Stochastic modeling of the drops breakup in LES with atomizing spray

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A stochastic subgrid model for large-eddy simulation (LES) of atomizing spray is developed. Following Kolmogorov's concept of viewing solid particle-breakup as a discrete random process, atomization of liquid blobs at high relative liquid-to-gas velocity is considered in the framework of uncorrelated breakup events, independent of the initial droplet size. Kolmogorov's discrete model of breakup is rewritten in the form of differential Fokker-Planck equation for the pdf of droplet radii. Along with the Lagrangian tracking of spray dynamics, the size and number density of the newly produced droplets is governed by the evolution of this pdf in the space of droplet-radius. The parameters of the model are obtained dynamically by relating them to the local Weber number with two-way coupling between the gas and liquid phases. Computations of spray are performed for the representative conditions encountered in idealized gas-turbine engine configurations. A broad spectrum of droplet sizes is obtained at each location with co-existence of large and small droplets. The present approach is computationally efficient and can capture the complex fragmentary process of liquid atomization.

1. Introduction

When liquid-jet is injected into high relative-velocity gas flow (high Weber number), the influence of interfacial forces on the atomization process is less pronounced. In these conditions, it is too difficult to disclose clearly a dominant mechanism of atomization. Turbulence, multiple droplets collision, cavitations, variations in operating conditions, stripping, etc., may contribute to the breakup. In every region of spray, droplets may be produced with some probability, over a large spectra of size, often independently on the prehistory of breakup. To this end, the stochastic approach for the breakup modeling has been proposed in [1, 2]. In [3], this approach was further developed and implemented in the framework of unstructured LES/spray model in the case of diesel-like configuration. In this paper, we briefly describe the stochastic atomization model in sprays and then we show an example of calculated results obtained by LES/spray approach in the case of air-blast atomization.

2. Fokker-Planck equation for particle-breakup

Let $N_{tot}(t)$ and $N(r,t)$ represent the total number of breaking particles and among them a number of particles with size $\rho \le r$, respectively, at discrete time instants $t = 0,1,2,\ldots$. These time moments are scaled by the breakup frequency ν, such that ($\nu t_{bu} = 1$), where t_{bu} is the time at which breakup occurs. Their corresponding expectations are given as $\overline{N}_{tot}(t)$ and $\overline{N}(r,t)$ respectively. Consider breakups of a given particle with size *r* within the time interval $[t,\ t+1]$. Let $Q(\alpha)$ be the mean number of secondary particles produced with size $\rho \le \alpha r$ ($0 \le \alpha \le 1$). According to Kolmogorov's hypotheses [4], the probability to break each parent particle into a given number of fragments is independent of the parent particle size. In other words, $Q(\alpha)$ does not depend on the history of breakup and is not influenced by other parent particles. It then follows that,

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

Introducing $x = \ln r$, Kolmogorov [4] pointed out that

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

Further, denoting $\xi = \log\alpha$ and $Q(\alpha) = Q(1)\cdot S(\xi)$, Eq. (1) can be rewritten as

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

By central limit theorem, Kolmogorov noted that from discrete model (3), the long-time limit form of $T(x,t)$ tends to be a Gaussian function. This implies that the number of droplets $N(r,t))$ is asymptotically governed by the log-normal distribution of particle size.

The spectrum $Q(\alpha)$ in (3) is principally unknown. However, the discrete model (3) can be represented at large times by its differential Fokker Planck approximation, where only two first moments of $Q(\alpha)$ intervene as coefficients of equation. For example, using parabolic scaling of variables $\tau = \beta^2 t$, $y = \beta x$, where β is a small scaling parameter (in a way that $\beta \to 0$ with $t \to \infty$), the relation (3) rewrites

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

Then expanding both the left-hand side and the expression under integral and assuming also that the integral $\int_{-\infty}^{0}\xi^3 s(\xi)d\xi$ is limited such that $\frac{1}{3!}\beta\frac{\partial^3 T}{\partial x^3}\int_{-\infty}^{0}\xi^3 s(\xi)d\xi$ becomes negligible if $\beta \to 0$, one obtains the Fokker-Planck approximation:

$$\frac{\partial T(x,t)}{\partial t} = -\nu\langle\xi\rangle\frac{\partial T(x,t)}{\partial x} + \frac{1}{2}\nu\langle\xi^2\rangle\frac{\partial^2 T(x,t)}{\partial x^2} \tag{5}$$

Here $\langle\xi\rangle = \int_{-\infty}^{0}\xi\, s(\xi)d\xi$ and $\langle\xi^2\rangle = \int_{-\infty}^{0}\xi^2\, s(\xi)d\xi$ are two first moments of ξ, and the time, which has been scaled in (3) by the breakup frequency, is transformed in (5) to its dimensional form. Equation (5) is written for the probability distribution. Setting further

$T(x,t)=\int_{-\infty}^{x}\Phi(x,t)dx$, the equation for the probability density distribution, $\Phi(x)$, can be written in the equivalent to (5) form :

$$\frac{\partial\Phi(x,t)}{\partial t}=-\nu\langle\xi\rangle\frac{\partial\Phi(x,t)}{\partial x}+\frac{1}{2}\nu\langle\xi^2\rangle\frac{\partial^2\Phi(x,t)}{\partial x^2} \tag{6}$$

The density distribution of radius, $f(r,t)$, which is the number distribution function normalized on the total number of particles ($\int_0^\infty f(r,t)dr=1$), can be expressed according to the rule $|f(r)dr|=|\Phi(x)dx|$. This gives

$$\begin{cases}\Phi(x)=e^x f(e^x)\\ f(r)=\frac{1}{r}\Phi(\ln r)\end{cases} \tag{7}$$

Using (7), the Fokker-Planck equation for the distribution $f(r,t)$ looks:

$$\frac{\partial f(r,t)}{\partial t}=\frac{\partial S(r,t)}{\partial r} \tag{8}$$

where $S(r,t)$ is a density of flux in the space of length scales given by the following expression

$$S(r,t)=-\nu\langle\xi\rangle r f(r,t)+\frac{1}{2}\nu\langle\xi^2\rangle r\frac{\partial}{\partial r}(r f(r,t)) \tag{9}$$

The solution of (6) yields:

$$\Phi(x,t)=\int_{-\infty}^{0}\frac{1}{\sqrt{2\pi\langle\xi^2\rangle\nu t}}\exp\left[-\frac{(x-x_0)^2}{2\langle\xi^2\rangle\nu t}\right]\Phi_0(x_0-\langle\xi\rangle\nu t)dx_0 \tag{10}$$

where $\Phi_0(x_0)$ is the distribution of the logarithm of droplet radius of the parent drop. Accounting for (7), this solution can be rewritten for the normalized distribution of radius, $f(r,t)$:

$$f(r,t)=\frac{1}{r}\int_0^\infty\frac{1}{\sqrt{2\pi\langle\xi^2\rangle\nu t}}\exp\left[-\frac{\left(\ln\frac{r_0}{r}+\langle\xi\rangle\nu t\right)^2}{2\langle\xi^2\rangle\nu t}\right]f_0(r_0)dr_0 \tag{11}$$

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

3. Implementation of Stochastic Breakup Model into Unstructured LES code

In the present LES computations, an Eulerian-Lagrangian code based on low Mach number equations is used [5]. This code is capable of handling complex geometries with unstructured and arbitrary shaped elements and is primarily developed for hi-fidelity computations of turbulent flows in realistic complex geometries. The algorithm has been validated for multiphase flows in a variety of configurations including turbulent flows through the channel, swirling coaxial combustor, and realistic industrial combustion chamber [6]. The influence of the high number density of droplets on the gas-phase flow are modeled through two-way

coupling between the gas and liquid phase. The standard particle-in-cell (PIC) methodology is employed where the effect of particles within a control volume is represented at its centroid.

The breakup is modeled stochastically along with Lagrangian tracking of individual drops or parcels of drops. To simplify computations, the sampling procedure was based on the logarithm of radius, $x = \ln r$. Consider a given primary blob that breaks into secondary droplets according to the following scenario. The starting distribution for the logarithm of droplet radius in this primary blob is

$$\Phi_0(x) = \delta(x_0 - x) \tag{12}$$

After the passage of time ($\nu t = 1$), the new droplets arise due to the blob breakup. The change of the initial distribution (12) is governed by Fokker-Planck equation and, as time progresses to $\nu t = 1$, the distribution of $x = \ln r$ becomes from (10):

$$\Phi(x) = \frac{1}{\sqrt{2\pi\langle\xi^2\rangle}} \exp\left[-\frac{(x - x_0 - \langle\xi\rangle)^2}{2\langle\xi^2\rangle}\right] \tag{13}$$

Therefore, the sampling procedure for new droplets ($\int_{-\infty}^{x} \Phi(x)dx = \eta, \quad 0 \prec \eta \prec 1$) is realized by the following function:

$$\int_{-\infty}^{x} \Phi(x,t)dx = \frac{1}{2}\left[1 + erf\left(\frac{x - x_0 - \langle\xi\rangle}{\sqrt{2\langle\xi^2\rangle}}\right)\right] \tag{14}$$

where *erf* is the error function and x_0 is the logarithm of the given parent blob. The number of newborn droplets is computed from the mass conservation in the primary and secondary droplets. The breakup process is interrupted when the radius of secondary parcel becomes equal to or less than the maximum stable radius, r_{cr}.

4. Critical radius and breakup frequency

The critical (or maximum stable) radius for break-up is obtained by a balance between the disruptive hydrodynamic and capillary forces:

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

where $|u_r|$ is the relative velocity, δ the surface tension coefficient, We_{cr} the critical Weber number, which is assumed to be of the order of six over a wide range of Ohnesorge numbers [7]. This expression can be further applied if $|u_r|$ is known. Estimating the mean square of relative droplet-to-gas velocity from the mean viscous dissipation and Stokes time scale [8], one writes:

$$\langle u_r^{\,2} \rangle \approx \varepsilon\tau_{st} \tag{14}$$

This gives the critical radius as follows [1]:

$$r_{cr} = \left(\frac{9}{2}\frac{We_{cr}\delta\nu}{\varepsilon\rho_l}\right)^{1/3} \tag{15}$$

This expression, however, requires a reliable knowledge of viscous dissipation rate. This can be obtained dynamically from the resolved scale energy flux in a LES computation.

The breakup frequency follows the standard expression:

$$\nu = B\frac{|u_r|}{r_0}\sqrt{\frac{\rho_g}{\rho_l}} \tag{16}$$

where r_0 is the radius of a given parent drop and $B = 1/\sqrt{3}$.

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

Providing values of $\langle\xi\rangle$ and $\langle\xi^2\rangle$ is a crucial and difficult problem. Our objective is to relate these terms to the characteristic flow parameters in order to obtain their values dynamically. It should be noted that in a long time limit, when all droplets are already broken, the density of flux in the space of radius $S(r, t\to\infty)$ may be set to zero, which implies some steady state distribution of broken droplets. Equating expression (9) to zero, the steady state solution verifies to be the power function:

$$f(r,t) \underset{t\to\infty}{\infty} \left(\frac{1}{r}\right)^{1-2\frac{\langle\xi\rangle}{\langle\xi^2\rangle}} \tag{17}$$

A power distribution is endowed with a remarkable property, namely with self-similarity or fractal property of complicated irregular shapes. As to breakup occurring at high relative velocity (high Weber number), the fractal structure of atomized spray implies (see observations in [9, 10]) that there is no typical length scale in the intermediate range of scales between scale of parent fluid element and maximum stable scale defined by the critical Weber number. This resembles an inertial interval of turbulent eddies in the well-known cascade process in the homogeneous turbulence at high Reynolds numbers. Therefore analogously to the concept of energy cascade from the large to small scales in a turbulent flow field , one yields :

$$We_0 = \frac{r_0\,\rho_g\,u_r^2}{\sigma} = We_{cr}\left(\frac{r_0}{r_{cr}}\right)^{5/3} \tag{18}$$

where $u_{r,cr}$ is the relative velocity, at which disruptive and capillary forces are balanced (similar to the turbulent velocity scale of smallest eddies). It follows from definition of α and ξ, that

$$\alpha_{\min} = \frac{r_{cr}}{r_j} = \left(\frac{We_{cr}}{We_j}\right)^{3/5} \text{ and } \xi_{\min} = 0.6\cdot\log\left(\frac{We_{cr}}{We_j}\right).$$

To this end, we assume in this paper that

$$\langle\xi\rangle = K\log\left(\frac{We_{cr}}{We_j}\right) \tag{19}$$

where constant K is of order of unity. As to computation of $\langle\xi^2\rangle$, let us remark that the diffusion coefficient in the Fokker-Planck equation is known from the Einstein's theory of Brownian motion to be the an energy of Brownian particles multiplied by their mobility. At the same time, the drift velocity in this theory is presented in form of drag force multiplied by the mobility. The ratio of diffusion-to-drift velocity is then given by the ratio of energy-to-drug force. In our case of breakup process, we associate the energy in Einstein's theory with

the disruptive energy while the force may be associated with capillary force. Then the diffusion-to-drift velocity ratio may be presented as disruptive energy-to-capillary force ratio. The last one is characterized by the Weber number. Coming back to the Fokker-Planck equation (8), (9), one can see that the diffusion-to-drift velocity ratio is scaled by the ratio $-\frac{\langle \xi^2 \rangle}{\langle \xi \rangle}$. In this situation it is logically to assume that

$$-\frac{\langle \xi^2 \rangle}{\langle \xi \rangle} = We_0 \tag{20}$$

Thus, both the parameters $\langle \xi \rangle$ and $\langle \xi^2 \rangle$ are obtained dynamically by computing the local values of We_0 and We_{cr}.

6. Example of computation of air-blast atomization

Air-blast atomization of liquid jet in a strong, turbulent cross flow depicting conditions in a gas-turbine combustion chamber was simulated. First, a periodic, turbulent channel flow was computed using the unstructured LES code. The bulk mean velocity normalized by the wall-shear velocity (1 m/s) is approximately 15.63, which gives the Reynolds number based on the bulk mean velocity and full channel width as 5600. The coarse grid 32 x 64 x 32 used in this simulation was able to give good results for the gas-phase turbulent quantities comparing to DNS. Liquid jet is injected through the lower wall at z = 0 plane in the vertical direction with velocity 1/10-th of the mean axial gas-phase velocity at the centerline of the channel (approximately, 18 m/s). The water jet is simulated by introducing 1 mm diameter blobs. Figure 1 shows the time evolution of gas-phase axial velocity contours in the $z = 0$ plane. Instantaneous snapshots of liquid spray are superimposed on the contour plots. The size of the circles is proportional to the droplet diameter. Axial velocity contours in a channel flow without liquid injection is also shown on the top part for comparison. It is seen that large-scale eddies transmit kinetic energy to the liquid jet, causing stretching, flapping, and breakup. A highly unsteady, `pulsating' formation of droplets with broad size-spectrum is observed. Figure 2 shows one-point correlation between gas-phase velocity and droplet diameter normalized by reference velocity (1m/s) and channel width (2m). The coupling between the gas-phase turbulent fluctuations and atomization is explored by computing one-point correlation between gas-phase streamwise velocity and droplet diameter. Strong correlation is observed in the core region of the liquid jet. The damping of turbulent fluctuations by the dense spray is evident from the contour plots shown in Fig. 1.

7. Conclusion

A stochastic model of secondary breakup involving Lagrangian tracking of droplets with LES of the gas-phase flow field was developed. Atomization was considered in the framework of cascade of uncorrelated breakup events providing droplet diameter distribution with the critical stable diameter independent of the initial size. Kolmogorov's discrete model of particle breakup was represented by its Fokker-Planck approximation governing the production of new droplets. The parameters of the model were computed dynamically based on the local Weber number. The role of LES is to provide accurate predictions of turbulent transport used in estimating the maximum stable diameter of droplets before breakup. In [3],

the present model was validated against available experimental data by Hiroyasu and Kadota (1974) and compared with other standard breakup models. Here in this paper, a breakup simulation is performed in the presence of turbulent cross flow to qualitatively demonstrate the air blast atomization.

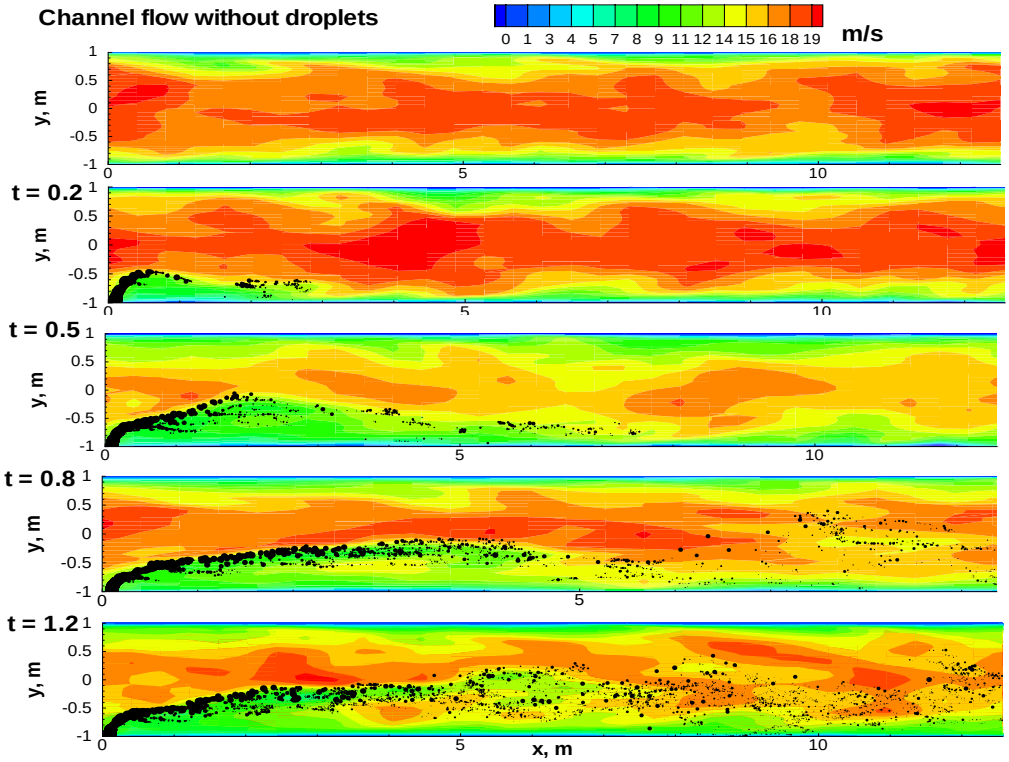

Fig. 1 Contours of axial velocity superimposed with instantaneous locations of the computational particles at $z = 0$. Droplets are injected from the bottom plane at $x = 0.01m$.

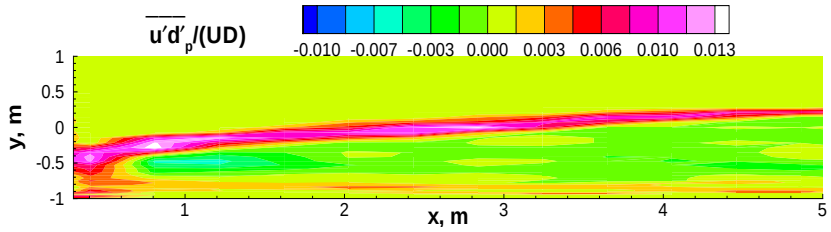

Fig. 2 One-point correlation between gas-phase velocity and droplet diameter normalized by reference velocity ($U = 1m/s$) and channel width ($D = 2m$).

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