parameters (ρ, u, w, E_t) are solved in the first-step and the species ($Y_k, k = 1{,}7$) with mass source terms are solved in the second-step. The approximation of the convection terms is performed by the ENO scheme of the third-order accuracy [8]. 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. For the approximation of the derivatives of the diffusion terms, the 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 represents difficult task in the case of the thermally perfect gas. This problem is connected by explicit representation of pressure through the unknown parameters. Here, the pressure is determined by using the following formula

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

where $\bar{\gamma} = h_{sm}/e_{sm}$ is an effective adiabatic parameter of the gas mixture, $h_{sm} = \sum_{i=1}^{N} Y_i \int_{T_0}^{T} c_{p_i} dT$, $e_{sm} = \sum_{i=1}^{N} Y_i \int_{T_0}^{T} c_{v_i} dT$ are the enthalpy and internal energy of the mixture minus the heat and energy of formation; $T_0 = 293K$ is the standard temperature of formation. The system of the original equations is solved by the use of the Euler method.

The dispersion behavior of the particles is then computed by numerically solving equations (2).

VI. Results and Discussion

The results of free mixing layer simulation with and without the particles is presented below.

The simulations of the hydrogen-air flows are performed in the dimensionless rectangular domain of 350 in stream-wise direction and 80 in transverse direction. The splitter plate thickness is $\delta = 0.3175$ cm. The initial momentum thickness $\theta = \int\left(\dfrac{\rho}{\rho_\infty}u^*(1 - u^*)dz\right)$ is 0.05 cm. At the inflow plane, hydrogen enters from the upper half of domain and air enters from the lower one. The hydrogen flow parameters are $M_0 = 2.0$, $T_0 = 2000$ K, $p_0 = 101325$ Pa and the air flow parameters are $M_\infty = 2.1$, $T_\infty = 2000$ K, $p_\infty = 101325$ Pa. The initial mass fraction of the upper flow is $Y_{H_2} = 0.5$, $Y_{N_2} = 0.5$ and the lower flow is $Y_{O_2} = 0.2$, $Y_{N_2} = 0.8$.

Isolines of hydrogen (H2) fraction is presented in Figure 2. Numerical result shows the pairing phenomenon between two adjacent vortices and formation of the new vortex which is moved downstream. This vortex enlargement process occurs randomly in space and time. From figure it is seen the spacing between two adjacent vortices and the size of vortex are increasing with time as in homogenous shear layer [2].

Here, the particles are injected at the inflow boundary of the mixture layer $z = H_1 - 5\delta$ and $z = H_1 + 5\delta$ at $x = 0$. For this case, the mimixing layer simulation is started at time t=0 and the interval between two consecutive injections is $N = 600$ of iteration. One parcel of particles is entered to the flow field for each N .

Figure 3 shows the particles' spread for the injection from

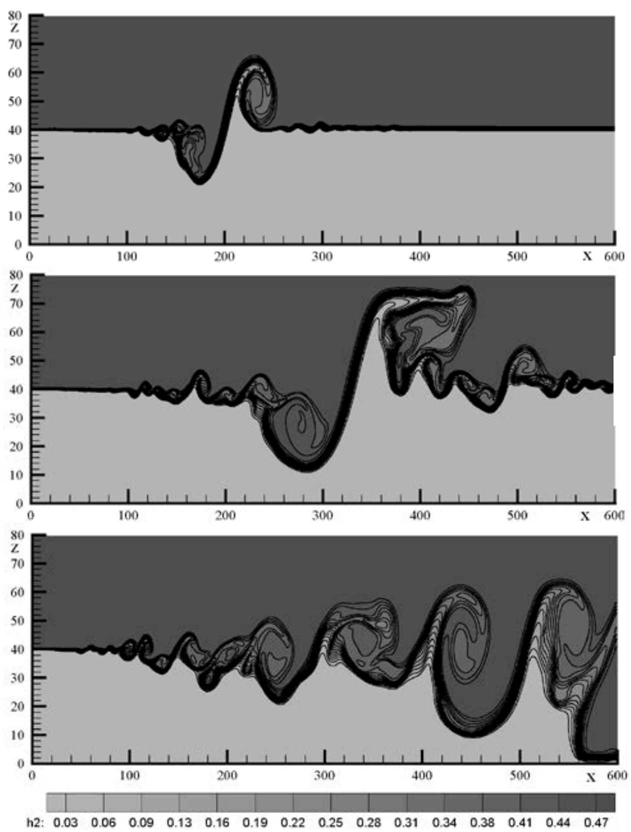

Fig. 2 distribution of hydrogen atom concentration at the three moments in time: a) t=350, b) t=800, c) t=1500

different points z. It is seen that since the lower flow rate is less than the upper flow rate, the particles carried away by the gas flow tend to the higher speed. Accordingly, particles at z=20 (Fig.2a) and z=30 (Fig.2b) are moving faster than that at z = 40 (Fig.2c) and z = 50 (Fig.2d).

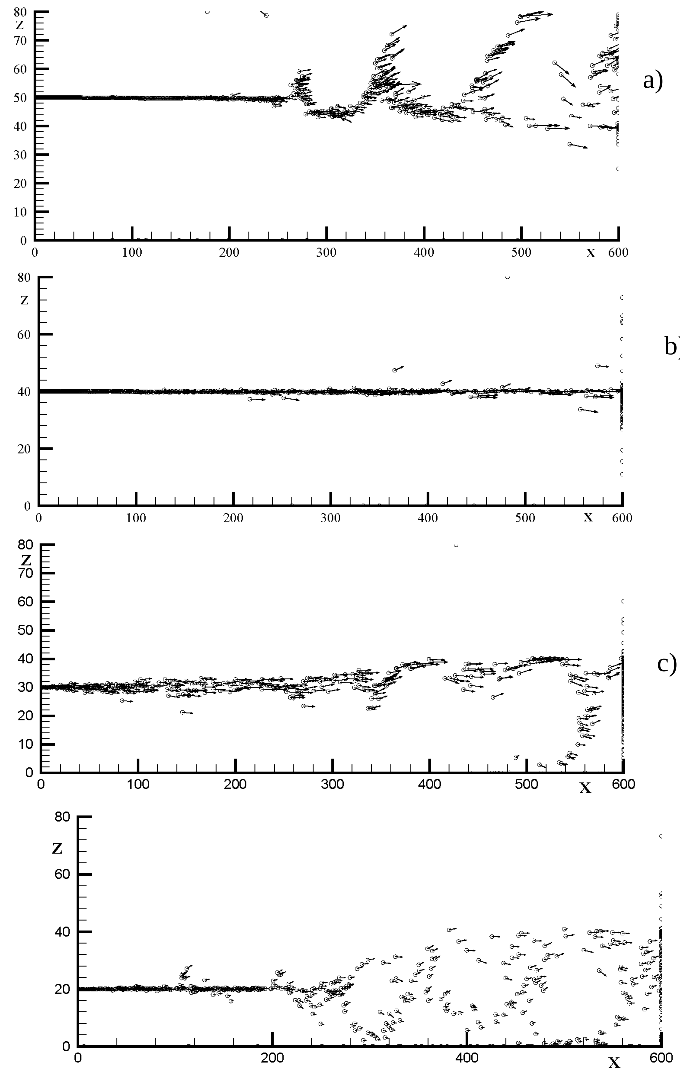

Fig. 3 the particles spread for the injection from the different points: a) z=20, b) z=30, c) z=40, d) z=50

Below is the analysis of the calculation results for the case when particles are injected simultaneously from the four points (Figure 4). The comparison of the flow patterns at different moments in time t = 350 (Fig. 4a), t = 800 (Fig. 4b) and t=1500 (Fig. 4c) illustrate that the particles in the lower flow reach the output boundary of the considered area faster than that in the upper flow. Also, the area of the lower flow at t=1500 (Fig. 4c) is completely filled with particles faster than the upper flow area.

Numerical calculation reveals density particle influence on their trajectory, namely the easy particles are captured by the vortical structures, whereas the heavy particles remain mostly unaffected by the eddies.

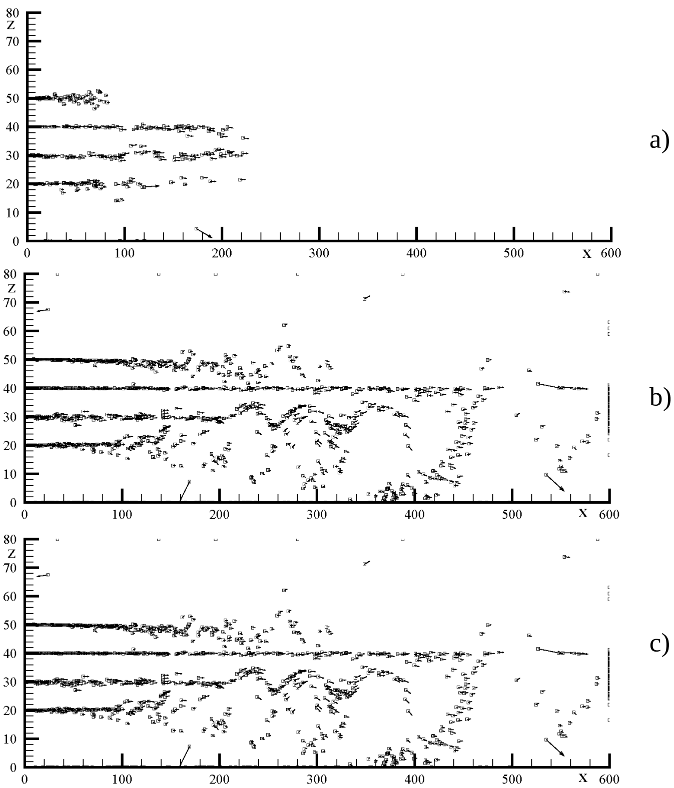

Fig. 4 the particles spread for the injection from the four points at the three moments in time: a) t=350, b) t=800, c) t=1500

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