Simulations of developing two-dimensional mixing layers with particle dispersion

Altyn Makasheva, Altynshash Naimanova, Nurtoleu Shakhan

Abstract—Numerical simulations of particle dispersion in a planar mixing layer formed by two co-flowing streams past a splitter plate are presented. The two-dimensional time-dependent gas-phase equations are solved numerically using the high-order essentially non-oscillatory (ENO) scheme. The particles are traced a Lagrangian approach assuming one-way coupling between the continuous and dispersed phases. The influence of large-scale coherent structures in a spatially-developing mixing layer on the particle dynamics is numerically studied. Detailed analysis reveals that the intermediate size particles are caughted by them, leading to their enhanced dispersion, while the large particles are mostly unaffected by the large eddies. However, the asymmetric entrainment of particles on the periphery of the mixing layer is presented for both cases.

Keywords—turbulent gas-particle flow, mixing layers, particle dispersion, multi-species flow , ENO-scheme.

I. INTRODUCTION

NUMEROUSE applications in natural sciences and engineering deal with particles in the mixing layers. Two-phase flows are subject of active experiments and measurements research [1]. Unfortunately, this approach is time consuming, particularly if a certain optimization process requires multiple and expensive experiments. For modeling gas- particle flows, the continuous phase is represented by an Eulerian description, while particle dispersions in the flow field can be modeled by either the Eulerian description [2] or Lagrangian description [3].

In the last decades, there has been progress in investigating particle transport in shear layers by the numerical simulation.

For example, the RANS [4], DNS [5] and stochastic separated models simulating Lagrangian particles were applied to predict the dispersion of inertial fuel particles in the supersonic turbulent flows.

The objective of the present paper is to study high speed turbulent gas-particle mixture layer. Eulerian approach is used for the numerical simulation of supersonic mixing layer of multi-species gas with 2D-DNS. The dispersion of particles is studied following their trajectories in the mixture layer. A Lagrangian approach is used to trace the particles which are transported by the fluid 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).

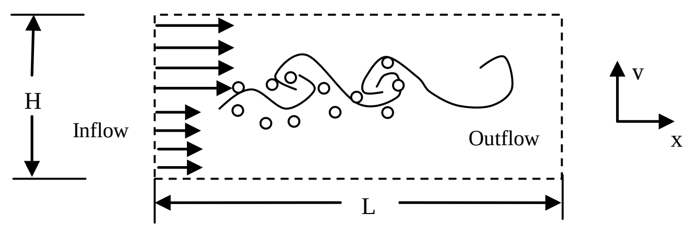

Fig. 1 illustration of the flow configuration

III. THE MATHEMATICAL MODEL AND GOVERNING EQUATIONS

A. Navier-Stokes Equation For Multi-Species Gas

The carrier gas is treated in the Eulerian manner as a compressible multi-species gas described the two-dimensional system of Navier-Stokes equations. We impose conservation of mass, momentum and total energy. The equations can be written as [6]:

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

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

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

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

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

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

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

$$\tau_{xz} = \tau_{zx} = \frac{\mu_l}{\mathrm{Re}}(u_z + w_x); \quad q_x = \frac{\mu_l}{\Pr \mathrm{Re}}\frac{\partial T}{\partial x}; \quad q_z = \frac{\mu_l}{\Pr \mathrm{Re}}\frac{\partial T}{\partial z};$$

where Y_k is the mass fraction of k th species, $k = 1...N$, 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. The coefficient of molecular viscosity of the mixture μ_l is given by Wilke's formula [7].

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:

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

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 [8].

The system of the equations (1) is written in the conservative, dimensionless form. The air parameters are $\rho_\infty, u_\infty, w_\infty, T_\infty, h_\infty, W_\infty, R_\infty$, hydrogen 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 pressure 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 distance scale.

B. Particle Equation in the Lagrangian Frame

The particles are tracked individually in Lagrangian manner. The particle collision effects are neglected. In addition, all the particles are assumed to collide with the walls elastically. The Lagrangian particle equations for the position, the velocity and the energy are given by

$$\begin{cases} \dfrac{\partial \vec{x}_p}{\partial t} = \vec{u}_p \\ \dfrac{\partial \vec{u}_p}{\partial t} = D_p\left(\vec{u} + \vec{u}' - \vec{u}_p\right) \\ m_p C_p \dfrac{d\, T_p}{d\, t} = 2\pi r_p K_{conv}\left(T - T_p\right) Nu_p + g \end{cases}, \qquad (2)$$

where $\vec{x}_p$ is the particle position vector, $\vec{u}_p$ is the particle velocity vector and $\vec{u}$ is the gas velocity, $\vec{u}'$ is fluctuating velocity of the gas phase, $\vec{g}$ 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 coefficient of heat transfer between the gas and the particle. D_p is the drag force with the particle radius r_p :

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

The drag coefficient C_D, corrected by R. Chein and J.N. Chung [9] is defined as:

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

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.

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 $x = 0$, $0 \le z < \mathrm{H}_1$.

$u_2 = M_\infty\sqrt{\dfrac{\gamma_\infty R_0 T_\infty}{W_\infty}}$, $w_2 = 0$, $p_2 = p_\infty$, $T_2 = T_\infty$, $Y_{k2} = Y_{k\infty}$ at $x = 0$, $\mathrm{H}_1 + \delta \le z \le \mathrm{H}_2$.

- for particles:

$\rho_p = \rho_{p0}$, $T_p = T_{p0}$ at $x = 0$, $z = H_1 - 5\delta$ and $z = 30$.

In the region $H_1 \le z \le H_1 + \delta$ 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 $\phi = (u, v, p, T, Y_k)$, $\theta = \int\left(\frac{\rho}{\rho_\infty}u^*(1-u^*)dz\right) = 0.15\,\text{cm}$ is the momentum thickness and $\delta = 0.3175$ cm is the splitter plate 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 [10].

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 has 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 [10]. The $\omega = 2\pi\left(\frac{\left(\sqrt{\frac{\gamma_0 R_0 T_0}{W_0}} + \sqrt{\frac{\gamma_\infty R_\infty T_\infty}{W_\infty}}\right)/2}{2\delta_w}\right)$ is the frequency of perturbation,

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

V. Method of Solution

Preliminary, in the regions of high gradients, i.e. in the mixing layer, the grid points are clustered near the splitter plate. In the calculations, we used coordinate transformations of the form:

$$\xi(x) = L\left[(\beta+1) - (\beta-1)\left(\frac{\beta+1}{\beta-1}\right)^{1-\frac{x}{a}}\right] \Big/ \left[\left(\frac{\beta+1}{\beta-1}\right)^{1-\frac{x}{a}} + 1\right],$$

$$\eta(z) = K + \frac{1}{\tau} arsh\left[\left(\frac{z}{z_c} - 1\right) sh(\tau K)\right],$$

$$K = \frac{1}{2\tau}\ln\left[\left(1 + (e^\tau - 1)\frac{z_c}{H}\right) \Big/ \left(1 + (e^{-\tau} - 1)\frac{z_c}{H}\right)\right]$$

$\beta > 1$ and $\tau > 1$ are the refinement parameters, a is the height of the computational domain in the generalized coordinates, and z_c is the point relative to which the refinement is carried out.

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 [11].

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 simulations of the hydrogen-air flow are performed in the dimensionless rectangular domain of 600 calibers in stream-wise direction and 80 calibers in transverse direction. 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 is $Y_{H_2} = 0.5$, $Y_{N_2} = 0.5$ for the upper flow and $Y_{O_2} = 0.2$, $Y_{N_2} = 0.8$ for the lower flow.

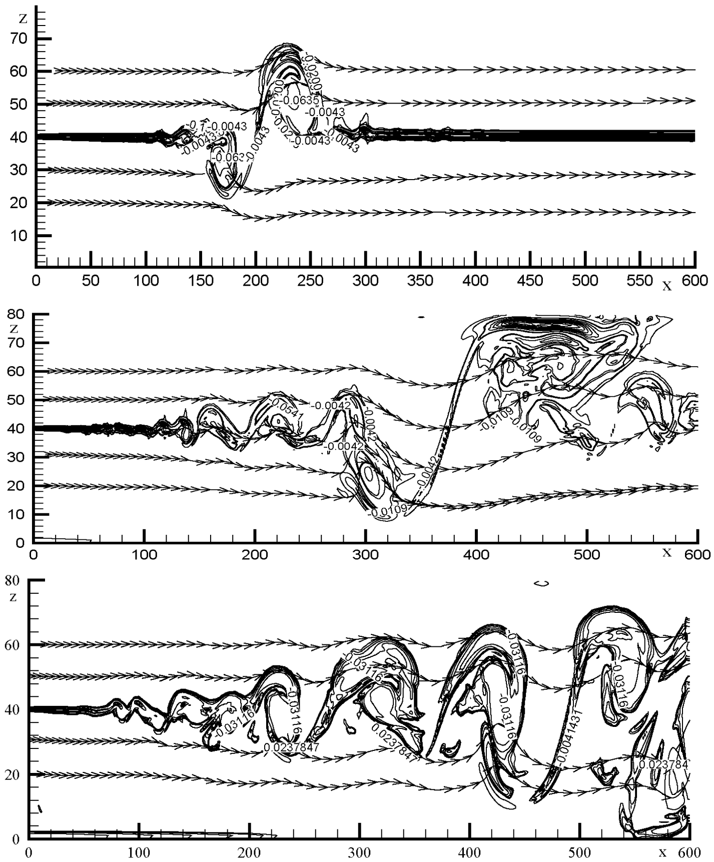

Fig. 2 sequence of vorticity contours at time: a) t=375, b) t=675, c) t=1450

The particles are injected randomly with value of velocity equal to velocity of gas at the point: $x=0$, $z=30$. The flow computation and the particle injection are started at t = 0. The time interval between two consecutive injections is $N=10$, i.e. starting at $t=0$, a one particle is injected into the flow field after every 10 iteration.

Numerical calculation is provided for the range of the diameters of the particles $5<d_p \le 150$.

Fig. 2 shows a sequence of vorticity contours at a) $t=375$, b) $t=675$ and c) $t=1350$ on the results of free mixing layer simulation. This figure illustrates the merging processes of vorticies, which responsible for the growth of the mixing layer downstream (the pairing and merging of vortices, their convection downstream, and the formation of a new vortex upstream in the mixing layer) .

The corresponding hydrogen contours are represented in Fig. 3. This picture clearly demonstrates the asymmetric entrainment which is an important feature of the mixing layer development.

It is known [12] that the small particles ($d_p<5$) follow the tracer (gas) particles in subsonic case. Here, the numerical experiments confirm that the smaller particles remain trapped in the eddies.

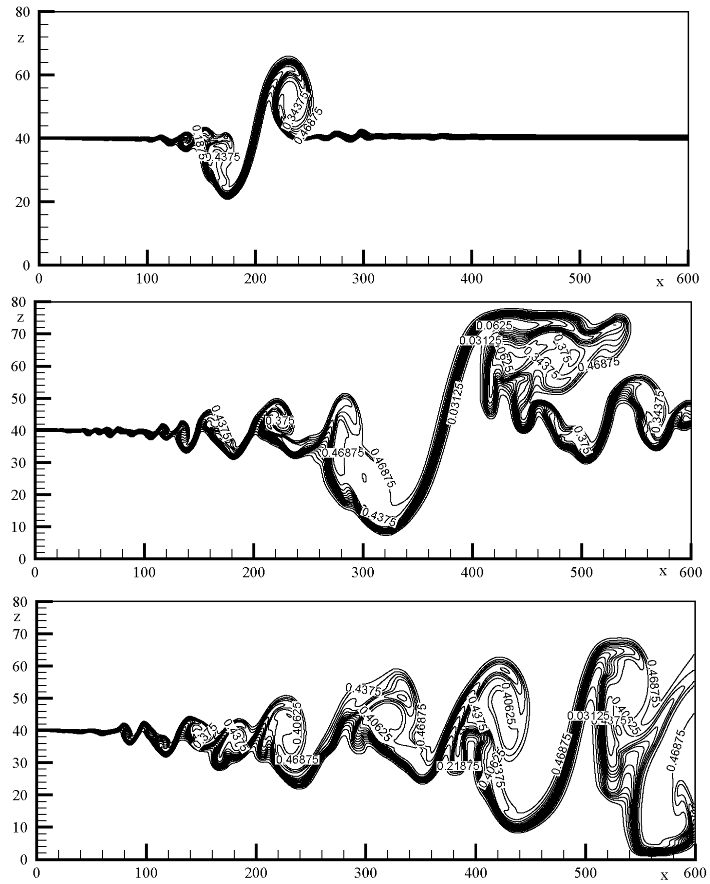

Fig.3 sequence of hydrogen atom concentration at time: a) t=150, b) t=375, c) t=1450

Fig. 4 ($d_p=50$) and Fig. 5 ($d_p=150$) represent the evolution of intermediate and large of particles at: a) $t=150$, b) $t=375$, c) $t=675$ and d) $t=1350$.

As follows from Fig. 4 ($d_p=50$) most of the intermediate size particles is convected through the mixing layer, but some of them are entrapped by the large-scale structures.

Increasing size of particles up to $d_p=150$ shows that almost all particles are convected through the mixing layer (Fig. 5) and the dispersion of particles is significantly greater than in preliminary case. Also from Figs. 5b,c it is visible that particles remain relatively unaffected by the large scale structures. In addition, comparison of Fig. 4 and Fig. 5 shows the asymmetric entrainment of particles on the periphery of the mixing layer for both cases.

The numerical experiments reveal the trajectory particles and strong influence of their involving in vertical structures on the injection location.

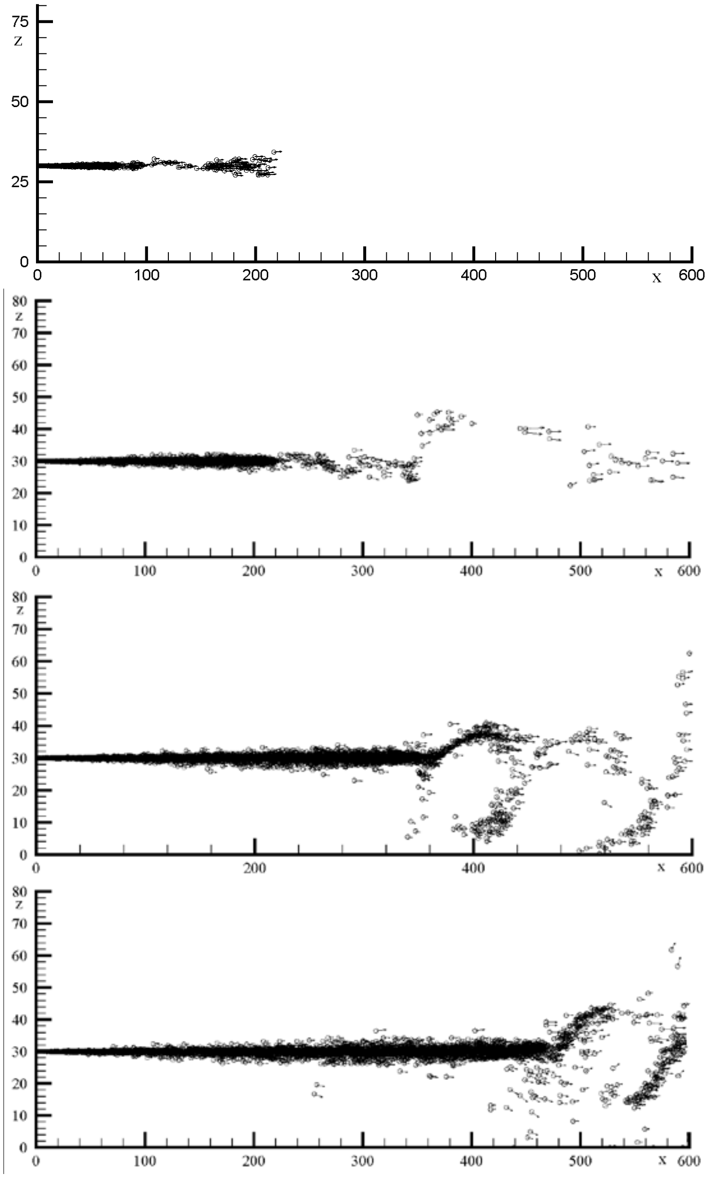

Fig. 4 distribution of particles at time: a) t=150, b) t=375, c) t=675, d) t=1350. The particle diameter $d_n = 50$.

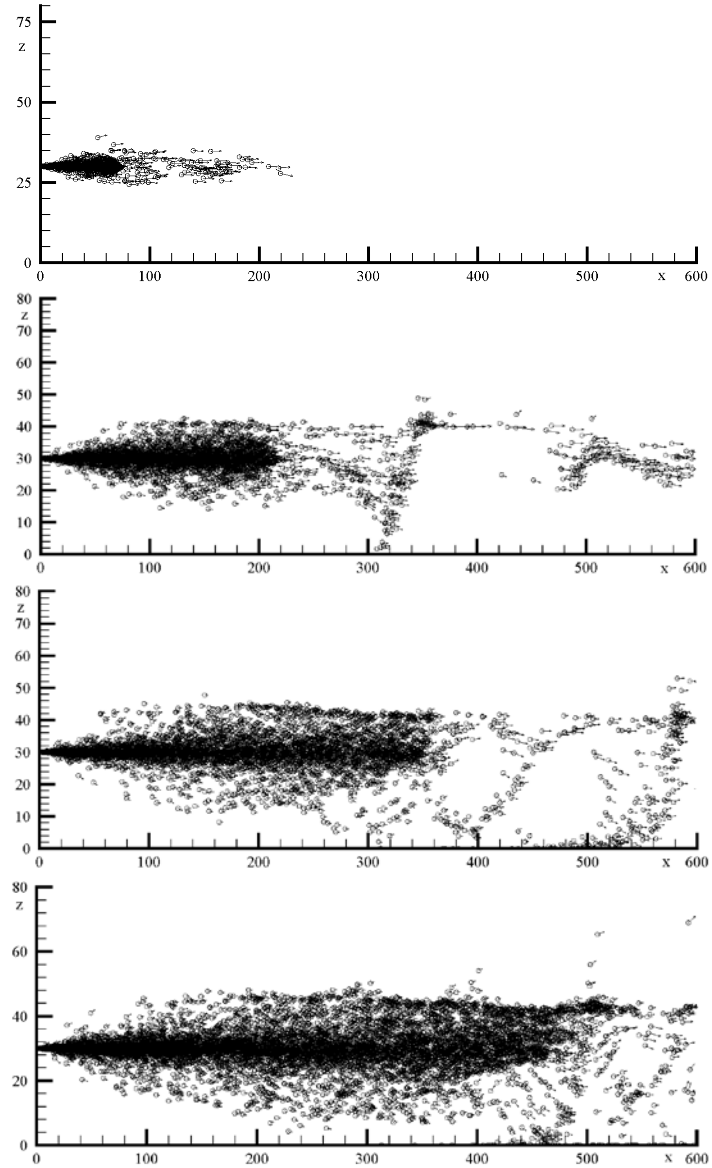

Fig. 5 distribution of particles at time: a) t=150, b) t=375, c) t=675, d) t=1350. The particle diameter $d_p = 150$.

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