Modeling Primary Atomization

Mikhael Gorokhovski
LMFA UMR 5509 CNRS Ecole Centrale de Lyon, 36 avenue Guy de Collongue, 69131 Ecully Cedex, France; Mikhael.Gorokhovski@ec-lyon.fr

Marcus Herrmann
Department of Mechanical Engineering, Stanford University, Bldg. 500, ME/FPC, 488 Escondido Mall, Stanford, CA 94305-3030, USA; Marcus.Herrmann@stanford.edu

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Abstract This review concerns recent progress in primary atomization modeling. The numerical approaches based on direct simulation are described first. While DNS offers the potential to study the physical processes during primary atomization in detail, thereby supplementing experimental diagnostics, it also introduces severe numerical challenges. These challenges and the numerical methods to address them are outlined, highlighting some recent efforts in performing detailed simulation of the primary atomization process. The second part is devoted to phenomenological models of primary atomization. Since earlier conventional models of break-up are well reported in available literature, only two recent developments have been highlighted: (i) stochastic simulation of the liquid jet depletion in the framework of fragmentation under scaling symmetry; (ii) primary atomization in terms of RANS mixing with a strong variation of density.
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Primary atomization represents an example of a complex gas-liquid flow: near the nozzle, the liquid, initially introduced as a continuous jet, disintegrates into filaments and drops by interaction with the gas. In addition to its academic interest, understanding primary atomization is important in analyzing the combustion process in propulsion and power related applications. Primary atomization is also important in a wide variety of other applications (liquid metals, environmental spraying, printing, food processing, etc.), as a significant parameter of the subsequent droplet formation and dispersion. This has led researchers to focus on theoretical and experimental analysis of this phenomenon.

When the liquid jet is injected into annular co-flowing gas at a high relative velocity, the jet breaks up due to momentum transfer from the gas to the liquid. This type of break-up is often referred to as air-blast atomization (19,23,27,54). A possible physical model was suggested in experimental studies by Hopfinger, Villermaux, Cartellier and Lasheras, and by their PhD students, Rehab (74,75), Raynal (72), Marmottant (57,58), Hong (42,43) and Varga (97,98). According to these studies, the liquid jet break-up is caused by instabilities occurring at the gas/liquid interface. After exiting the nozzle, the surface of the liquid jet is subject to the Kelvin-Helmholtz instability. As this instability develops, the most unstable wavelength, $\lambda_{KH}$, is determined by the thickness of the incoming vorticity layer formed in the gas flow inside the nozzle (72), and by the liquid-to-gas density ratio. These primary waves are exposed to the high-speed gas stream and accelerated. This leads to the development of secondary interfacial instabilities. It is shown in (42,43,97,98) that the acceleration of primary waves gives rise to a Rayleigh-Taylor instability with characteristic wavelength $\lambda_{RT}$, which
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When a high-speed liquid jet is discharged into stagnant dense air, less of a consensus has been reached in identifying the dominant mechanism of initial break-up: many interdependent phenomena may instigate this process. The experimental study showed that amongst the important phenomena are turbulence (26, 87, 105, 106) and cavitation pockets (4, 5, 15, 88) within injection holes, drop shedding (81), unsteadiness of the injection velocity (22).

It has been established that a large number of dimensionless scaling parameters are involved in primary atomization. In air-blast atomizers, these include the Weber number $We = \frac{\rho_g (u_g - u_l)^2}{\sigma}$; the non-dimensional thickness of the incoming boundary layer from inside the nozzle $\delta_y / D_g - D_l$; the ratio $\frac{\lambda_{RT}}{\lambda_{KH}}$ characterizing the spectrum of drops produced near the injector; the gas-to-liquid density, mass and dynamic pressure ratios $\rho_l / \rho_g$, $m = \frac{\rho_g u_g (D_g^2 - D_l^2)}{\rho_l u_l D_l^2}$ and $M = \frac{\rho_g u_g^2}{\rho_l u_l^2}$; the Ohnesorge number $Oh = \frac{\mu_l}{\sqrt{\rho_l \sigma D_l}}$, measuring the relative importance of interfacial viscous stress and surface tension. For a high-speed liquid jet atomized in still air, the list of relevant parameters also includes the level of turbulence and the cavitation number in the injection hole: $l_{\text{tur}} / D_l$, $\sqrt{k_{\text{tur}}} u_l$ and $CN = \frac{1/2 \rho_l u_l^2}{p_g - p_{\text{vap}}}$, where $p_{\text{vap}}$ is the saturation vapor pressure at the given temperature. Evaluating the influence of all these parameters in different regimes of break-up, and in realistic operating conditions (high velocities and pressures; small length-and-time scales, strongly non-homogeneous 3D gas-liquid flow) is a difficult task for experimentalists. The numerical modeling of primary atomization may provide a way of overcoming this problem and this review concerns recent progress in such...
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The first category of numerical approaches concerns direct simulation of primary atomization, which is the subject of Section 2. These approaches are based on integration of the Navier-Stokes equations, identifying the gas/liquid interface at each time step. Using this technique, liquid fragments break apart when the progressively stretched filament becomes smaller than the typical size of a numerical cell. Such approaches provide accurate local estimates of the gas/liquid mixture close to the injector, and may help in understanding the physics of primary atomization. However, when the Weber number is very large, the computational expense associated with the resolution of all length scales is very high. When the relative velocity between liquid and gas is more than, say, a hundred meters per second, droplets with diameters of a dozen or so microns may be produced, which is usually smaller than the resolution of the numerical grid. As a result, alongside direct numerical simulation, there is a need to develop phenomenological models, with more modest CPU requirements. The objective of conventional models is to represent statistically the essential features of the initial break-up. Although these models contain the mechanisms of the initial break-up of the liquid jet (surface instabilities in Reitz’s et. al. models (6,36,69,76) and drop shedding (107); "spontaneous" break-up in Tanner’s model (92), jet turbulence in Huh and Gosman’s model (44), cavitation in Arcoumanis and Gavaises’s model (2,3,51)), they use round "blobs" injected from the nozzle exit and hence do not really describe the primary atomization process. To compensate for this to some extent, Section 3 is devoted to two recent developments in phenomenological modelling of primary atomization.
2 Direct Numerical Simulation of Primary Atomization

The detailed physical mechanisms by which primary atomization occurs are as of this date not well understood. Thus direct numerical simulation (DNS) of the primary atomization process can serve as a valuable tool to study the involved mechanisms in detail. In DNS, the goal is to resolve all time and length scales solving the governing equations directly. Since most primary atomization applications occur at low Mach numbers and the two fluids involved are immiscible, the flow is governed by the unsteady Navier-Stokes equations in the variable density, incompressible limit,

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \rho \mathbf{u} = -\nabla p + \nabla \cdot \left( \mu \left( \nabla \mathbf{u} + \nabla^T \mathbf{u} \right) \right) + \rho \mathbf{g} + \mathbf{T}_\sigma \quad (1)
\]

\[
\nabla \cdot \mathbf{u} = 0. \quad (2)
\]

Here, \( \mathbf{u} \) is the velocity, \( \rho \) the density, \( p \) the pressure, \( \mu \) the dynamic viscosity, \( \mathbf{g} \) the gravitational acceleration, and \( \mathbf{T}_\sigma \) the surface tension force which is non-zero only at the location of the phase interface \( x_f \).

Although a DNS approach reduces epistemic uncertainty, the numerical requirements are extremely challenging:

- length and time scales vary over several orders of magnitude,
- the phase interface constitutes a discontinuity in material properties,
- surface tension forces are singular forces active only at the phase interface,
- turbulence and the turbulent primary atomization process are inherently three dimensional,
- topology changes of the phase interface occur frequently.

While the second and third properties are typical for most flows involving liq-
uid/gas interfaces, the others are specifically significant in primary atomization DNS.

The following sub-sections will address the numerical requirements outlined above and discuss state of the art numerical solution strategies for to address them.

2.1 Length and time scales

In a DNS, the goal is to reduce epistemic uncertainty by resolving all necessary time and length scales inherent in the flow and thus eliminating the need to model the effect of any unresolved scales. In a single phase turbulent flow, the smallest length scale that must be resolved is the Kolmogorov length scale $\eta$. Multiphase flows add an additional smallest length scale that requires resolution, the size of the smallest liquid structure $\zeta$. Unfortunately, when topology change of the phase interface is involved, that length scale approaches zero, since the process of pinching involves at the very instance of breakup, a zero sized connecting ligament. Such resolution requirements together with the break down of the continuum assumptions inherent in the Navier-Stokes equations makes simulation of the details of the topology change process unfeasible in the context of DNS of the turbulent primary breakup process. Thus, modeling has to be introduced to address topology change. This will be discussed in a later section.

Using adequate topology change models, the smallest liquid structure $\zeta$ that then should be resolved is of the order of the smallest drop generated by the initial breakup. Depending on the interface tracking/capturing method used, this implies a grid resolution of about 2-5 grid cells per $\zeta$.

As an example, consider the primary breakup of a Diesel jet. There, smallest
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drop diameters near the nozzle of the order of 1 µm have been observed (104) with the Kolmogorov length scale being of the same order of magnitude. This implies an about one order of magnitude finer resolution requirement for the primary breakup DNS as compared to a single phase DNS. Fortunately, such high resolution is required only at and near the phase interface. Away from it, the usual single phase DNS resolution requirements apply.

2.2 Describing the motion of the phase interface

To perform a DNS of the primary atomization process, the location and motion of the phase interface has to be described with high accuracy. Neglecting phase transition effects, the phase interface constitutes a material surface whose motion is described by

\[
\frac{d\mathbf{x}_f}{dt} = \mathbf{v}(\mathbf{x}_f)
\]

where the subscript \(f\) refers to a point on the phase interface. The straightforward way of describing the motion of the phase interface is to solve Eq. (3) for a collection of marker particles placed onto the phase interface. This is the so-called interface tracking approach. While flow solver grid nodes can be used as marker particles, thereby ensuring phase interface conforming flow solver grids, such an approach would require almost constant regridding or rezoning (84) due to the complex flow field at the phase interface during primary atomization. Instead, in the surface marker method, the marker points are connected to form a separate surface grid that is advected according to Eq. (3) in a Lagrangian way inside a fixed flow solver grid (93,94). Although not inherently mass conserving, this approach nonetheless shows excellent mass conservation properties. It’s drawback is that topology changes are not handled automatically, see Sec. 2.5. It has thus
not been applied to the DNS of primary breakup, yet.

An alternative to interface tracking methods are interface capturing methods. Here, the phase interface is imbedded into a fixed grid via the use of an additional scalar. Two principle methods have emerged in this class: the Volume of Fluid method (40,62,84) and the level set method (65,66,85). In the former method, a marker function $\psi$ is defined as the liquid volume fraction in each computational grid cell,

$$\psi = \frac{1}{V} \int_V H(x - x_f) dx$$

(4)

with $H$ the Heaviside function, resulting in a simple advection equation describing the motion of the phase interface,

$$\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi = 0.$$  

(5)

One of the major advantages of the Volume of Fluid method making it a popular interface tracking method is that it can be constructed to be inherently liquid volume conserving. However, due to the discontinuous nature of $\psi$ at the phase interface, see Eq. (4), special geometric algorithms have to be employed to solve Eq. (5) to avoid unacceptable numerical diffusion of $\psi$ (35,77).

In level set methods, a scalar $\phi$ is defined to be equal to some constant value $\phi_0$ at the location of the phase interface, and $\phi > \phi_0$ in fluid 1 and $\phi < \phi_0$ in fluid 2. From this definition and Eq. (3) the level set equation follows,

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0.$$  

(6)

Since the above definition of the level set scalar defines $\phi$ only at the location of the phase interface, there is significant latitude in defining $\phi$ away from it. For numerical reasons, one would like $\phi$ to be a smooth function, thus one of the most popular definition is that of a signed distance function, i.e. $|\nabla \phi| = 1$, see
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for example (89). The major drawback of the level set method is that it does not inherently preserve liquid volume. Since volume errors are proportional in size to the employed grid resolution, grid refinement strategies, like structured adaptive mesh refinement (63) or the Refined Level Set Grid Method (RLSG) (39) can be employed to limit their impact. An alternative to grid refinement is to augment and correct the level set scalar by an additional numerical scheme, for example the CLSVOF or MCLS methods coupling level set and volume of fluid (71,90) or the particle level set method, coupling marker particles and level sets (25).

Defining $\phi$ as the signed distance, is, as indicated above, not a requirement. Instead, in the so-called conservative level set method (64), $\phi_0 = 0.5$ and $\phi$ away from the interface is defined to be a smeared out version of the liquid volume fraction $\psi$, i.e.

$$\phi = \frac{1}{2} \left( \tanh \left( \frac{d}{2\varepsilon} \right) + 1 \right),$$

where $d$ is the minimum distance to the phase interface. Solving Eq. (6) in conservative form in conjunction with re-initializing $\phi$ according to Eq. (7) does show good volume conservation properties (64) even in complex interface geometries (20).

So far, in DNS of the primary atomization process, the VOF (10,100), CLSVOF (60), conservative level set (20), and RLSG method (46) have all been successfully employed.

2.3 Treating the discontinuity in material properties

In most technical applications involving primary atomization, the smallest scales that need to be resolved in a DNS, i.e. the Kolmogorov scale $\eta$ and the size of the smallest drops $\zeta$ are still orders of magnitude larger than the thickness
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of the phase interface itself. Thus, on the resolved scales, the phase interface constitutes a discontinuity in material properties. Under the common assumption that material properties $\alpha$, like density and viscosity, are constant in each of the fluids, their respective values at any point $\mathbf{x}$ in the computational domain are defined as

$$\alpha(\mathbf{x}) = \alpha_2 + H(\mathbf{x} - \mathbf{x}_f)(\alpha_1 - \alpha_2),$$  \hspace{1cm} (8)

where indices 1 and 2 denote values in fluid 1, respectively 2, and $H$ is the Heaviside function.

Two different numerical approaches are commonly used to deal with the jump in material properties. In the first, geared towards finite volume schemes, the discrete control volume value $\alpha_{cv}$ of any quantity $\alpha(\mathbf{x})$ is defined as the control volume average,

$$\alpha_{cv} = \frac{1}{V_{cv}} \int_{V_{cv}} \alpha(\mathbf{x}) d\mathbf{x} = \alpha_2 + \psi(\alpha_1 - \alpha_2),$$  \hspace{1cm} (9)

where the last part follows from Eqs. (8) and (4). This approach is thus ideally suited for Volume of Fluid methods and the conservative level set method, since the volume fraction $\psi$ is readily available. Note, that Eq. (9) does treat the phase interface as a discontinuity in the finite volume sense.

For finite difference methods, Eq. (8) directly holds at the node location $\mathbf{x}_i$, however, some amount of artificial smearing is typically introduced, resulting in

$$\alpha_i = \alpha_2 + \psi(\alpha_1 - \alpha_2)$$  \hspace{1cm} (10)

for VoF methods and

$$\alpha_i = \alpha_2 + H_{\epsilon}(\phi - \phi_0)(\alpha_1 - \alpha_2)$$  \hspace{1cm} (11)

for level set methods, where $H_{\epsilon}$ is a smeared out version of the Heaviside function.

An alternative approach that avoids smearing of the phase interface discontinuity
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is the ghost fluid approach (41,45) applicable to finite difference methods. Here, although formally still in a single fluid formulation, the two phases are effectively solved separately and coupled by imposing the appropriate jump conditions at the phase interface. The method relies on knowing these jump conditions and being able to evaluate $x_f$ in Eq. (8) within each computational cell with good accuracy. It is thus ideally suited for level set methods.

2.4 Surface tension forces

Even though Weber numbers of technically relevant turbulent primary atomization processes calculated using integral scales are typically very large, seemingly indicating that surface tension forces are unimportant, primary atomization can occur on scales significantly smaller than the integral scale, resulting in relatively small local Weber numbers. In fact, there is experimental evidence (58) that the actual primary breakup process is governed by capillary forces determining the resulting drop size distribution. Hence the accurate treatment of surface tension forces is crucial for DNS. On scales relevant to DNS, surface tension forces $T_\sigma$ are singular forces active only at the location of the phase interface,

$$T_\sigma = \sigma \kappa n_f \delta(x - x_f) = -\nabla \cdot \left((1 - n \otimes n)\sigma \delta(x - x_f)\right), \quad (12)$$

where $\kappa$ is the mean curvature of the phase interface, $n_f$ is its normal vector, and $\delta$ is the delta function concentrated on the phase interface. The first part of Eq. (12) forms the basis of the so called Continuum Surface Force (CSF) method (14), whereas the last part is the basis for the Continuum Surface Stress (CSS) method (55, 84). Depending on the chosen interface capturing method, two different approaches are common to discretize the delta function in Eq. (12).
For VoF methods, interpreting $\psi$ as a color function (14),

$$n_f \delta(x - x_f) \approx \nabla \psi,$$  \hspace{1cm} (13)

whereas for level set methods, a regularized, spread out version of the delta function is commonly used (24, 70). Both effectively spread the surface tension force into a small neighborhood normal to the phase interface. The alternative approach is to use the ghost fluid method (41, 45). Here, the surface tension force is acting through the pressure jump condition at the phase interface,

$$[[p]] = \sigma \kappa + 2[[\mu]]n^T \cdot \nabla u \cdot n,$$  \hspace{1cm} (14)

and thus does not require a discretization of the delta function. As is obvious from Eq. (14), surface tension forces result in a change of pressure across the phase interface. In the CSF and CSS method it is therefore crucial, that on a discrete level, the pressure gradient across the phase interface, Eq. (1) and the surface tension force balance exactly. While this is guaranteed in VoF schemes on staggered grids, this is not the case in collocated formulations or level set formulations using spread out delta functions, resulting in significant so-called spurious currents. These erroneous velocities limit the range of capillary/Laplace numbers that can be simulated in an accurate and stable manner (84). For collocated schemes, Francois et al. (29) recently proposed a so-called balanced force algorithm for VoF methods on Cartesian grids that ensures the required discrete balance, while Herrmann (39) presented a corresponding scheme for level set methods on structured and unstructured grids.

Using either the ghost fluid method or the CSF/CSS method in the discrete balance form is however not sufficient. The phase interface curvature has to be calculated with good accuracy as well. This is especially problematic for VoF
method, since $\psi$ is discontinuous at the phase interface, thus requiring convolution operations (103), a height function approach (37,91), or higher order interface reconstruction methods like PROST (77). For level set methods, discretization of the curvature at node locations $\kappa = \nabla \cdot (\nabla \phi / |\nabla \phi|)$ (66) is at best first order accurate requiring surface based evaluation of curvature (39) for higher accuracy.

2.5 Topology changes

As discussed in Sec. 2.1, resolution of the actual instance of topology change cannot be resolved in a DNS of turbulent primary atomization. Pinching models are thus required. The choice of model used, depends on the interface tracking/capturing method. In interface capturing methods, topology change is initiated automatically, once two interface segments enter into the same computational grid cell. These methods thus contain an inherent breakup length scale of the order of the local grid size, making the topology change process grid dependent, a clearly undesired feature. However, it can be argued that while in most primary atomization situations the exact moment of topology change might not be predicted accurately, nevertheless the error in volume of the broken off liquid structure is only of the order of the volume of the local grid cell, thus not significantly affecting drop sizes larger than several local grid cell volumes. Still, due to the inherent grid dependency, it is incumbent on an interface capturing DNS to demonstrate grid independence. It should be noted that interface tracking methods based on marker particles never result in topology changes unless they are "manually" introduced. While this intervention is a cumbersome and at times costly procedure (93), these methods nonetheless offer the potential to introduce a physics based breakup length scale, independent of the local grid size. Some
similar efforts have been presented in (38) for the RLSG method.

2.6 Current state of the art

Direct numerical simulation of the turbulent primary atomization process is still in its infancy due to the associated high computational cost and numerical challenges. Nonetheless a number of studies have shown the potential for analyzing the atomization process using numerical methods. Most studies are not DNS in the sense outline above. They employ a single phase LES formulation in the single phase regions of the flow and extend that formalism to regions containing the phase interface. They thus neglect all LES subgrid terms that arise from the presence of the phase interface and the associated jump in material properties and surface tension forces. As such, they can be called LES in name only and should rather be viewed as quasi-DNS, or under-resolved DNS of the phase interface combined with LES of the single phase regions of the flow (9, 10). Nonetheless, quasi-DNS/LES simulations can yield valuable insight into the primary atomization process and the resulting drop size distribution, if it can be shown that the small scale non-resolved phase interface dynamics will not influence the larger scale, resolved phase interface dynamics. A measure for this pre-requisite is the grid-convergence of the resolved scale drop size distribution: refining the grid should not alter the resulting resolved scale drop size distribution.

Using the quasi-DNS/LES approach, de Villiers et al. (100) performed relatively coarse simulations of the Diesel jet breakup under typical operating conditions. They performed a one level grid convergence study and found that although their resulting drop size distributions are of $\chi^2$ type, for different grid sizes, these distributions are significantly different, even for larger drop sizes. This indicates
that for their employed grid resolution, the quasi-DNS/LES assumption is questionable.

Bianchi et al. (9, 10) reported on similar Diesel jet atomization simulations using a slightly higher grid resolution. They studied the influence of the turbulence in the injector pipe and found that this has a strong impact on both intact core length and atomized mass, but only a weak impact on the resulting drop size distribution. However, grid dependency results were not reported leaving the question of applicability of the quasi-DNS/LES approach unanswered.

While the former two studies use VoF interface capturing and are in the atomization regime, Menard et al. (60) employ the CLSVOF method in conjunction with a ghost fluid method to study the Diesel jet atomization in the second wind induced regime. Instead of simulating part of the injection system, they prescribe turbulent fluctuations at the nozzle exit with a procedure due to Klein et al. (47). They do not apply any LES subgrid models in the single phase regions and thus aim to perform a DNS. However, their grid resolution is too coarse for a true DNS with $\Delta x/\eta \approx 3$ and more importantly $\zeta$ limited to drops with Weber numbers larger than 10 resolved by a single grid point. Still, their grid sizes are a factor 2 finer than that of Bianchi et al. (10). Unfortunately no grid convergence results or resulting drop size distributions are reported.

Finally, Desjardins et al. (20) report promising results for Diesel jet atomization using a conservative level set approach in conjunction with a ghost fluid method. Figure 1 shows two snapshots of the phase interface at different times during the injection. In the upper frame, most of the droplets have been generated by shedding of the mushroom shape at the tip of the jet. However, in the lower frame, generation and break-up of ligaments occur in many different places
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throughout the whole length of the jet. A zoom on the middle part of the jet is presented in Fig. 2. The surface topology appears extremely complex, composed of stretched out ligaments and droplets. A clear liquid core can be seen behind these structures. Many different droplet sizes and shapes are obtained, ranging from the smallest possible resolvable droplets to large liquid blobs more than ten computational cells wide. However, as with most other DNS simulations, no quantitative comparison to experimental data and no grid convergence study was performed.

For co-axial atomizing configurations, Kim et al. (46) used a RLSG method in conjunction with a balanced force algorithm to perform near DNS simulations of a low density ratio liquid jet. They report qualitative agreement with the postulated subsequent physical processes involved in atomization, determined experimentally by Marmottant and Villermaux (58), see Fig. 3, i.e. initial Rayleigh limit Kelvin-Helmholtz instability, followed by a Rayleigh-Taylor instability resulting in ligament formation that are subsequently stretched by the surrounding fast moving gas stream resulting in pinch off followed by a capillary breakup of the detached ligament into drops of varying sizes. In order to limit the computational cost, broken-off small near spherical drops are removed from the interface capturing representation and added as drops into a Lagrangian spray model preserving their volume, center of mass, and momentum. They performed a limited grid convergence study observing indications for grid converged drop size distributions for drops that are resolved by at least two grid points (46).

In addition to the discussed studies, a number of two-dimensional studies of primary atomization have been performed (13,68,108,109). It must be stressed, however, that these cannot be considered DNS of turbulent primary atomization,
due to the inherent three dimensional nature of the break up process. They do, however, represent a class of models for the atomization process, with their inherent, albeit questionable, modeling assumption that initial breakup occurs in the form of torus detachment from the liquid core. However, none of the quasi-DNS simulations discussed above, seem to support this hypothesis.

Finally, the numerical studies of Klein (48) and Pan and Suga (67) should be mentioned. The former performs three dimensional DNS of turbulent film phase interfaces (48), whereas the latter simulates laminar liquid jets in the second wind induced regime (67). Neither study, however, involves breakup and thus avoids a number of critical issues associated with atomization.

3 Phenomenological Approach in Primary Atomization Modeling

3.1 Stochastic primary atomization under scaling symmetry

This approach, referred to as the stochastic approach, was initially applied to the simulation of secondary atomization (1, 30, 31, 78, 80, 101) and has been further developed for primary air-blast atomization in (32, 33). It combines LES in the turbulent gas flow with stochastic simulation of the liquid jet depletion: the 3D structure of the liquid core with surrounding drops that are pinched off from the core, are simulated stochastically. The frequency of break-up is assumed to be high enough in order to consider the liquid jet depletion as a fragmentation cascade with scaling symmetry. The $\lambda_{RT}$-to-$\lambda_{KH}$ ratio, and the kinetic energy transfer from the gas to the liquid are parameters of the stochastic process.

**Statistical universalities.** Kolmogorov (49) considered the break-up of solid carbon particles as a random discrete process. He assumed the probability of
breaking each parent particle into a given number of parts is independent of the size of the parent particle. In the context of the central limit theorem he predicted that, after a large number of break-up events, such a discrete process should yield a log-normal distribution of particle sizes. Using a scaling formulation, Kolmogorov’s scenario states that each break-up event reduces the typical size of a fragment, \( r \Rightarrow \alpha r \ (r_{M+1} = r_M e^{\ln \alpha}) \), by an independent random multiplier \( \alpha \), which is governed by the fragmentation spectrum \( q(\alpha) \), \( \int_0^1 q(\alpha) d\alpha = 1 \).

An alternative to Kolmogorov’s discrete stochastic process is provided by the mathematical models described in (17, 18, 28, 59, 73, 111, 112), which are based on the analytical solution of the fragmentation equation, without appealing to the central limit theorem. In these models, the particle-size distribution evolves continuously with increasing time, instead of the growing number of breakage events in discrete models.

In the case of constant fragmentation frequency \( \nu \), the kinetic fragmentation equation for the normalized distribution function \( f(r, t) \) has the following form:

\[
\frac{1}{\nu} \frac{\partial f(r)}{\partial t} = \int_0^1 \frac{1}{\alpha} f \left( \frac{r}{\alpha} \right) q(\alpha) d\alpha - f(r) \tag{15}
\]

The steady-state solution of this equation, \( f(r) = \int_0^1 \frac{1}{\alpha} f \left( \frac{r}{\alpha} \right) q(\alpha) d\alpha \), is the delta function

\[
f(r) = \delta(r) \tag{16}
\]

and the following question can be asked: How does the distribution \( f(r, t) \) evolve towards the ultimate steady-state solution (16)? Since the solution of the fragmentation equation (15) requires knowledge of \( q(\alpha) \), which is, in principal, unknown, this question cannot be completely answered. However, due to scaling symmetry, the evolution of \( f(r, t) \) goes through at least two intermediate asymp-
totic distributions. Evaluating these distributions does not require the knowledge of the entire spectrum \( q(\alpha) \) - only its first two logarithmic moments, and, at large times, only the ratio of these moments determine the behavior of the solution of Eq.(15).

These two universal forms are given in (31) as follows. The asymptotic solution of Eq.(15) can be derived as:

\[
rf(r, t) = \frac{1}{\sqrt{2\pi \langle \ln^2 \alpha \rangle \nu t}} \exp \left( -\frac{\langle \ln \alpha \rangle^2}{2 \langle \ln^2 \alpha \rangle \nu t} \right) \times \\
\times \exp \left( -\frac{(\ln \frac{r}{R})^2}{2 \langle \ln^2 \alpha \rangle \nu t} \right) \left( \frac{r}{R} \right)^{\frac{\langle \ln \alpha \rangle}{\langle \ln^2 \alpha \rangle}}
\]

where \( R = \exp^{(\ln r) \alpha} \) denotes the initial length scale and \( \langle \ln \alpha \rangle = \int_0^1 \ln \alpha q(\alpha) \, d\alpha \). This expression confirms the main result of Kolmogorov 1941 concerning the log-normal asymptotic shape of the size distribution resulting from fragmentation under scaling symmetry. Increasing time still further, it is seen that the "log-normal" multiplier in Eq.(17) tends to unity and hence the long-time particle-size distribution is determined by a power law with just one universal parameter \( \langle \ln^2 \alpha \rangle / \langle \ln \alpha \rangle \):

\[
rf(r, t \to \infty) \propto \left( \frac{r}{R} \right)^{\frac{\langle \ln \alpha \rangle}{\langle \ln^2 \alpha \rangle}}
\]

The power law (18) implies that size of particle has a fractal distribution. The fractal geometry of an atomizing liquid jet has been observed photographically in many experiments (see, for example, (16, 57, 86, 110)). The identification of \( \langle \ln^2 \alpha \rangle / \langle \ln \alpha \rangle \) may be seen from the solutions for the logarithmic moments of the continuous model (1) (34):

\[
\langle \ln r \rangle \approx \nu t \langle \ln \alpha \rangle; \quad \langle (\ln r - \langle \ln r \rangle)^2 \rangle \approx \nu t \langle \ln^2 \alpha \rangle,
\]

where the mean quantity is denoted by angled brackets. Hence the ratio \( \langle (\ln r - \langle \ln r \rangle)^2 \rangle / \langle \ln \alpha \rangle \) has the time-independent constant value \( \langle \ln^2 \alpha \rangle / \langle \ln \alpha \rangle \), regardless of dispersion.
\( \langle (\ln r - \langle \ln r \rangle)^2 \rangle \):

\[
\frac{\langle (\ln r - \langle \ln r \rangle)^2 \rangle}{\langle \ln r \rangle} = \frac{\langle \ln^2 \alpha \rangle}{\langle \ln \alpha \rangle}
\]  
(19)

The statistical universality of fragmentation also implies that at large times (high fragmentation frequency \( \nu \)), the fragmentation equation reduces to the Fokker-Planck equation. Indeed, the kernel in the fragmentation equation (15) may be expanded as

\[
\frac{1}{\alpha} f \left( \frac{r}{\alpha} \right) = \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} \left( \frac{\partial}{\partial r} r \right)^n f(r) \ln^n \alpha \quad \text{(Saveliev et. al. (82,83))},
\]

leading to an infinite number of terms containing the moments \( \langle \ln^k \alpha \rangle \) in the fragmentation equation. However, the asymptotic distribution (17), depends solely on the first two logarithmic moments, \( \langle \ln \alpha \rangle \) and \( \langle \ln^2 \alpha \rangle \). This means that, although each term with \( \langle \ln^k \alpha \rangle, k > 2 \), may be significant, setting them to zero will not change the long time asymptotics of the solution. The consequence is that at high fragmentation frequency \( \nu \), Eq.(15) takes exactly the following form:

\[
\frac{1}{\nu} \frac{\partial f(r)}{\partial t} = - \langle \ln \alpha \rangle \frac{\partial r f(r)}{\partial r} + \frac{1}{2} \langle \ln^2 \alpha \rangle \frac{\partial}{\partial r} r \frac{\partial r f(r)}{\partial r}
\]  
(20)

The Fokker-Planck equation Eq.(20) describes the log-Brownian stochastic process. The corresponding stochastic equation is

\[
\dot{r} = \nu \langle \ln \alpha \rangle r + \sqrt{\nu \langle \ln^2 \alpha \rangle / 2r \Gamma(t)}
\]  
(21)

where \( \Gamma(t) \) is the Langevin process: \( \langle \Gamma(t) \rangle = 0; \langle \Gamma(t) \Gamma(t') \rangle = 2 \delta(t - t') \).

**Stochastic model of liquid jet depletion.** In the technique (32, 33, 49), the random interface of the liquid core is simulated using the spatial trajectories of constituent stochastic particles. The one-point distribution, \( f(x, t; r) \), defined such that \( f(x, t; r)dr \) is the probability that the radial location of the liquid core interface, \( r \), at axial position \( x \) and time \( t \) lies in the element \( dr \) about \( r \), is given by

\[
f(x, t; r) = \langle \delta(r(x, t) - r_{SP}) \rangle,
\]

where \( r_{SP} \) is the position of a stochastic particle.
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and $\delta(r(x, t) - r_{SP})$ denotes the Dirac function. The main steps in the modeling are:

(i) stochastic particles are injected one after another, thus yielding the random geometry of the liquid core; each particle trajectory ends after a length of time determined by kinetic energy transfer from the gas flow to the liquid.

(ii) the radial motion of a stochastic particle is governed by Eq.(21), where the fragmentation parameter (19) is determined from $\langle \ln^2 \alpha \rangle / \langle \ln \alpha \rangle = \ln \left( \frac{\lambda_{RT}}{\lambda_{KH}} \right)$. The axial particle velocity is taken equal to the convection velocity of liquid surface waves (21), $u_l = \frac{\sqrt{p_g} u_g + \sqrt{p_l} u_l}{\sqrt{p_g} + \sqrt{p_l}}$. The path of each stochastic particle lies in a plane with random azimuth.

(iii) the statistics of the core surface are used to obtain the size and position characteristics of the drops surrounding the core, sampled with the total mass rate equal to inflowing liquid mass rate.

(iv) LES is used to simulate the gas flow and is conditioned by the presence of the liquid core. The blobs formed around the core are dragged along by such a conditioned flow of gas and subject to secondary atomization and coalescence, both modeled by an inter-droplet collision mechanism (101).

Figure 4 shows comparisons with measurements of Werquin (102) for two liquid injection velocities of the near injector distribution of liquid fraction in a round liquid jet atomized by parallel co-flow of air. It is seen that the simulation reproduces qualitatively the experimental observation. Figures 5 shows simulation results for an atomizing liquid jet injected at different velocities into high-speed (140 m/s) co-flowing gas. Here, the inlet conditions correspond to those of the experimental study by Lasheras et al. (53). Evidently, this approach cannot reproduce the real filamentary structure of an atomizing spray. However, the
results of such statistical simulation agree with physical intuition: increasing the parameter \( M = \frac{\rho_g u_g^2}{\rho_l u_l^2} \) (99) causes the liquid core to shorten and the diameter of drops around the core to decrease. What is more, the predicted far-field of the spray has length scales in reasonable agreement with measurements.

### 3.2 Eulerian RANS approach and transport of the mean inter-facel density

This approach was proposed by Vallet, Burluka and Borghi in (95,96) and applied in simulation of primary atomization of a Diesel spray (7,8,12) and air-blast atomizers (52, 61). The approach is based on homogeneous formulation of two-phase medium: in each unit volume, two random motions may exist simultaneously; the liquid and the gas move through each other independently. Each motion is connected with its own "effective" mass: motion of the liquid is connected with \( \rho_l^* = \alpha \rho_l \), where \( \alpha \) is the instantaneous liquid volume fraction and \( \rho_l \) is the constant density of the liquide, whereas motion of the gas is connected with \( \rho_g^* = (1 - \alpha) \rho_g \), where \( \rho_g \) is the constant gas density. The total true density of the gas-liquid mixture is the sum \( \rho = \alpha \rho_l + (1 - \alpha) \rho_g \). Introducing the local liquid mass fraction \( Y_l \), one writes

\[
\frac{1}{\rho} = \frac{Y_l}{\rho_l} + \frac{1 - Y_l}{\rho_g} \tag{22}
\]

For such a gas-liquid mixture, the bimodal mass-weighted pdf (11) of \( Y_l \)-distribution may be defined: \( \tilde{P}(Y_l) = \gamma \delta(Y_l - 1) + (1 - \gamma) \delta(Y_l) \), where \( \gamma = \bar{Y}_l \) is the Favre-averaged liquid mass fraction. With this pdf and Eq.(22), the time-averaged mass fraction, \( \overline{Y}_l \), is equal to the time-averaged liquid volume fraction: \( \overline{Y}_l = \overline{\alpha} \), and, also, \( \overline{pY}_l = \rho_l \overline{\alpha} \), \( \overline{p} = \frac{\rho_g}{1 - \overline{Y}_l(1 - \rho_g/\rho_l)} \). The sum of two motions is governed by the mixture conservation law of the density \( \overline{p} \) and of the mass flow density
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\[ \rho u_i = \rho \bar{u}_i \] (\( \bar{u}_i \) is the local mass-averaged velocity). In mass weighting of the last one, the contribution of liquid is significant; thereby the introduced here "two-phase turbulent kinetic energy" \( \rho \bar{k} = \frac{1}{2} \rho (u_i - \bar{u}_i)(u_i - \bar{u}_i) \) contains the velocity slip between liquid and gaseous phases.

This approach considers the primary atomization in the framework of turbulent RANS (11) mixing of a jet with high density (assigned to the liquid) spreading in the gaseous environment. Similar to classical assumption in turbulence, it is assumed that the turbulent Reynolds number, along with the turbulent Weber number, are high; thereby the turbulent dispersion of the jet is independent of those numbers. At small scales, following Kolmogorov (50), the formation of droplets of maximum stable size is linked to the surface tension \( \sigma \), the gas viscosity \( \mu_g \) and also, to the turbulent stretching.

**Large-scale mixing.** The turbulent dispersion of liquid jet is computed from standard transport equation for \( \rho \bar{Y}_l \). However the diffusion term in this equation, containing the turbulent flux \( \rho u_i'' \bar{Y}_l'' \), is coupled with the local slip velocity \( \rho u_i'' \bar{Y}_l'' = \rho \bar{Y}_l(\bar{u}_i, i - \bar{u}_i) \) (\( \bar{u}_i, i \) is the time-mean velocity of the liquid fluid particle). Hence its gradient closure is not completely appropriated. Additionally to this, due to high density variation, the pressure-gradient drift fluxes \( u_j'' \frac{\partial \rho}{\partial x_i} \) and \( Y_l'' \frac{\partial \rho}{\partial x_i} \) contribute significantly to the turbulent transport \( \rho u_i'' \bar{Y}_l'' \), \( \rho u_i'' u_j'' \) and \( \rho \bar{k} \). This motivated authors to use the technique of algebraic stress modelling (79).

With the bimodal shape of PDF, the pressure driven fluxes may be obtained in the following form:

\[ Y_l'' = \rho \bar{Y}_l \left( 1 - \bar{Y}_l \right) \left( \frac{1}{\rho_l} - \frac{1}{\rho_g} \right) ; \quad u_j'' = \rho u_i'' \bar{Y}_l'' \left( \frac{1}{\rho_l} - \frac{1}{\rho_g} \right) \] (23)

(last expression in Eqs.(23) is probably based on expansion \( u_i (Y_l) \approx a + b (Y_l - \bar{Y}_l) \).)

**Transport equation of the mean interface density.** The new Eulerian
variable $\Sigma$, a mean amount of interfacial surface per unit volume, is introduced in this approach. The knowledge of local $\Sigma$ allows to estimate the mean radius of round droplets $r = 3\rho\tilde{Y}_l/\rho_l\Sigma$, which are available for advection in a Lagrangian way.

Similar to the Marble and Broadwell’s flame surface density in turbulent combustion (56), the transport equation of $\Sigma$ is presumed with terms of convection, diffusion, production (surface stretching) and destruction (coalescence):

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_j \Sigma}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D \frac{\partial \Sigma}{\partial x_j} \right) + \frac{1}{\tau_{\text{prod}}} \Sigma - \frac{1}{\tau_{\text{destr}}} \Sigma^2$$

In this equation, the production of interface density is addressed to the turbulent stretching; expressions of turbulent time scales are used. In equilibrium, when turbulent stretching is balanced by capillary forces, i.e. the critical Weber number is of order of unity, it follows from Eq.(24) that $\frac{1}{\tau_{\text{destr}}} = \frac{1}{\tau_{\text{prod}}r_{eq}}$, which may be expressed in terms of maximum stable radius $r_{eq}$: $\frac{1}{\tau_{\text{destr}}} = \frac{\rho_l r_{eq}}{3\tau_{\text{prod}}\tilde{Y}_l}$. Different expressions of $r_{eq}$ are available from (30) and (96). In RANS computation of the rocket combustion (52), Jay, Lacas and Candel modify Eq.(24) taking into account for the Kelvin-Helmholtz instability effect.

The Eulerian mixing model of primary atomization naturally lends itself to the RANS codes which are in widespread use. In the case of a Diesel spray atomization, Figure 6 (8) shows that this model matches well the DNS presented in (60). At the same time, the model is affected by the drawbacks of the RANS approach: the presumed form of Eq.(24) is supposed to be universal, independently of the specific geometry of the flow and its boundary conditions; the transport of $\Sigma$, which is modelled in (24) by diffusion-like hypothesis, and thereby, neglects the spatial grouping of liquid elements, is of concern.
4 The future

The advent of ever more powerful computers will enable the simulation of the primary atomization process with ever higher resolution, enabling simulations in the near future employing at least adequate resolution. This puts simulating the atomization process as a whole into reach, if the primary atomization simulation is coupled to a secondary atomization model. Developments along these lines have been reported in (38, 46) transferring broken off, near spherical small liquid structures into a Lagrangian particle/parcel model that describes secondary atomization.

However, due to fractal nature of primary atomization in a high Weber and Reynolds number flow, the problem of full resolution of liquid scales will persist even with very powerful computers. Introducing similarities of break-up at small scales and discovering the renormalized formulation of Navier-Stokes equations, which will describe interacting gas-liquid flow "effectively", similar to LES equations of turbulent flow, is the future of modelling primary atomization. Another problem which motivates the future work stems from recent developments in a high-pressure propulsion systems, when primary atomization takes place in supercritical conditions. In these conditions, the surface tension and laminar viscosity are negligible and the concept of interfacial surface has no more sense. Describing primary atomization in such conditions is an open problem for researchers.

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Figure 1: Two successive snapshots of the turbulent atomization of a liquid Diesel jet (20).

Figure 2: Zoom into the chaotic structure of the interface of the atomizing liquid Diesel jet (20).
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Figure 3: Co-axial atomization mechanisms. Initial Rayleigh limit Kelvin-Helmholtz instability (top left), Rayleigh-Taylor instability (top right), ligament stretching (bottom left), and ligament detachment and drop generation (bottom right) (46). RLSG captured phase interface is shown in blue, and Lagrangian spray drops are depicted in yellow.
Figure 4: Modeling liquid core geometry and averaged liquid fraction field (32) compared to measurements from (102). Here the round liquid jet issued from the central tube ($D_l = 1.8$ mm) at $u_l = 0.68$ m/s (on the upper part) and $u_l = 1.36$ m/s (on the bottom part) is atomized by a parallel flow of air issued at $u_g = 60$ m/s from the annular duct ($D_g = 3.4$ mm).
Figure 5: LES of the gas flow (velocity of injection $u_g = 140 \text{ m/s}$) combined with stochastic simulation of the liquid jet depletion (33) in experimental conditions (53); on the left-hand side, $u_l = 0.13 \text{ m/s}$; on the right hand-side, $u_l = 0.55 \text{ m/s}$; coordinates are dimensioned in the inner nozzle orifice diameter. $D_l = 3.8 \text{ mm}$; the nozzle diameter of the annular air jet is $D_g = 5.6 \text{ mm}$. 
Figure 6: Application of Eulerian RANS model (8) (upper part) to the Diesel spray atomization ($u_{inj} = 100 \text{ m/s}$, $d_{inj} = 100 \text{ µm}$, $\rho_g = 25 \text{ km/m}^3$, $\rho_l = 670 \text{ km/m}^3$); on the bottom: comparison with mean distributions from quasi-DNS of (60); from the left to the right : the liquid mass fraction, the interface density, the turbulent flux $\bar{\rho}u_i'Y_l''$, the kinetic turbulent energy.