Spray formation: an inverse cascade

Yue Ling,¹ Daniel Fuster,¹ Gretar Tryggvason,² and Stéphane Zaleski¹

¹Institut Jean le Rond d'Alembert, Sorbonne Univ,

UPMC Univ Paris 06, CNRS, UMR 7190, F-75005, Paris, France ²Department of Aerospace & Mechanical Engineering,

University of Notre Dame, Notre Dame, IN 46556, United States

We present a study of droplet formation in a gas-liquid mixing layer using direct numerical simulation. It is seen that two mechanisms compete to generate the droplets: fingering at the tip of the waves and hole formation in the thin liquid sheet. The three dimensional liquid structures are much shorter than the longitudinal wavelength of the instability at the first instant of their formation. As time evolves, the structures evolves to larger and larger scales, in a way similar to the inverse cascade of length scales in droplet impact and impact crown formation.

The breakup of fluid masses is a phenomenon of enormous complexity, with diverse physical setups and mechanisms. When the fluid masses break into large numbers of small droplets one speaks of atomization [1, 2]. Atomization in the gas-liquid mixing layer, where a highspeed gas stream emerges from an orifice parallel to a lower-speed liquid stream, has been studied in great detail [3, 4]. The resulting Kelvin-Helmholtz instability generates large coherent structures that grow in size as they propagate downstream, together with equally growing wave-like structures [5] on the liquid-gas interface. The standard picture of atomization [1] is that twodimensional wave structures form near the orifice, then destabilize into three-dimensional finger or ligament-like structures which eventually break into droplets. This sequence and its variants are called primary atomization and is supposed to be followed by the breakup of large drops further downstream whenever they interact with sufficiently high-velocity gas flow. This second event is called secondary atomization. As a result of the breakup of ligaments by a Rayleigh–Plateau instability initialized in a random manner, Gamma distributions of droplet sizes have been predicted [3, 6]. Another mechanism for primary atomization is the formation of holes in the thinsheet-like structures that appear in the waves prior to the formation of ligaments and fingers. These holes-in-thinsheets structures are quite similar to the holes that form in bag-breakup secondary atomization [7, 8]. The hole formation has been seen more rarely by experimentalists and is thus less firmly documented.

In order to better understand the mechanisms underlying atomization processes, experimentalists have switched from the coaxial round jets typical of industrial applications to a quasi-planar setup that is more favorable for detailed analysis [9–11]. This setup has allowed precise measurements and detailed visualizations of the droplet-forming process. In the quasi-planar configuration, it is possible to compare the growth and frequency of the Kelvin-Helmholtz instability in the linear regime as predicted by numerical simulation, linear stability theory and experiments [12]. Three-dimensional analysis is, for obvious reasons [13–15], less advanced, despite a large number of results in the references already cited. In this work we simulate a model of the quasi-planar experiment of [9] in order to better understand the mechanisms of droplet formation.

The computational domain is a box of dimensions $L_x \times L_y \times L_z$, where we inject two streams, liquid and gas separated by a solid plate of size $\ell_x \times e_y \times L_z$ through the boundary at x = 0. The thickness of the liquid and gas streams are H and $H - e_y$, respectively. In order to minimize the effects of the finite size of the domain, the dimensions of the box are large in the x and y dimensions $L_x = 16H$ and $L_y = 8H$ (while L_z is set to 2H). Special care is taken to specify the exit conditions to minimize the recirculating flow and avoid excessive reinjection of coherent structures near the inlet. It is not possible with present technology and numerical methodology to perform simulations at this setup that: a) use the physical parameters, such as the large liquid-to-gas density ratio, exactly as in the experiments [9]; b) are fully resolved down the smallest physical scales, (the tiny submicron droplets generated are three orders of magnitudes smaller than H; c) continue for a long enough time to yield a statistical analysis of the observed structures. To alleviate these problems we choose a set of parameters that allow faster and easier simulations while still placing the flow in the high-speed atomization regime. The gas and the liquid are injected with velocities U_g and U_l . The thickness of the boundary layers on the liquid and gas sides of the separator plate are taken to be identical and denoted by δ . The values of the corresponding dimensionless parameters are given in Table I, using standard notations.

Μ	r	m	$\operatorname{Re}_{g,\delta}$	$We_{g,\delta}$	Re_g
$\overline{\rho_g U_g^2 / (\rho_l U_l^2)}$	$ ho_l/ ho_g$	μ_l/μ_g	$\rho_g U_g \delta / \mu_g$	$\rho_g U_g^2 \delta / \sigma$	$\rho_g U_g H/\mu_g$
20	20	20	1000	10	8000

Table I: Dimensionless parameters.

We solve the Navier-Stokes equations for incompressible flow with sharp interfaces and constant surface tension. The fields are discretized using a fixed regular cubic grid, and use a projection method for the time stepping to incorporate the incompressibility condition. The advection of the velocity fields is done using the QUICK scheme, and the viscous term is treated explicitly. The interface is tracked using a Volume-of-Fluid (VOF) method with a Mixed Youngs-Centered Scheme to determine the normal vector and a Lagrangian-Explicit scheme for the VOF advection [16]. Curvature is computed using the height-function method. Surface tension is computed from curvature by a well-balanced Continuous-Surface-Force method. Density and viscosity are computed from the VOF fraction C by an arithmetic mean. The whole method is implemented in the a free code *PARIS* [17] and described in [18].

The simulations are performed on three grids called M0, M1 and M2, so that Mn has $H/\Delta x = 32 \times 2^n$ points in the liquid layer. The domain is initially filled with gas and liquid progressively enters it. An approximate steady state is reached at about $U_g t/H = 200$ and the simulations are then continued until $U_g t/H = 400$. For the M2 mesh, the simulation was performed using 2048 processors and the total simulation time is about 5×10^5 CPU hours. The results presented correspond to the M2 mesh, unless stated otherwise.

A global view of the atomizing liquid jet is shown in Fig. 1. The gas-gas and the gas-liquid mixing layers can be identified from the z-vorticity plotted on the backplane. The characteristics of the wave formation on the gas-liquid interface correspond to the convective instability regime, where small perturbations present in the region upstream grow as they advect downstream. This is consistent with the theoretical predictions of [19] and the experimental and 2D simulation results of [12]. The interfacial wave grows and forms a thin liquid sheet which in turn breaks into ligaments and droplets. The unbroken part of the liquid sheet eventually reattaches to the domain bottom. Turbulence develops from the mixing layers and the downstream flow becomes fairly violent and chaotic.

Although the turbulent flow in the gas-liquid mixing layer leaves three-dimensional "foot prints" on the interface, the wave remains approximately two-dimensional, as it grows. The wave evolution can be seen in the 2D snapshots of the interface on the plane z = 0.6H in Fig. 2 (a). If the *x*-axis is scaled by the Dimotakis speed,

$$U_D = \frac{\sqrt{\rho_l}U_l + \sqrt{\rho_g}U_g}{\sqrt{\rho_l} + \sqrt{\rho_g}},\qquad(1)$$

with respect to the origin of the wave formation x_0 and t_0 , the waves at different time collapse, except the amplitude, see Fig. 2 (b). This approximate self-similar wave structure has also been observed in single-wave simulations [5].

As the wave appears as an obstacle to the gas, the gas flow separates at the top of the wave and a recirculation



Figure 1: The atomizing jet. The z-vorticity is shown on the backplane. The sampling boxes for droplet statistics are indicated by dotted lines.



Figure 2: The interface in the z = 0.6H plane, showing the formation of the quasi-singularity at the wave crest. The time interval between the lines is H/U_q . (a)

Original scale; (b) x-axis scaled by the Dimotakis speed U_D .

region is formed downstream, as indicated by the arrows in Fig. 2 (b). Under the influence of the downstream recirculation and the upstream gas flow, the curvature of the wave at the crest increases and eventually a quasisingularity (very small radius of curvature) is formed. The quasi-singularity is also observed in experiments as shown in the comparison with the numerical result in Fig. 3.

Various interface structures appear after the quasisingularity forms, as depicted in Fig. 4. At first, a thin sheet is formed at the wave crest. Tiny fingers are seen at the tip of the sheet, which then break into very small isolated cylinders and droplets. The thickness of the liquid sheet, the diameter of the fingers, and the size of



Figure 3: 3D view of the quasi-singularity at the wave crest. (a) Present simulation; (b) Experiment [10].



Figure 4: A sequence of snapshots for the process of wave breakup and droplet formation. The time interval between the snapshots (indicated by different colors) is $1.25H/U_q$.

the droplets are typically very small and their sizes seem to be dictated by the radius of curvature of the quasisingularity.

As time evolves, the length scales of these structures increase, instead of remaining constant. As shown in Fig. 4, the diameter, length and spacing of the fingers and the droplets increase as time advances. This increase in length scale is reminiscent of the inverse cascade of length scales in droplet impact and impact crown formation [20, 21]. The growth of the finger diameter can be ascribed to the Taylor-Culick rim growth mechanism observed in many complex two phase flow situations [22]. A thicker rim is destabilized at larger wavelengths by the Rayleigh–Plateau instability and thus the wavelength between fingers is expected to grow. As a consequence of that, the droplets generated further downstream are typically larger than those formed closer to the nozzle.

Beyond forming fingers at the tip, the hole formation within the sheet is another mechanism that contributes



Figure 5: Hole formation and the resulting breakup of the liquid sheet. A 3D view of the interface is shown on the left and the interface and the pressure in the mid-plane is plotted on the right.

to the eventual breakup of the liquid sheet. The evolution of the recirculating vortex behind the wave can be seen through the flow pressure in Fig. 5. The departure of the vortex stretches the liquid sheet formed at the wave crest in the downstream direction and its thickness continues to decrease [10]. At a certain stage, holes are formed in the liquid sheet, as indicated in Fig. 5. The expansion of the holes eventually causes the sheet to rupture, producing a large amount of ligaments, which later break into droplets. Hole formation in a real liquid sheet is generally due to the disjoining pressure and holes only form when the thickness of the sheet is down to only tens of nanometers. In the present simulation, the disjoining pressure is not included and the sheet breaks at a much larger thickness. The holes seen here are therefore a numerical artifact due to insufficient mesh resolution. Nevertheless, results of different mesh resolutions show that refining the mesh only delay the hole formation but has little effect on the scale of the ligaments generated (assuming that the mesh is fine enough to resolve these ligaments). The droplet size distributions, to be shown later, also support this conclusion.

The existence of different droplet formation mechanisms is also demonstrated in the analysis of the probability distribution function (PDF) of droplet sizes. To obtain the PDF for droplets formed by different mechanisms, we consider droplets in three different sampling boxes (see Fig. 1). The boxes all span the full width (z direction) of the domain. The first box $(4 \le x/H \le 5.5)$ and $0.5 \le y/H \le 2$) is used to collect droplets formed close to the quasi-singularity; while the second box $(8 \le x/H \le 9.5)$ and $2 \le y/H \le 3.5$) samples droplets generated after the fingers grow and the sheet breaks up due to hole formation. Finally, the third box $(12 \le x/H \le 12.5)$ and $0.5 \le y/H \le 5$) captures the PDF for all the droplets formed from the atomizing liquid jet. The sampling time interval for all cases is from $U_g t/H = 200$ to 400. The PDF results are shown in Fig. 6. For both the first and second box, exponential decay of the number of droplets with increasing diameter are observed:

$$PDF(d_p) \sim \exp(-d_p/\lambda),$$
 (2)

where λ is a characteristic length scale. This observation of exponential decay at larger droplets is consistent with previous experimental and numerical results [3, 4, 18], but here the λ for different boxes is different. Specifically, $\lambda_1 \approx 0.00875H$ is smaller than $\lambda_2 \approx 0.02H$. Correspondingly, more small droplets are formed in the region near the quasi-singularity ($\langle d_n \rangle / H = 0.01975$) while the size of droplets formed after the fingers grow and the sheet ruptures is typically larger ($\langle d_p \rangle / H = 0.0255$). Since the droplets collected by the third box include droplets generated by all formation events, the decay rate characteristic length scale λ is seen to increase in d_p from λ_1 to λ_2 gradually. The log-normal and gamma distribution functions are employed to fit the PDF data. The highly skewed log-normal distribution, denoted by log-normal-1 in Fig. 6(c), is shown to well capture the inverse cascade in spray formation.

Finally, we examine the effect of grid resolution on the the droplet size PDF. It is seen that the large decay rate characteristic length scale λ_2 is well captured by M1 and M2 and partially captured by M0. The size distributions of large droplets for different meshes are in good agreement, which seems to affirm that numerical breakup of thin liquid sheet due to insufficient grid resolution has little effect on the size of the droplets that are eventually formed. Nevertheless, to capture the small droplets formed near the quasi-singularity a fine mesh has to be used, since both M0 and M1 completely miss the small droplets generated by this mechanism. Even with the M2 mesh, the calculated λ_1 is close to the mesh size (0.0078H). Therefore, the radius of curvature at the quasi-singularity may not be well resolved. Furthermore, the approximate log-normal distribution profile also seems to suggest tiny droplets may be missed in the M2 simulation. To better resolve the formation of these very small droplets, a finer mesh is required and this is relegated to future works. Although the M2 mesh used here may not be fine enough to capture the tiny droplets, the results have achieved converged distribution for the larger droplets and seem to capture the major characteristics of the spray formation process.

This project has been supported by the ANR MODEMI project (ANR-11-MONU-0011) program, and the FIRST project supported by the European Commission under the 7th Framework Programme under Grant Agreement No. 265848. This work was granted access to the HPC resources of TGCC-CURIE and CINES-Occigen under the allocations 2015-x20152b7325 made by GENCI. We would also acknowledge PRACE (2014112610) for awarding us access to resource CINECA-FERMI and LRZ-SuperMUC based in Italy and Germany. The support of Alessandro Grottesi and Luigi Calori from CINECA, Italy to the technical work is gratefully acknowledged.



Figure 6: The droplet size PDF. Figures (a) (b) and (c) are obtained in different sampling boxes for the M2 mesh. The bin width for all the cases is 0.00125H.

- J. C. Lasheras and E. J. Hopfinger. Liquid jet instability and atomization in a coaxial gas stream. Annu. Rev. Fluid Mech., 32:275–308, 2000.
- [2] J. Eggers and E. Villermaux. Physics of liquid jets. Rep. Prog. Phys., 71:036601, 2008.
- [3] E. Villermaux, Ph. Marmottant, and J. Duplat. Ligament-mediated spray formation. *Phys. Rev. Lett.*, 92:074501, 2004.
- [4] P. Marmottant and E. Villermaux. On spray formation. J. Fluid Mech., 498:73–111, 2004.
- [5] J. Hoepffner, R. Blumenthal, and S. Zaleski. Selfsimilar wave produced by local perturbation of the kelvin-helmholtz shear-layer instability. *Phys. Rev. Lett.*, 106:104502, 2011.

- [7] M. Pilch and C. A. Erdman. Use of breakup time data and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop. Int. J. Multiphase Flow, 13:741–757, 1987.
- [8] M. Jain, R. S. Prakash, G. Tomar, and R. V. Ravikrishna. Secondary breakup of a drop at moderate weber numbers. *Proc. R. Soc. Lond. A Mat.*, 471:20140930, 2015.
- [9] J.-P. Matas, S. Marty, and A. Cartellier. Experimental and analytical study of the shear instability of a gasliquid mixing layer. *Phys. Fluids*, 23:094112, 2011.
- [10] J. J. S. Jerome, S. Marty, J.-P. Matas, S. Zaleski, and J. Hoepffner. Vortices catapult droplets in atomization. *Phys. Fluids*, 25:112109, 2013.
- [11] J.-P. Matas, S. Marty, M. S. Dem, and A. Cartellier. Influence of gas turbulence on the instability of an airwater mixing layer. *Phys. Rev. Lett.*, 115:074501, 2015.
- [12] D. Fuster, J. P. Matas, S. Marty, S. Popinet, Hoepffner J., A. Cartellier, and S. Zaleski. Instability regimes in the primary breakup instability regimes in the primary breakup instability regimes in the primary breakup region of planar coflowing sheets. J. Fluid Mech, 736:150– 176, 2013.
- [13] M. Gorokhovski and M. Herrmann. Modeling primary atomization. Annu. Rev. Fluid Mech., 40:343–366, 2008.
- [14] R. Lebas, T. Menard, P. A. Beau, A. Berlemont, and F.-X. Demoulin. Numerical simulation of primary break-up and atomization: Dns and modelling study. *Int. J. Mul-*

 $tiphase \ Flow, \ 35:247-260, \ 2009.$

- [15] J. Shinjo and A. Umemura. Simulation of liquid jet primary breakup: Dynamics of ligament and droplet formation. Int. J. Multiphase Flow, 36:513–532, 2010.
- [16] G. Tryggvason, R. Scardovelli, and S. Zaleski. Direct numerical simulations of gas-liquid multiphase flows. Cambridge University Press, 2011.
- [17] T. J. Arrufat, S. Dabiri, D. Fuster, Y. Ling, L. Malan, R. Scardovelli, G. Tryggvason, P. Yecko, and S. Zaleski. The PARIS-Simulator code. Available from http://www.lmm.jussieu.fr/zaleski/paris/index.html.
- [18] Y. Ling, S. Zaleski, and R. Scardovelli. Multiscale simulation of atomization with small droplets represented by a lagrangian point-particle model. *Int. J. Multiphase Flow*, 76:122–143, 2015.
- [19] T. Otto, M. Rossi, and T. Boeck. Viscous instability of a sheared liquid-gas interface: Dependence on fluid properties and basic velocity profile. *Phys. Fluids*, 25:032103, 2013.
- [20] A. L. Yarin. Drop impact dynamics: splashing, spreading, receding, bouncing.... Annu. Rev. Fluid Mech., 38:159–192, 2006.
- [21] L. V. Zhang, P. Brunet, J. Eggers, and R. D. Deegan. Wavelength selection in the crown splash. *Phys. Fluids*, 22:122105, 2010.
- [22] C. Josserand and S. Zaleski. Droplet splashing on a thin liquid film. Phys. Fluids, 15:1650–1657, 2003.