STATISTICAL MODELING OF THE AIR-BLAST ATOMIZATION IN THE LAGRANGIAN COMPUTATION OF LIQUID SPRAY

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I. INTRODUCTION

When injection of liquid jet takes place into coflowing motion of high relative velocity gas, a wide range of turbulent eddies may impact on the liquid jet causing its breakup. This regime of atomization is often referred to as the air-blast atomization and is widely used in practical systems. The physics of air-blast atomization is very complex [1-5]. In addition to the gas turbulence-induced breakup, many other's random processes such as multiple droplets collision, turbulence in liquid, variations in the cavitating flow inside the injector, etc., contribute to the phenomenon of breakup. This implies that at each spray location, the spectra of size of produced droplets can be very large. Then the question of what are the probabilities of sizes that are involved into atomization, arises in the breakup modeling. Due to the complexity of phenomenon, it is too difficult to disclose clearly a dominant mechanism of air-blast breakup with expectation of a characteristic size of droplet. To this end, the basic idea behind the simulation undertaken in this paper, is as follows. The process of air-blast breakup is considered in the framework of cascade of uncorrelated breakage events in series , independently from the initial distribution of sizes. The stochastic modeling of droplets production under this hypotheses down to the critical (or maximum stable) size is the subject of this paper.

The cascade idea of breakup comes from the early work of Kolmogorov written in 1941 [6]. In this work, Kolmogorov described the breakup of solid particles as a discrete random process, where the probability to break each parent particle on a given number of parts is independent of the parent particle size. From Lyapunov's theorem, Kolmogorov has pointed out that such a general assumption leads to the log-normal distribution of particle size in the long-time limit. In this paper, the Kolmogorov's discrete model has been reproduced in the form of evolution equation for distribution function. The asymptotic solution of this equation has been applied to simulate the drop breakup alongside with Lagrangian model of spray dynamics. Performed computations of air-blast atomization are related to a spray close to the rocket engine configuration.

II. KOLMOGOROV'S (1941) THEORY OF THE PARTICLE BREAKUP.

Let us consider an ensemble of breaking solid particles at discrete time moments $t=0,1,2,....$ These time moments are scaled by the breakup frequency ν ($t=\nu t$). According to Komogorov[6], the number of particles $N(r,t)$ of size $\rho \le r$ was selected amongst all particles $N(t)$ at a given moment t. The expectations of total number of particles and of particles of size $\rho \le r$ were denoted as $\overline{N}(t)$ and $\overline{N}(r,t)$ correspondingly. Considering an outcome of breakup per unit time $[t,\ t+1]$ of a given parent particle of size r, the mean number $Q(\alpha)$ of secondary particles of size $\rho \le \alpha r$ ($0 \le \alpha \le 1$) was introduced. According to hypotheses of Kolmogorov, the probability to break each parent particle on a given number of parts is independent of the parent particle size. In other words, $Q(\alpha)$ does not depend of prehistory of breakup and is not influenced by others parent particles. By this assumption, Kolmogorov writes:

$$\overline{N}(r,t+1)=\int_0^1 \overline{N}\left(\frac{r}{\alpha},t\right) dQ(\alpha) \tag{1}$$

Introducing the logarithm of particle-size $x=\ln r$, Kolmogorov pointed out that

$$T(x,t)=\frac{\overline{N}(e^x,t)}{\overline{N}(t)}=\frac{N(e^x,t)}{N(t)} \tag{2}$$

Further, denoting $\xi=\ln\alpha$ and $Q(\alpha)=Q(1)\cdot S(\xi)$, equation (1) is rewritten by Kolmogorov in the following form:

$$T(x,t+1)=\int_{-\infty}^{0} T(x-\xi,t)\,dS(\xi) \tag{3}$$

By Lyapunov's theorem, Kolmogorov stated that from discrete model (3), the long-time limit form of $T(x,t)$ tends to Gaussian function. Then the main result of Kolmogorov's work is that $N(r,t))$ is asymptotically governed by log-normal law.

III. THE ASYMPTOTIC DIFFERENTIAL FORM OF THE DISCRETE KOLMOGOROV'S MODEL.

Here the discrete model (3) is represented by its differential approximation in the long time limit. Using parabolic scaling of variables $\tau = \varepsilon^2 t$, $y = \varepsilon x$, where ε is a scaling parameter and t is scaled by breakup frequency, the equation (3) can be written as

$$T(y,\tau+\varepsilon^2)=\int_{-\infty}^{0} T(y-\varepsilon\xi,\tau)s(\xi)d\xi \tag{4}$$

Expanding both the left-hand side and the expression under integral in (4), one gets

$$T(y,\tau+\varepsilon^2)=T(y,\tau)+\varepsilon^2\frac{\partial T(y,\tau)}{\partial\tau}+O(\varepsilon^4)$$

$$T(y-\varepsilon\xi,\tau)=T(y,\tau)-\varepsilon\xi\frac{\partial T(y,\tau)}{\partial y}+\frac{1}{2!}(\varepsilon\xi)^2\frac{\partial^2 T(y,\tau)}{\partial y^2}-\frac{1}{3!}(\varepsilon\xi)^3\frac{\partial^3 T(y,\tau)}{\partial y^3}+O(\varepsilon^4)$$

Substituting these expansions in (4) and coming back to variables t and x, one yields:

$$\frac{\partial T(x,t)}{\partial t}+O(\varepsilon^4)=-\langle\xi\rangle\frac{\partial T(x,t)}{\partial x}+\frac{1}{2!}\langle\xi^2\rangle\frac{\partial^2 T(x,t)}{\partial x^2}-\frac{1}{3!}\frac{\partial^3 T(x,t)}{\partial x^3}\varepsilon^3\int_{-\infty}^{0}\xi^3 s(\xi)d\xi+O(\varepsilon^4) \tag{5}$$

where $\langle\xi\rangle=\int_{-\infty}^{0}\xi\, s(\xi)d\xi$ and $\langle\xi^2\rangle=\int_{-\infty}^{0}\xi^2\, s(\xi)d\xi$ are two first moments of ξ. Assuming that the integral $\int_0^1|\ln\alpha|^3\, dQ(\alpha)$ is limited, the equation (5) can be written in the long-time limit $\varepsilon\to 0$ ($t\to\infty$), as

$$\frac{\partial T(x,t)}{\partial t}+v\langle\xi\rangle\frac{\partial T(x,t)}{\partial x}=\frac{1}{2!}v\langle\xi^2\rangle\frac{\partial^2 T(x,t)}{\partial x^2} \tag{6}$$

The dimensional time has been used in (6). The solution of (6) is Gaussian function. This repeats the main result of Kolmogorov[6]. At the same time, an influence of the initial distribution before breakup starts can be taken into account by using (6). The solution of (6) verifies to be:

$$T(x,t)=\int_{-\infty}^{0}\frac{1}{\sqrt{2\pi\langle\xi^2\rangle\nu t}}\exp\left[-\frac{(x-x_0)^2}{2\langle\xi^2\rangle\nu t}\right]T_0(x_0-\langle\xi\rangle\nu t)dx_0 \qquad (7)$$

where $T_0(x_0)$ is the initial distribution of the logarithm of droplet radius and x_0 is logarithm of radius of the parent drop. One can rewrite equation (6) for the normalized distribution of radius $f(r)$:

$$\frac{\partial f(r)}{\partial t}=-\nu\langle\xi\rangle\frac{\partial}{\partial r}(r\,f(r))+\frac{1}{2}\nu\langle\xi^2\rangle\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}(r\,f(r))\right) \qquad (8)$$

The solution of this equation has the following form:

$$f(r,t)=\frac{1}{r}\int_{0}^{\infty}\frac{1}{\sqrt{2\pi\langle\xi^2\rangle\nu t}}\exp\left[-\frac{\left(\ln\frac{r_0}{r}+\langle\xi\rangle\nu t\right)^2}{2\langle\xi^2\rangle\nu t}\right]f_0(r_0)dr_0 \qquad (9)$$

where $f_0(r_0)$ is the initial distribution of droplet radius before breakup starts.

IV. IMPLEMENTATION INTO COMPUTATIONAL CODE KIVA II

IV.1 General procedure

The right hand side of equation (8) can be added to the transport spray equation[7] as a source term due to drop breakup. The modeling of the spray equation is often based on Lagrangian formulation[8]. The spray is considered to be composed of discrete parcels of particles, each of which represents a group of droplets of similar size, velocity and position. These groups of droplets are followed as they interact and exchange momentum and energy with surrounding gas. The basic ideas of this method, including the modeling of turbulent dispersion of

particles, are presented in [9]. Here, the Lagrangian tracking is coupled with stochastic computing of breakup. Two additional physical processes were included in the Monte Carlo procedure. Namely, the product droplet velocity has been modeled and the breakup has been considered down to the local magnitude of the critical (or maximum stable) radius, r_{cr}. The liquid fuel was injected in the axial nozzle direction in form of discrete parcels of drops with characteristic size equal to the exit nozzle radius. The injection velocity was determined from the known liquid injection rate.

Let us consider the motion of a given $j-th$ primary parcel that undergoes breakup. Before breakup starts, the distribution function associated with this parcel, is Dirac function at radius of the parent drop. After passage of time, which is inversely the breakup frequency, the new droplets arise due to breakup. In sequel, the droplet-radius distribution function changes. We suppose that the new distribution may be described according to solution (9) taken at $\nu t = 1$ with $\langle \xi \rangle$ and $\langle \xi^2 \rangle$ as parameters of the model. In order to alleviate computations, we can proceed the following way. Let us assume that once every breakup time scale, all outcomes of breakup in the given parent parcel are in mean (over many computations), recovered by one new parcel that replaces the parent one. The radius of droplet associated with produced parcel is sampled from (9). The new number of droplets is computed by mass conservation from the primary parcel to the secondary one. After the sampling procedure, the current time, t, prescribed for produced parcel is counted from zero and Lagrangian tracking is continued up to the moment ($\nu t = 1$) of the further breakup.

In computations, we used expressions obtained for the distribution of the logarithm of radius. The starting distribution for the logarithm of droplet radius in $j-th$ primary parcel is

$$T_{0_j}(x_0) = \delta(x_0 - x_j) \tag{10}$$

Using this distribution function in (7) at $\nu t = 1$, one can express the solution by the error function erf:

$$T_j(x,t) = \frac{1}{2}\left[1 + erf\left(\frac{x - x_j - \langle \xi \rangle}{\sqrt{2\langle \xi^2 \rangle}}\right)\right] \tag{11}$$

The product droplet velocity is computed by adding to the primary parcel velocity a velocity $\mathbf{w}_{bu}$, which is randomly distributed in a plane normal to the relative velocity vector between the parent droplet and gas. The quantity of $|\mathbf{w}_{bu}|$ is determined by the mean local Sauter radius of parent drops, r_{32}, and the breakup frequency, ν:

$$|\mathbf{w}_{bu}| = r_{32}\nu \tag{12}$$

IV.2 Critical radius, breakup frequency

The critical (or maximum stable) radius is determined when disruptive hydrodynamic forces are balanced by capillary forces:

$$r_{cr} = We_{cr}\delta / \rho_g u_r^2 \tag{13}$$

where u_r is the relative between liquid and gas velocity, δ is the surface tension coefficient, We_{cr} is the critical Weber number, which can be taken of order one over a large interval of Ohnesorge numbers [10,11]. In the paper, written in 1949 [12], Kolmogorov considered the stretched drop of insoluble liquid that was submerged in a turbulent flow. Using the Obuchov-Kolmogorov's scaling law for the velocity difference across a size when the surface tension force becomes significant, Kolmogorov introduced a critical size of produced droplets as:

$$r_{cr} = \frac{1}{2}\left(\frac{We_{cr}\delta}{\varepsilon^{2/3}\rho_g}\right)^{3/5} \quad \text{if } 2r >> \eta \tag{14}$$

$$r_{cr} = \frac{1}{2}\left(\frac{We_{cr}\delta\nu}{\varepsilon\rho_g}\right)^{1/3} \quad \text{if } 2r << \eta \tag{15}$$

where ε is the mean viscous dissipation rate and ρ_g is density in the gas.

An estimation of r_{cr} by using experimental data from [4] gives an enhanced magnitude of r_{cr} comparing to the measurements. In order to account for the inertia of liquid, namely for the density of the liquid ρ_l, the expression (14) can be modified. Estimating the mean square of relative droplet-to-gas velocity by mean viscous dissipation and Stokes time scale[13,14],

$$\left\langle u_r^{\,2} \right\rangle \approx \varepsilon \tau_{st} \tag{16}$$

one yields a new expression for critical radius:

$$r_{cr} = \frac{36^{1/3}}{2}\left(\frac{We_{cr}\delta\nu}{\varepsilon\rho_l}\right)^{1/3} \tag{17}$$

Using the experimental data from [4]: water density, 1000 kg/m^3; gas viscosity, 1.5×10^{-5}m^2/s; gas orifice size, 2.1 mm; surface tension, 0.07 kg/s^2; gas injection velocity, 140 m/s and by setting the turbulent gas velocity at one tenth of the gas injection velocity, one gives for critical radius 3×10^{-5} m, which is of the same order that was measured in [4]. At the same time, expressions (17) requires a reliable knowledge of viscous dissipation rate, which is a problem in the turbulence computation. For these reasons, the critical radius is calculated in this work by the standard expression (13), where $u_r = \mathbf{v}_g - \mathbf{v}_P$ is calculated by the mean relative velocity between gas and liquid particle, computed by the model of turbulent dispersion of particles [13]. Note that introducing the turbulent Weber number, $We_{tur} = \frac{\rho_g l_{tur} u_{tur}^2}{\delta}$, and using (16), one may write for the critical Weber number:

$$We_{cr} = \frac{1}{36}\frac{\rho_l}{\rho_g} Re_{tur}\, We_{tur}\left(\frac{2r_{cr}}{l_{tur}}\right)^3 \tag{18}$$

Assuming that at scales where breakup takes place Re_{tur} is of order of unity and $l_{tur} \approx \eta$, one may propose:

$$\frac{2r_{cr}}{\eta} = 3.3\left(\frac{We_\eta}{We_{cr}}\right)^{-\frac{1}{3}}\left(\frac{\rho_g}{\rho_l}\right)^{\frac{1}{3}} \tag{19}$$

The choice of the breakup frequency has to be stated from the physics of atomization. In this paper, the breakup time scale is taken from [15-17]:

$$\nu = B\frac{\left|\mathbf{v}_g - \mathbf{v}_P\right|}{r_{32}}\sqrt{\frac{\rho_g}{\rho_l}} \tag{20}$$

where r_{32} is the local Sauter mean radius of parent drops and $B = 1/\sqrt{3}$ is taken from TAB model [18].

IV.3 Choice of parameters $\langle\xi\rangle$ and $\langle\xi^2\rangle$

Multiplying (8) by r and integrating over the entire $r-$range give us an expression for the first moment

$$\langle r\rangle = \langle r\rangle_{t=0} \exp\left[\nu\left(\langle\xi\rangle + 0.5\langle\xi^2\rangle\right)t\right] \tag{21}$$

The condition

$$\langle\xi\rangle < -\frac{1}{2}\langle\xi^2\rangle \tag{22}$$

provides for $\dfrac{\langle r\rangle}{\langle r\rangle_{t=0}} < 0$. In this paper, the magnitude for $\langle\xi^2\rangle$ is supposed to be proportional to the maximal dispersion of radius $\langle\xi^2\rangle \propto \ln 1 - \ln\dfrac{r_{cr}}{r_{32}}$. Replacing in (19) η by the local Sauter mean diameter of parent drops, one may assume that

$$\langle\xi^2\rangle \approx -\ln\frac{r_{cr}}{r_{32}} \approx const \cdot \ln\left(\frac{We_{r_{32}}}{We_{cr}}\right)^{1/3} \tag{23}$$

and $\langle\xi\rangle$ is an arbitrary parameter to be taken according to (22) and (23).

V. EXAMPLE OF LAGRANGIAN COMPUTATION OF THE ATOMIZING SPRAY

The configuration and inlet parameters from the CORIA's injector[19] are used in the computation. In this experiment, the round jet of water issues from the central tube ($D_l = 1.8mm$) at low velocity and atomizes by a parallel coflow of air issuing at high velocity from an annular duct ($D_g = 3.4mm$). An example of spatial distributions of drops in the spray, the schematic of the injector and the evolution in time of distributions of droplet-size probability density function (pdf) at two cross sections in the near-nozzle region are given in Fig.1. The pdf distributions are scaled on the total drops number crossing the given section at the given time moment. The statistics of radius at (3-5) mm shows mostly the large unbroken drops of size of the injector orifice that are accompanied by small striped droplets. From pdf's

at (7-9) mm, it is seen that the probability to find drops of size of the injector orifice is essentially decreased while new droplets are produced with radius from 50 μm to 250 μm. These figures and zooming given in Fig.2 show that a broad spectra of droplet size is presented by computations with a co-existence of large drops and small droplets. Computations are performed for different inlet air and water velocities represented in [19] providing for the different magnitudes of the parameter $J = \frac{\rho_g u_g^2}{\rho_l u_l^2}$ and the inlet Weber number. The qualitative agreement have been obtained between measured impact liquid core and the estimated length of the zone presented by computed blobs of size of the injector orifice. The modified numerical code with the stochastic model of breakup is specifically target on the computation of the spray combustion in the configuration likely to rocket engine.

VI. CONCLUSION

A new sub-grid-scale stochastic model of drops air-blast breakup is presented in this paper. The stochastic process is considered in the framework of cascade of uncorrelated breakage events in series down to the critical size, independently from the initial distribution of sizes. To this end, the Kolmogorov's discrete model of particle breakup has been reproduced in the form of evolution equation for distribution function. The asymptotic solution of this equation has been applied to simulate the drop breakup alongside with Lagrangian model of spray dynamics. Performed computations of air-blast atomization are related to a spray close to the rocket engine configuration. A broad spectra of droplet size is simulated at each spray location with a co-existence of large drops and small droplets. The evolution of shape of the droplet-size pdf's is shown at different sections in downstream direction.

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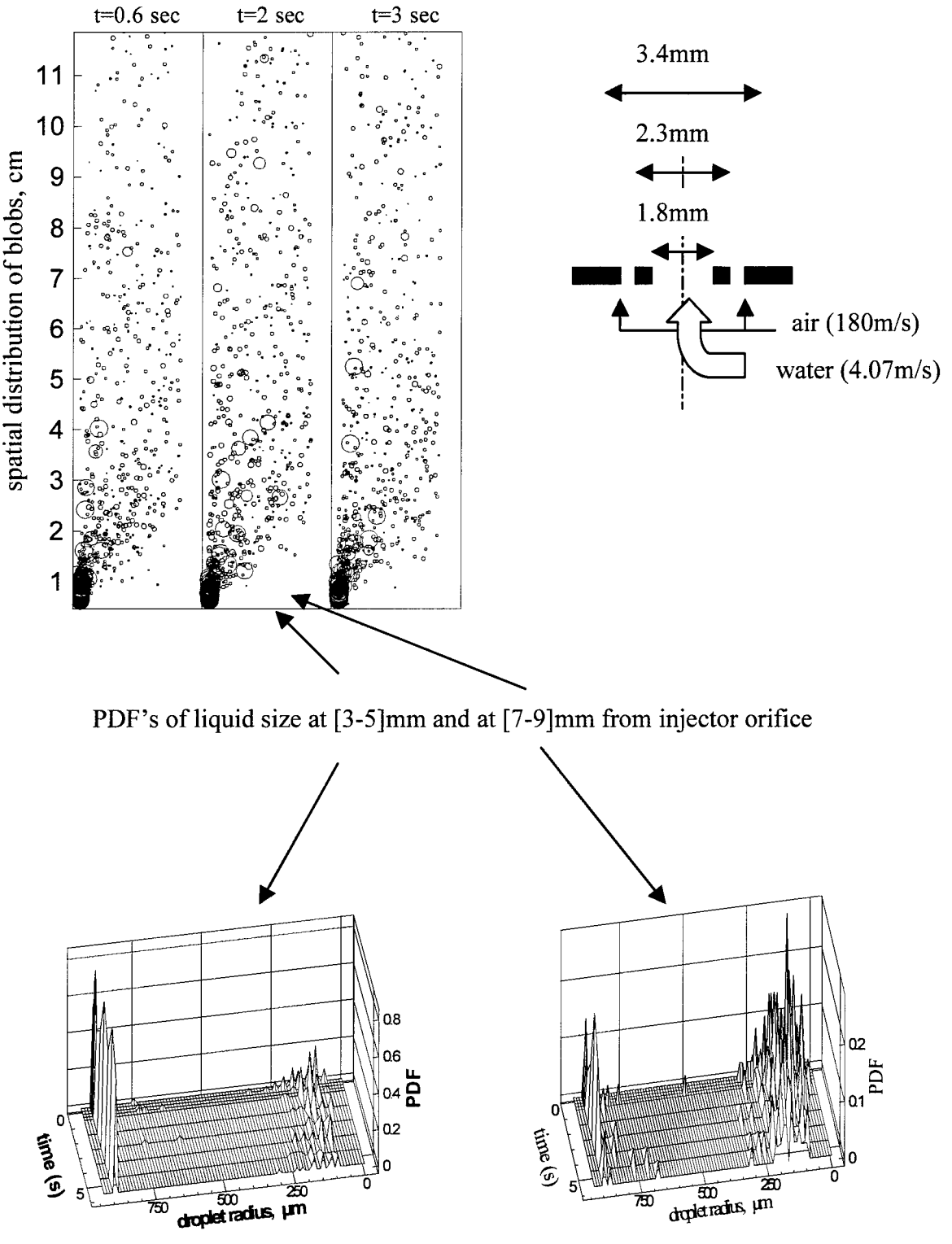

Fig.1 Computed one-side spatial distributions of drops and PDF's of size at different sections. CORIA GDR injector.

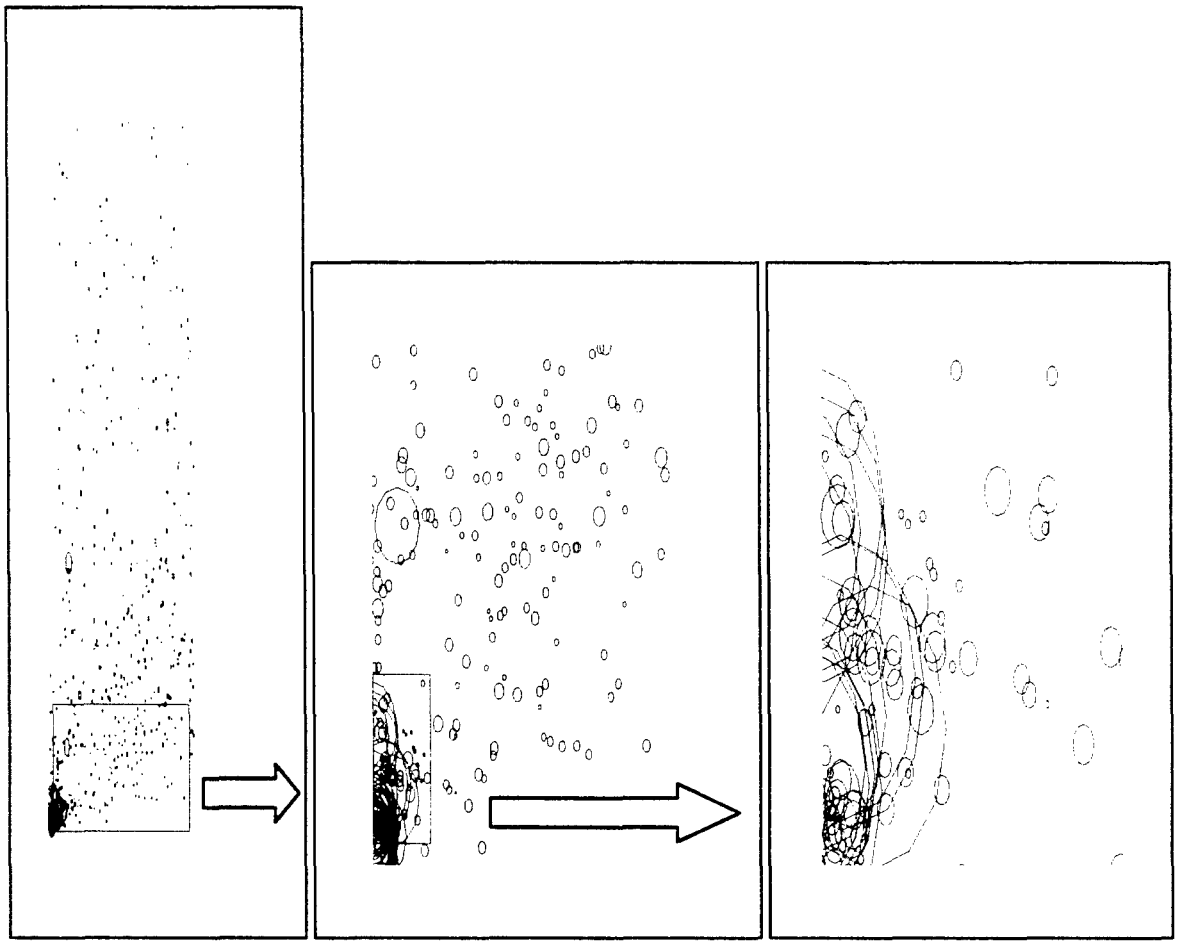

Fig.2 Zooming of spatial distributions of blobs computed in the near-injector region.