1. INTRODUCTION.

When a liquid jet at small velocity is injected into a gas motion, the physics of fragmentation is very complex (shearing of liquid bulk and generation of vorticity, instabilities on the gas/liquid interface, entrainment of liquid filaments by gas flow with instabilities, collisions, coalescence, shearing of those). Several direct numerical approaches were designed to simulate such fragmentation [1]-[4]. These methods are based on integration of the instantaneous Navier Stokes equations, with capturing of the gas/liquid interface at each time step. The fragments are created when the stretched liquid filament is getting within the finite-difference cell. If the flow is not “very turbulent”, these approaches may provide accurate local estimates of gas/liquid mixture, and then may help to understand the physics of primary atomization. However in practical applications, the primary atomization takes place at high Weber number, and exact resolution of primary atomization may become a difficult task. If the relative velocity between liquid and gas is more than hundred meters per second, the large resolved scales in the liquid may produce the fragments of order of dozen of microns, which is substantially less than the grid size. Also, if the flow is highly intermittent, a liquid subgrid filament may, contrary to fragmentation, relax its form up to large scales. Is such a long-range interaction significant in the prediction of primary atomization at high Weber number, is the open question. Complementary to those deterministic approaches, the need comes to develop another methods, more engineering and less limited on CPU resources. One of such is the approach proposed in [5]. In this approach, the atomization is viewed as a turbulent mixing of a dense jet in the gas flow. This mixing is simulated in the framework of RANS approach. In each spray location, the local mean size of droplets can be computed from the transport equation for the mean interface density. The form of this equation is presumed and supposed to be universal, independently of geometry of the flow, of initial and boundary conditions. The transport of the mean interface density is modelled by the gradient hypothesis, thereby the diffusion-like motion of liquid elements is assumed. In this paper, we propose another engineering model of the primary air-blast atomization, in which the position between atomizing liquid jet and the gas flow is defined only at a certain probability. The geometry of injected liquid bulk is assumed to be fluctuating so strongly that its statistics is characterized by universalities under scaling symmetry. These universalities were identified in [6]. The statistics behind these universalities is principally non-Gaussian, implying an evolution towards fractal properties of interface with parameters controlled by local mechanism of atomization. From statistics of the instantaneous geometries of liquid bulk in the vicinity of injector, the liquid drops are sampled using presumed distribution of size and conservation of the liquid mass. The drops are subjected to the secondary atomization and coalescence. These processes are simulated stochastically as a result issued from inter-drop collision [7]. The stochastic model of spray atomization is coupled with LES computation in the gaseous flow: at each time step, the computed velocity field is conditionally averaged on the liquid void in the vicinity of injector. This conditioned velocity field controls...
dynamics of produced drops. The numerical procedure comprises the following steps: (a) LES computation of the gas flow up to the statistically stationary state; (b) simulation of primary atomization and conditioning of the resolved velocity field on the presence of non-depleted liquid bulk in the vicinity of injector; (c) sampling of drops, dragging procedure by conditioned velocity field simulation of secondary atomization and coalescence; (d) verification of statistical stationarity. The results of computation at different inlet velocities of the gas and the liquid were compared with experimental visualisation of the liquid void distribution in the vicinity of injector [8]. In the far-field of the spray, the computed mean Sauter diameter is compared with presented in [9] measurements.

2. MODELING OF DISTRIBUTION OF THE LIQUID IN THE VICINITY OF INJECTOR.

2.1 Notation of “Stochastic Floating Cutter Particle”. In Fig. 1, the different realizations are shown schematically of a atomizing liquid jet injected into high velocity co-flowing gas; each realization is presented as a corrugated non-depleted liquid core surrounded by disintegrated liquid fragments. For the statistical description of these realizations, our four main assumptions are as follows:

(i) at different times, the geometrical configurations of non-depleted core represent an ensemble of independent realizations

(ii) many degree of freedom intervene in the fluctuation of the liquid core due to high Weber number; these fluctuations are strong enough that following one geometrical realization, its instantaneous thickness in the downstream direction does not depend on the instantaneous thickness in the upstream direction (scaling symmetry assumption)

(iii) the stochastic process of each geometrical realization is piloted by fastest wave growth of Rayleigh-Taylor instability

(iv) the distribution of liquid in the vicinity of injector is controlled mainly by statistics of spatial positions of non-depleted liquid bulk; the contribution of disintegrated fragments is neglected in this distribution.

In order to realize (ii), we introduce a stochastic particle moving in the physical space according to the stochastic equations that are specific for the scaling symmetry hypothesis (the equations are demonstrated hereafter). This particle is called a “floating cutter”. Its motion in the space determines one geometrical realization of non-depleted liquid bulk. This motion continues during the “life” time of the particle, which is defined by time scale from competition between momentum exchange and the inertia of liquid jet:

$$\tau_{\text{life}} = \frac{\rho_l u^2_{\text{g0}} - \rho_l u^2_{\text{l0}}}{2 \rho_l} \frac{1}{d_0}$$

Here $\rho_g u^2_{\text{g0}} / 2$ and $\rho_l u^2_{\text{l0}} / 2$ are initial momentums in gas flow and liquid jet, respectively; $\rho_l$ is the density of liquid; $d_0$ is diameter of injector. In correspondence with (iii), the parameter of governing stochastic equations is coupled with fastest wave growth of Rayleigh-Taylor instability, computed by inlet parameters. To satisfy (i), we inject simultaneously an ensemble of “floating cutter” particles; each life-history of one particle represents one independent realization of geometry of non-depleted liquid core. According to (iv), the statistics of these geometries is used to form blobs, which are subjected to the secondary atomization and coalescence.

Fig.1 Schematic of different geometrical realizations in primary air-blast atomization
2.2 Scaling symmetry assumption and log-Brownian stochastic process for “floating cutter” particle.

Following the scaling symmetry scenario, each fragmentation reduces the typical thickness of the liquid core in down-stream direction, \( r \Rightarrow \alpha r \), by an independent random multiplier \( \alpha \), which is governed by the fragmentation intensity spectrum \( q(\alpha) \), \( \int_0^\infty q(\alpha) d\alpha = 1 \).

If the breakup frequency, \( \nu \), is independent on \( r \), the normalized distribution of size, \( f(r,t) \), evolves according to the following integro-differential equation:

\[
\frac{\partial f(r)}{\partial t} = -\nu f(r) + \int_0^\infty q(\alpha) \frac{d\alpha}{\alpha} - \nu f(r)
\] (2)

Here, to fulfill the evolution of distribution function, the fragmentation spectrum \( q(\alpha) \) has to be different from delta function. Expanding the kernel \( \frac{d\alpha}{\alpha} \) on powers of \( \ln \),

\[
\frac{\partial f(r)}{\partial t} = -\nu f(r) + \frac{\partial}{\partial r} \left( h + g \frac{\partial^2 f}{\partial r^2} \right)
\] (3)

The solution of (3) requires the knowledge of all moments of spectrum \( q(\alpha) \). However it has been shown in [6] that although each term on the right hand side of (3) can be significant, their renormalized sum, in the case of scaling symmetry, is determined solely by first two logarithmic moments of \( q(\alpha) \). Then equation (3) reduces exactly to the Fokker-Planck equation:

\[
\frac{\langle \ln^2 \alpha \rangle}{\langle \ln \alpha \rangle} = \frac{r_{cr}}{r_c}
\] (5)

where \( r_{cr} \) is the maximum stable size and \( r_c \) is the length scale, to which the dominant physics of atomization must be prescribed. Let us formulate the stochastic process corresponding to (4) in the framework of the Langevin equation. For the stochastic variable \( r \), the general Langevin equation has the form

\[ \dot{\alpha} = h(r,t) + g(r,t) \Gamma(t) \]

where \( \Gamma(t) \) is the Langevin force assumed to be a Gaussian random value with zero mean and \( \delta \) -correlation in time: \( \langle \Gamma(t) \rangle = 0 \);

\( \langle \Gamma(t) \Gamma(t') \rangle = 2\delta(t-t') \). Using first two (non-zero) coefficients of the Kramers-Moyal expansion [11] the general Fokker-Planck equation then has the form:

\[
\frac{1}{v_n} \frac{\partial f}{\partial t} = -\frac{\partial}{\partial r} \left( h + g \frac{\partial^2 f}{\partial r^2} \right) + \frac{\partial}{\partial r} \left( g \frac{\partial^2 f}{\partial r^2} \right)
\] (6)

This equation can be rewritten in the following form:

\[
\frac{1}{v_n} \frac{\partial f}{\partial t} = -\frac{\partial}{\partial r} \left( h + g \frac{\partial^2 f}{\partial r^2} \right) + \frac{\partial}{\partial r} \left( g \frac{\partial^2 f}{\partial r^2} \right)
\] (7)

Rewriting equation (4) as:

\[
\frac{\langle \ln \alpha \rangle}{v_n} \frac{\partial f}{\partial t} = -\frac{\partial}{\partial r} \left( h + g \frac{\partial^2 f}{\partial r^2} \right) + \frac{\partial}{\partial r} \left( g \frac{\partial^2 f}{\partial r^2} \right)
\] (8)

and comparing the later with (7), one yields the Langevin stochastic equation:

\[
\dot{\alpha} = h \langle \ln \alpha \rangle + \sqrt{\nu} \langle \ln^2 \alpha \rangle/2 r \Gamma(t)
\] (9)

which corresponds to the classical Brownian process in the space of \( x = \ln r \).

At the starting location of the liquid/gas interface, we inject the ensemble of stochastic “floating cutter” particles. In the radial direction, the velocity of “floating cutter” particle with index \( i \) is defined by:

\[
V_{ri} = \nu \langle \ln \alpha \rangle r_i + \sqrt{\nu \langle \ln^2 \alpha \rangle/2} r_i \Gamma(t)
\] (9)

and therefore its radial position is computed from:
\[ \frac{dr_i}{dt} = V_{ip} \quad (10) \]

In the axial direction, we assume that the acceleration of “floating cutter” particle is controlled by gradient of kinetic energy of relative liquid-to-gas motion:

\[ \frac{dU_{ip}}{dt} = \frac{1}{2} \rho_g \left( u_g - U_{ip} \right) \left( u_g - U_{ip} \right) \frac{1}{r_i} \quad (11) \]

where \( u_g \) and \( \rho_g \) are the local velocity and density in the gas flow, respectively. The axial position of “floating cutter” particle is defined from:

\[ \frac{dX_{ip}}{dt} = U_{ip} \quad (12) \]

The initial conditions for (9)-(12) are:

\[
\begin{align*}
    r(t = 0) &= r_0 \\
x_{ip}(t = 0) &= 0 \\
V_{ip}(t = 0) &= 0 \\
U_{ip}(t = 0) &= u_{l0}
\end{align*}
\]

(13)

where \( u_{l0} \) is the initial velocity of liquid jet and \( r_0 \) is the radius of injector.

2.3 Identification of parameters

Following analysis given in [12], the significant contribution to primary air-blast atomization comes from Raleigh-Taylor instability of filaments entrained by the gas flow. To this end, the length scale, associated with the fastest Raleigh-Taylor wave instability growth, is introduced in our model. In [13], this scale is expressed as a function of Weber and Ohnesorge numbers.

\[ \lambda_{RT} = 9.02 \frac{1 + 0.45 Z^{0.5}}{1 + 0.87 W_{e2}^{1.07}} r_0 \quad (14) \]

where

\[ W_{e1} = \rho_l (u_{g0} - u_{l0})^2 r_0 / \sigma, \quad W_{e2} = \rho_g (u_{g0} - u_{l0})^2 r_0 / \sigma, \quad Re_t = \left( u_{g0} - u_{l0} \right) r_0 / \nu_t, \quad Z = W_{e1}^{0.5} / Re_t, \quad T = Z W_{e2}^{0.5}. \]

Using (14), the expression (5) writes:

\[ \left\langle \ln^2 \alpha \right\rangle = \ln \left( \frac{r_{cr}}{\lambda_{RT}} \right) \quad (15) \]

and

\[ \left\langle \ln \alpha \right\rangle = \text{const} \ln \left( \frac{r_{cr}}{\lambda_{RT}} \right) \quad (16) \]

where \( \text{const} \) is of order of unity and the critical scale is expressed by

\[ r_{cr} = \frac{W_{e2} \sigma}{\rho_g (u_{g0} - u_{l0})^2}. \]

2.4 Comparison with experimental visualization.

In [8], the diagnostics of scalars in two-phase dense jets by plane laser has been developed. The distributions of liquid void in the of coaxial injector were presented. In this experiment, the round liquid jet issues from the central tube (\( D_l = 1.8\, \text{mm} \)) at low velocity (from 0.68 m/s to 4.07 m/s) and atomizes by a parallel flow of air issued at high velocity (from 60 m/s to 180 m/s) from an annular duct (\( D_g = 3.4\, \text{mm} \)). In the region close to injector, our previous work [14] showed that compared to [8], the model (9)-(16) agrees well with experimental visualization of liquid void statistics in near-injector region for different values of parameter \( M = \frac{\rho_l u_{l0}^2}{\rho_g u_{g0}^2} \). Besides, it has been shown that the shape of the typical size distribution at different axial positions, close to injector, evolves from the narrow peak towards lognormal form similar to experiment.

3. LES COMPUTATION OF THE GAZ FLOW

The gaseous round jet was computed in the framework of LES approach, using the CTR/Stanford numerical code [15]. This code resolves three-dimensional incompressible filtered Navier-Stokes equations. The MAC-grid is used, applying the second-order central differences in space and Crank-Nicolson discretization in time, with semi-implicit numerical integration using Newton-Raphson iterations. The sub-grid momentum transport term was modeled by dynamic approach of Germano [16]. This code was verified by comparison with DNS and measurements in jet flows [17, 18].

4. SECONDARY ATOMIZATION AND COALESCENCE IN THE RESOLVED VELOCITY FIELD CONDITIONNED ON THE PRESENCE OF LIQUID IN THE VICINITY OF INJECTOR

The computed spatial distribution of non-depleted liquid bulk is used to sample drops, which are subjected to the secondary atomization and coalescence. These drops are sampled in locations, where the probability to find the non-depleted liquid bulk is in between 0.01 and 0.9. The presumed distribution of size of formed drops was taken in the following form:
where the typical size $r_{typ}$ is computed assuming the balance between the local turbulent energy, stretching the liquid element, and the work done by the surface tension forces:

$$
    r_{typ} = \frac{1}{2} \left( \frac{\sigma}{\rho g} \right)^{\frac{2}{5}} \varepsilon^{-2/5},
$$

where $\varepsilon$ is the dissipation rate.

Here following [9]:

$$
    \varepsilon = \frac{u_2^2}{(1+m)D_g} \text{ and } m = \frac{\rho u_0 (D_e-D)^2}{\rho u_0 (D_e-D)^2 + \rho u_0 D^2}
$$

The sampling procedure of drops is organized in a way that the injected liquid mass is continuously conserved in the produced drops. These drops interact with the resolved velocity field in the gas flow $u_g$, conditioned on the presence of non-depleted liquid bulk:

$$
    \frac{d x_d}{dt} = u_d, \quad \frac{d u_d}{dt} = \frac{f}{St_g} \left( \langle u_g \rangle - u_d \right)
$$

Here $x_d$ and $u_d$ are the position and the velocity of the drop, respectively. The local conditioned gas velocity $\langle u_g \rangle$ is computed by:

$$
    \langle u_g \rangle = u_g - (1-P_l) \varepsilon + u_{f0} P_l
$$

where $P_l$ denotes the probability to find the non-depleted liquid bulk.

The details of stochastic modelling of secondary atomization and coalescence can be found in [7]. In this model, the coalescence or break-up issue from consideration of inter-drop collision. The collision frequency is calculated from O’Rourke model [19]. The outcome of collision (alternative to have the break-up or the coalescence) is defined by the Weber number of colliding partners.

5. EXAMPLES OF COMPUTATION AND COMPARISON IN THE FAR-FIELD OF SPRAY.

Fig. 2, Fig 3 demonstrates simulation of atomizing liquid jet injected at different velocities into high-speed (140m/s) coflowing gas. Here the intake parameters are used from experimental work [9]. For different axial positions, Fig3 compares the computed mean Sauter diameter with the measurements. It is seen that for different velocities of injection, this diameter is predicted relatively well. Fig. 2 shows snapshot of spatial distributions of the liquid and the gaseous conditioned velocities for different values of the parameter $M = \frac{\rho_g u_0^2}{\rho u_0 D}$. It should be noted that our stochastic modeling can not reproduce a real filamentary structure of atomizing spray; it represents conventionally the expected spatial distributions of scales of atomized liquid phase, when operating conditions are varying. In this optics, the distributions, shown in Fig.2, correspond to physical intuition: with increasing of parameter $M$, the liquid core is becoming shorter (the comparison with [8] showed its good quantitative prediction), the length scale of fragments decreases; these fragments are entrained by the jet flow of the gas, and finally, the far-field of the spray is supplied by scales, which are relatively in agreement with measurements (Fig. 3).

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Fig. 2. Simulated atomizing liquid jet injected into high velocity co-flowing gas ($u_{g0} = 140 \text{ m/s}$) at different injection velocities ($u_{l0} = 0.13 \text{ m/s}; 0.55 \text{ m/s}; 2.8 \text{ m/s}$)
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