

A Computational Framework for Simulating and Analyzing Primary Atomization in Electrically Charged Diesel-type Jets

Brendan Christensen; Bret Van Poppel; Mark Owkes

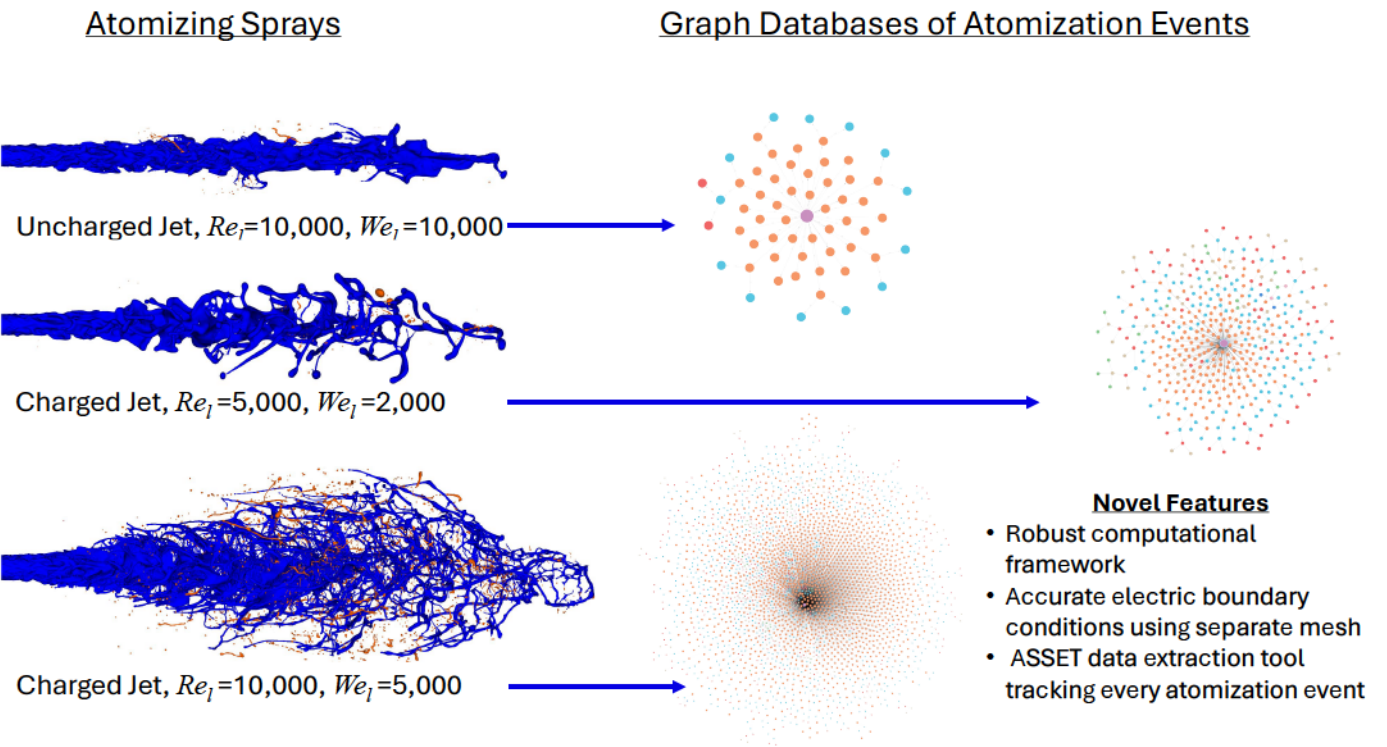
Accessibility Disclaimer:

For a more accessible version of this document, please submit an accessibility request form through the Montana State University Library website.

Graphical Abstract

A Computational Framework for Simulating and Analyzing Primary Atomization in Electrically Charged Diesel-type Jets

Brendan Christensen, Bret Van Poppel, Mark Owkes



A Computational Framework for Simulating and Analyzing Primary Atomization in Electrically Charged Diesel-type Jets

Brendan Christensen^a, Bret Van Poppel^b, Mark Owkes^a

^aMontana State University, Department of Mechanical and Industrial Engineering, Bozeman, MT, USA

^bUnited States Military Academy, Department of Civil and Mechanical Engineering, West Point, NY, USA

Abstract

A robust computational framework for simulating primary atomization in electrically charged liquid hydrocarbon jets is developed, tested and demonstrated in this work. First-principles-based numerical methods developed specifically for high-fidelity direct numerical simulations of electrohydrodynamic (EHD) flows are implemented within a conservative flow solver using an unsplit, geometric volume-of-fluid transport scheme that includes EHD effects. The numerical framework globally conserves mass, momentum, and the electric charge density even at the gas-liquid interface where discontinuities exist. A novel approach using a separate mesh is used to obtain accurate boundary conditions of electric potential on the computational domain. Simulations employ a recently developed physics extraction tool that tracks every breakup and coalescence event occurring during an atomizing spray. Data characterizing the atomization processes are stored in a Neo4j graphical database providing an easily accessible format to query and study the atomization process. The framework is demonstrated in five simulations focused on a region of interest relevant to primary atomization and varying fluid and EHD parameters, confirming the robustness of the methodology and its tools. Statistics for droplet size, breakup and coalescence events, onset of primary atomization, and spray cone angle are reported for all simulations revealing earlier and enhanced liquid breakup and greater spray dispersion with increasing electric charge. Some comparison with experimental work reveals the role of electric stress in de-stabilizing the jets and breakup consistent with the Plateau-Rayleigh mechanism.

Keywords: Electrohydrodynamics, Atomization, Direct numerical simulation, Data extraction, Volume of Fluid method

1. Introduction

Electrohydrodynamics is an interdisciplinary topic that describes the complex interaction between fluid mechanics and electric fields, explored since Lord Rayleigh revealed the competing forces and resulting dynamics of a liquid drop that is radially stressed by an applied electric field [1] and subsequently by many researchers. EHD may enable improved spray control and finer atomization so that fuel injection schemes can be inexpensively developed for the small combustion engine class. Moreover, EHD may provide efficient enhancements to hydrocarbon fuel atomization that could benefit a much broader range of engines and even other, non-combustion applications, such as pharmaceutical coating and micro- or nano-thin-film deposition [2].

The enhancement of atomization through the injection of electric charge into semi-insulating or dielectric liquids has drawn notable interest over the past several decades, progressing from pioneering work by Taylor [3, 4, 5, 6], Melcher [7, 8], Saville [9], Kim and Turnbull [10] and others. Kelly [11] extended the original demonstration of Kim and Turnbull. Lehr and Hiller [12] used experimental methods to confirm the observations of Kim and Turnbull, and Kelly, and predicted an

injected charge density limit due to the observed phenomenon of corona discharge. Shrimpton and co-workers have studied the technique of “charge injection” through experimental [13, 14, 15] and numerical [16, 17] investigations.

Notwithstanding these efforts, the complex interactions among electrostatic charge, electric fields, and the dynamics of atomizing liquids are not well understood. Considering the challenges and expense of experiments, high-fidelity numerical simulations should be able to provide some clarity to the underlying fundamentals and dynamics of EHD atomization. While numerical simulations of realistic liquid breakup are computationally expensive to resolve small structures and require large, parallel resources to perform these simulations, recent advances in scientific computing, numerical methods, and statistical tools render simulation a viable method of investigation. Leveraging these developments, several numerical studies have been conducted over the past few decades, including early work by Baygents and co-workers [18], Collins and co-workers [19], Tomar and co-workers [20], Feng [21, 22], Sherwood [23], and Shrimpton [24]. Hu [25], Paknemant [26], Hokmabad [27], Du [28], Xie and co-workers [29], Dong and co-workers [30], Holgate [31], and Frederich [32], among many others, have explored EHD systems for a range of electrical parameters, reporting two-dimensional results for mostly static droplets and structures under an externally applied electric field. Schnitzer, Yariv and co-workers employed an electrokinetics approach to ana-

Email addresses: brendan.christensen@montana.edu (Brendan Christensen), vanpoppelb@gmail.com (Bret Van Poppel), mark.owkes@montana.edu (Mark Owkes)

lyze EHD phenomena for conducting drops [33] and to address the Taylor-Melcher leaky dielectric model commonly used to describe the role of electric stress in poorly conducting liquids [34, 4, 8, 35]. López-Herrera and co-workers simulated Taylor cone-jets solving the electrokinetic equations [36], one of the most recent of many works exploring semi-conducting or ionic liquids. Few works published to date report fully three-dimensional, high-fidelity multiphase simulations of electrically charged Diesel-type jets—liquids with very low conductivity and few charge carriers—to elucidate primary atomization mechanisms and processes that are comparable to classic experiments, such as [15, 14, 24].

The distribution of electric charges within an atomizing flow is governed by two main fluid characteristics: the charge advection and charge mobility timescales [37, 38]. The ratio of these timescales, defined here as the electric Reynolds number (Re_e) [39], dictates how fast the electric charges are advected by the flow relative to how fast they relax to the fluid interface. Thus, the EHD fluid properties and flow characteristics control the resulting charge distribution within atomizing flows. Van Poppel [40] employed first-principles-based numerical methods in high-fidelity direct simulations of electrically charged liquid hydrocarbon jets undergoing electrostatic-enhanced primary atomization. Subsequently, Owkes and Sheehy [41] improved upon these methods to include charge mobility and conducted three-dimensional simulations of electrically charged liquid jets to assess the effects of Re_e on atomization efficiency.

The objectives of this work are (i) to establish a computational framework for simulating primary atomization in electrically charged Diesel-type jets; (ii) to provide statistics that quantify key breakup events and electrohydrodynamic properties of the spray from the recent development and integration of novel tools; (iii) and to identify the role of electric stress and breakup mechanisms in primary atomization. The framework detailed in this work extends EHD numerical schemes and integrates two novel, recently developed tools to perform fully three dimensional direct numerical simulations of liquid jets subject to a self-precipitating electric field due to the presence of bulk charge in the liquid. The computational approach employs a state-of-the-art numerical framework that globally conserves mass, momentum, and electric charge density even at the gas-liquid interface where discontinuities exist [42]. The Navier-Stokes solver’s numerical scheme sharply handles the discontinuous electric charge density, allowing robust and accurate simulations. A conservative unsplit geometric volume-of-fluid (VOF) employing semi-Lagrangian transport is used with a piece-wise linear interface reconstruction (PLIC), leveraging the combination of VOF and PLIC to efficiently capture breakup mechanisms and small satellite droplets [43] through its sharp and accurate representation of the phase interface.

Simulation results and analysis assess the effects of EHD on atomization quality, droplet size, and primary atomization events and processes. To better address the electric boundary conditions, known to be challenging for EHD flows, simulations employ a recently developed, novel approach using a separate mesh to obtain accurate boundary conditions of electric potential on the computational domain [44, 45]. Known

as *e-Mesh*, this mesh is much larger than the flow solver domain, implemented with well-defined boundary conditions for the electric potential, ϕ , and used to compute electric boundary conditions accurately and efficiently for the flow-solver domain. Another improvement is the implementation of a novel physics extraction tool that tracks every breakup and coalescence event occurring during an atomizing spray. Data characterizing the atomization processes are stored in a Neo4j graphical database providing an easily accessible format [46, 47] for analyzing primary and secondary atomization processes, although this work reports only the results of primary atomization events.

This paper is organized with §2 describing the governing equations and interface boundary conditions with relevant simplifications followed by §3 which summarizes the numerical approach employed in the flow solver and the *e-Mesh* tool. Data extraction employing the ASSET tools is summarized in §4 with some details provided for clarity and completeness. The simulation domain and parameters are provided in §5. Simulations are compared and primary atomization statistics and mechanisms are reported and discussed in §6.

2. Mathematical Formulation

This work solves the full set of governing equations to predict the dynamics of the flow (velocity and pressure), gas-liquid interface topology, and electric charge distribution within the liquid phase. The dynamics of the charge distribution are controlled by diffusion and the electric field created by the presence of space charge in the liquid domain. While assuming a constant charge density (insulating fluid) or surface charge (conducting fluid) has been done, notably reported in [19] among many others, predicting the non-trivial charge dynamics is important for accurate simulations. The formulation presented here couples the electrostatic and hydrodynamic phenomena for a poorly conducting liquid through the Maxwell stress tensor and implements gas-liquid interface boundary conditions.

2.1. Governing Equations

Conservation of mass and momentum for a variable density, low Mach number flow are given as

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}_i) = 0, \quad (1)$$

and

$$\frac{\partial \rho_i \mathbf{u}_i}{\partial t} + \nabla \cdot (\rho \mathbf{u}_i \otimes \mathbf{u}_i) = -\nabla p_i + \nabla \cdot (\boldsymbol{\sigma}_i^f + \boldsymbol{\sigma}_i^e) + \rho_i \mathbf{g},$$

where $\mathbf{u}_i$ is the velocity field, p_i is the hydrodynamic pressure, ρ is the mass density, $\mathbf{g}$ is gravitational acceleration. The subscript i represents the phase and can take the value g for the gas phase or l for the liquid phase. The viscous stress tensor, $\boldsymbol{\sigma}_i^f$, is given by

$$\boldsymbol{\sigma}_i^f = \mu_i \left(\nabla \mathbf{u}_i + \nabla \mathbf{u}_i^T \right) - \frac{2}{3} \mu_i \nabla \cdot \mathbf{u}_i \mathbb{I}, \quad (2)$$

with $\mathbb{I}$ the identity tensor and μ_i is the dynamic viscosity.

The Maxwell stress tensor, σ_i^e is used to define the electric body force, $f_i^e = \nabla \cdot \sigma_i^e$, and leads to,

$$f_i^e = q_i E_i - \frac{1}{2} E_i^2 \nabla \varepsilon_i + \nabla \cdot \left(\frac{1}{2} \rho_i \frac{\partial \varepsilon_i}{\partial \rho_i} E_i^2 \right), \quad (3)$$

where ε_i is the electric permittivity, q_i is a volumetric electric charge density, and E_i is the electric field vector. The three terms of f_i^e represent the Coulomb (or Lorentz) force, the dielectric force, and the electrostrictive force, respectively. Assuming incompressibility and material homogeneity within a phase,

f_i^e reduces to the Coulomb force in the bulk [48, 37] as

$$f_i^e = q_i E_i. \quad (4)$$

The electric displacement vector, D , is assumed to vary linearly with the electric field vector, as

$$D_i = \varepsilon_i E_i. \quad (5)$$

The electric field vector is irrotational, hence it can be expressed as the gradient of the scalar electric potential, ϕ_i , as

$$E_i = -\nabla \phi_i. \quad (6)$$

The Gauss law can be employed for a dielectric material to relate the electric displacement vector to the volumetric charge, as

$$\nabla \cdot D_i = \nabla \cdot \varepsilon_i E_i \quad (7)$$

which can be simplified to the Electric Potential Poisson Equation, as

$$\nabla \cdot (\varepsilon_i \nabla \phi_i) = -q_i. \quad (8)$$

Charge conservation and current density are described by

$$\frac{\partial q_i}{\partial t} + \nabla \cdot J_i = 0, \quad (9)$$

$$J_i = K_i q_i E_i - \mathcal{D}_i \nabla q_i + q_i u_i, \quad (10)$$

where J_i is the current density, $\mathcal{D}_i$ is the molecular diffusion coefficient and K_i is the ionic mobility coefficient.

2.2. Interface Boundary Conditions

The interface boundary and jump conditions are essential to capturing the dominant mechanisms influencing the flow and atomization. While the velocity and tangential electric field components are continuous across the interface, the mass density, viscosity, and electric displacement vector experience jumps, described by

$$[u \cdot n]_\Gamma = 0, \quad (11)$$

$$[u \cdot t_j]_\Gamma = 0, \quad \text{for } j = 1, 2 \quad (12)$$

$$[\rho]_\Gamma = \rho_l - \rho_g, \quad (13)$$

$$[\mu]_\Gamma = \mu_l - \mu_g, \quad (14)$$

$$[\varepsilon]_\Gamma = \varepsilon_l - \varepsilon_g, \quad (15)$$

$$[D]_\Gamma = n \cdot [\varepsilon E]_\Gamma = q_s, \quad (16)$$

$$n \times [E]_\Gamma = 0, \quad (17)$$

where $[(\cdot)]_\Gamma$ represents the jump of “(·)” across the interface, Γ , and for example, $[D]_\Gamma$ represents the jump of the electric displacement vector across the interface, n and t represent the normal and tangential vector components at the interface, subscripts l and g represent quantities in the liquid and gas phases, respectively, and q_s the surface charge. The electric charge is modeled as volumetric space charge that migrates throughout the liquid, which implies negligible surface charge and leads to the normal component of the electric displacement vector being continuous. However, the jump in electric permittivity across the phase interface imposes a discontinuity in the normal component of the electric field, and Eq. (16) can be written as

$$n \cdot [D]_\Gamma = n \cdot [\varepsilon E]_\Gamma = [\varepsilon E_n]_\Gamma = 0. \quad (18)$$

A direct consequence of the irrotational jump condition, Eq. (17), ensures that the tangential components of the electric field, and therefore the electric potential, ϕ , are continuous,

$$[E_{t1}]_\Gamma = 0, \quad [E_{t2}]_\Gamma = 0, \quad \text{and} \quad (19)$$

$$[\phi]_\Gamma = 0. \quad (20)$$

The pressure interface jump condition includes contributions from viscous, electric and surface tension forces, and is represented as

$$-[p]_\Gamma + [n^\top \cdot (\sigma^e + \sigma^f) \cdot n]_\Gamma = -\gamma \kappa, \quad (21)$$

which can be simplified as

$$[p]_\Gamma - 2[\mu]_\Gamma n^\top \cdot \nabla u \cdot n - \gamma \kappa = \left[\frac{1}{2} \varepsilon E_n^2 \right]_\Gamma - \left[\frac{1}{2} \varepsilon E_t^2 \right]_\Gamma, \quad (22)$$

where $[p]_\Gamma$ is the jump across the interface, γ the surface tension coefficient, and κ the local interface curvature. The tangential shear stress balance, again employing negligible surface charge, yields

$$[n^\top \cdot (\sigma^f) \cdot t_i]_\Gamma = 0. \quad (23)$$

Additional details are provided in [40, 41].

3. Numerical Approach

The simulations in this paper were conducted using the NGA computational platform, which employs a staggered grid with pressure and any scalars stored at the cell center and velocity components stored on cell faces [49]. Away from the interface, we use second-order finite difference operators that conserve mass, momentum, electric charge density, and kinetic energy. Near the interface, where discontinuities exist, special numerical methods are required. For convection, we use an unsplit, geometric, semi-Lagrangian framework. The framework is based on Owkes and Desjardins [50] and is used to transport the volume-of-fluid (VOF) representation of the phase interface, momentum, and electric charge density. Due to the staggered grid, consistent transport of both VOF and momentum is complex, requiring that the fluxes of mass used to transport VOF and momentum are discretely equal. This is achieved by discretizing VOF on a mesh twice as fine as the flow solver and

computing fluxes on all faces of pressure and momentum cells, implemented as an unsplit, geometric, semi-Lagrangian with details provided in Owkes and Desjardins [51]. The resulting scheme is second-order and conserves mass, momentum, and scalars even near the interface where discontinuities exist. The interface is using a piece-wise linear interface reconstruction (PLIC) [52] with interface normal vectors computed using the efficient least-squares VOF interface reconstruction algorithm (ELVIRA) [53]. Interface curvature is computed with the adjustable curvature evaluation scale (ACES) method [54]. NGA is fully parallelized with a message passing interface (MPI) protocol and scales well to tens of thousands of cores [55].

The electric field is computed from the electric potential using Eq. 6, which depends on the boundary conditions as well as the distribution of electric charge within the domain. The electric potential Poisson equation, Eq. 8, provides a relationship between the electric charge, q_i , and the electric potential, ϕ_i , and is solved using the *hypre* library of routines for scalable parallel solutions of linear systems [56, 57]. The pressure and electric potential Poisson equations are solved utilizing the ghost fluid method [58] and a black box solver [59].

The challenge of obtaining accurate electric potential boundary conditions on the computational domain for electrohydrodynamic flows is well documented, for example in [40, 41] among many others. For the model used in this work, grounded ($\phi = 0$) conditions exist at the boundaries of the computational domain. For smaller computational domains with higher electric charge concentrations, some mesh-alignment of the spray can result. To eliminate this numerical artifact of the computational model, a second domain called e-Mesh is introduced that spans from the nozzle to surfaces that represent physical boundaries that are grounded. The e-Mesh grid is implemented with well-defined boundary conditions and the charge density field, which is transferred from the flow domain. The electric Poisson equation, Eq. 8, is solved in e-Mesh to obtain a potential field and values of ϕ are transferred from e-Mesh to the boundaries of the flow domain to compute ϕ in the flow domain. Solving for the potential on the e-Mesh and then interpolating to the boundaries of the smaller flow domain allows for accurate boundary conditions of ϕ on the flow domain where they are needed but not well defined. The electric potential field, ϕ , is computed on e-Mesh and values are interpolated to the Navier-Stokes mesh using a tri-cubic interpolation scheme. Figure 1b shows the enlarged and coarse e-Mesh domain surrounding the much smaller and finer Navier-Stokes mesh. The e-Mesh is fully described in [44] and demonstrated in a numerical study in [45].

4. Data Extraction

Simulations employed the atomization simulation statistics extraction tool (ASSET), a recently developed physics extraction tool that identifies every breakup and coalescence event occurring during an atomizing spray. Data characterizing the atomization processes were stored in a Neo4j graphical database providing an easily accessible format. An in-depth description

of the process is available in previous works [46, 47], but a brief synopsis is included here for clarity.

ASSET operates at the same time as the simulation and runs every timestep, identifying droplets, which meet the criteria for either breakup or coalescence within that step. The algorithm works by assigning two integer identification numbers to every liquid structure within the domain. The first of these values ($\mathcal{S}$) is reassigned every timestep using a connected-component algorithm to identify every independent liquid structure. A second value ($\mathcal{L}$) is transported as a scalar value with the liquid and is only reassigned when a new droplet is formed either from breakup or coalescence. The sequence of events for one timestep is as follows:

1. Transport & Coalescence: $\mathcal{L}$ values are transported consistently with the liquid volume fraction via flux volumes. If multiple $\mathcal{L}$ values flux into a single computational cell, the liquid structures associated with the $\mathcal{L}$ values coalesce and these $\mathcal{L}$ values are stored for later processing of the coalescence event.
2. $\mathcal{S}$ assignment: A band-growth algorithm [60] assigns unique $\mathcal{S}$ values to structures separated by at least one full gas cell.
3. Structure statistics calculation: Each structure is added to a linked list with properties like volume, velocity, principal axis lengths, and average charge density.
4. Coalescence processing: Structures identified as coalescing are processed into a single structure. This structure is assigned a new $\mathcal{L}$ and the structures are tagged for data extraction.
5. Breakup identification and processing: Distinct structures (identified with multiple $\mathcal{S}$ values that contain the same $\mathcal{L}$ values were previously the same structure and therefore broke up. These structures are assigned new $\mathcal{L}$ values and tagged for data extraction.
6. Data extraction: Statistics from all identified coalescence and breakup structures are saved, along with old and new $\mathcal{L}$ values into the Neo4j database to construct a droplet “genealogy”.

5. Computational Domain and Simulations

Five liquid Diesel-type jets were simulated with liquid injection through a circular port of diameter D_{jet} , covering a range of relevant electrohydrodynamic and flow parameters. Simulation parameters are summarized in Table 1, with bulk velocity, U_{jet} . The domain size employed was $L_x = 24D_{\text{jet}}$, and $L_y = L_z = 8D_{\text{jet}}$ discretized on a uniform mesh of different sizes commensurate with the number of cells across the nozzle diameter, CAD, reported in Table 1. The Navier-Stokes computational domain is illustrated in Figure 1a. The electric potential boundary conditions implemented through e-Mesh for the charged simulation are Neumann on the upstream x -face, and Dirichlet ($\phi = 0$) on the downstream x -face and y - and z -faces. Figure 1b displays the e-Mesh surrounding the Navier-Stokes domain to provide a degree of scale and illustrate the e-Mesh stretching scheme employed to improve efficiency with

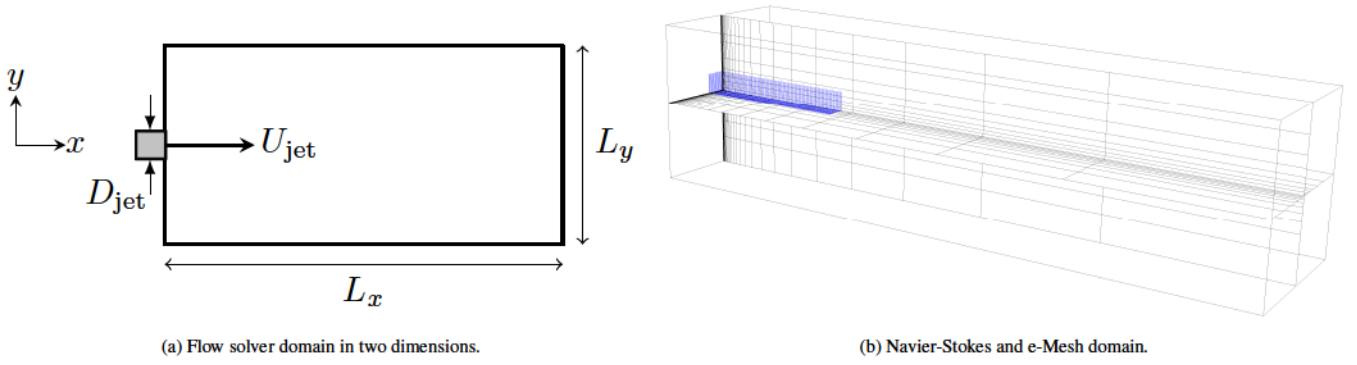


Figure 1: Simulation domain (left); Navier-Stokes mesh in blue and e-Mesh in black (right) showing relative scale of each domain.

Table 1: Non-Dimensional simulation parameters.

Sim ID	Reynolds, Re_l $\rho_l U_{\text{jet}} D_{\text{jet}} / \mu_l$	Weber, We_g $\rho_g U_{\text{jet}}^2 D_{\text{jet}} / \gamma_l$	Electro-inertial, N_{ei} $q_l^2 D_{\text{jet}}^2 / (\epsilon_l \rho_l U_{\text{jet}}^2)$	Density ratio ρ_l / ρ_g	Visc. ratio μ_l / μ_g	Resolution* $D_{\text{jet}} / \Delta x$
Lo_00	5000	2	Uncharged	1000	50	30 (60)
Lo_05	5000	2	0.05	1000	50	30 (60)
Lo_10	5000	2	0.1	1000	50	30 (60)
Hi_00	10000	10	Uncharged	1000	50	30 (60)
Hi_10	10000	10	0.1	1000	50	30 (60)
Domain Size $L_x = 24D_{\text{jet}}$, $L_y = L_z = 8D_{\text{jet}}$ *Parentetical value represents VOF resolution described in §3						

refinement near the nozzle and coarse spacing further from the injection location. As an initial investigation, EHD parameters were chosen similar to those reported in [41] and bulk hydrodynamic parameters similar to those reported in [47]. The electric Reynolds number, Re_e —a ratio of the residence time of liquid in the domain to the charge relaxation timescale [39]—is maintained at a moderate level of approximately 780 for all charged simulations, thereby permitting some charge mobility representative of poorly conducting liquids but limiting charge relaxation within the domain.

6. Results

Five cases were run for analysis and comparison, varying global Weber and Reynolds numbers and electro-inertial (N_{ei}) values. The cases are outlined in Table 1. The Lo_00 and Lo_05 simulations are shown separately in Figure 2 because these cases show minimal liquid breakup for analysis, although case Lo_05, Figure 2b, exhibits minimal droplet shedding. Figure 3 displays renderings of the Lo_10, Hi_00, and Hi_10 simulations in Figures 3a, 3b, and 3c, colored by liquid volume attached to the continuous liquid core (blue) and structures detached from the core (orange), illustrating the utility of the ASSET extraction tool for analyzing primary atomization mechanisms resulting from breakup events.

Figure 3a is shown next to experimental work reported by Shrimpton and co-workers [15, 14] for comparison of this case. The experimental work has hydrodynamic and electric parameters that closely match the Lo_10 case (see Table 1) with ex-

perimental values of $Re_l = 4,900$, $We_g \approx 2.1$, and $N_{ei} \approx 0.09$. The comparison reveals strong qualitative similarities, including the point of primary atomization onset, droplet size, and other structures within the disintegrating jets. The presence of numerous ligaments oriented radially outward from the axial centerline bears a strong resemblance to the experimental photograph, and the radial orientation of liquid structures is attributable to mutual repulsion arising from the space charge field.

Unlike simpler jet-to-dripping regimes, case Hi_00 did not exhibit a clear pinch-off point. Some droplet shedding was observed in Hi_00; however, complete disintegration of the liquid core was not evident. The presence of electric charge in the liquid plays a role in primary atomization, leading to initial de-stabilization. Electric effects on secondary atomization processes are expected to be small for these simulations due to the low values of electric charge compared to inertial and surface tension forces. The mutual repulsion of unipolar electric charge leads to greater spray dispersion through the action of the Coulomb force in the liquid bulk, thereby altering droplet trajectories and velocities after separating from the liquid core. The influence of electric charge is evident in Figures 3a (Lo_01) and 3c (Hi_01), particularly compared to their uncharged companion simulations in Figures 2a (Lo_00) and 3b (Hi_00), revealing the influence of electric effects in de-stabilizing the jet. The wider plume in Figure 3b, completely filling the domain, suggests a strong interplay among inertial, viscous, surface tension, and electric effects. Generally, increasing electric charge moves the initial

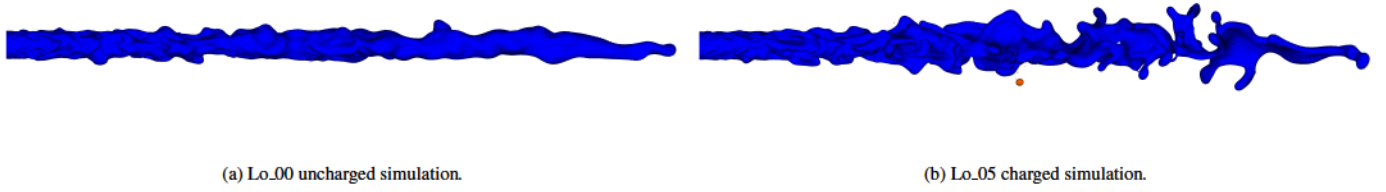


Figure 2: The Lo.00 (uncharged) and Lo.05 (low electric charge) simulations, showing minimal liquid breakup.

jet de-stabilization and point of atomization onset upstream, increases the number of structures dislodged from the liquid core and “radial fullness” of liquid in the domain, and widens the spray cone angle. The radial orientation of liquid structures in simulations with greater electric charge is attributable to Coulombic repulsion that arises from the space charge field, and is similar to that discussed elsewhere, for example in Tang and Gomez [61] among others. Coulombic repulsion leads to an electric field oriented radially from the liquid core, thereby confirming that the Coulomb force is a disruptive force that gives rise to the shape and orientation of the structures dislodged from the liquid core.

6.1. Uncharged and Charged Simulation Comparison

The uncharged and charged simulations demonstrate the robustness of the computational framework and their recently integrated tools, highlighting the notable differences in atomization processes due to electrostatic effects. Hydrodynamic and electric parameter values are listed in Table 1 for cases Hi.00 and Hi.10, identical except that there is no background electric potential and no liquid charge density in the uncharged simulation (Hi.00). The two cases are compared to elucidate the effects of electric charge and the corresponding electric field on the breakup mechanisms driving primary atomization while also demonstrating the accuracy and utility of the ASSET and e-Mesh tools. Figures 2a and 3c provide a visual comparison of the atomizing jets for the uncharged case (3a, Hi.00) and charged case (3c, Hi.10) at the simulation final time step. The presence of electric charge within a realistic Diesel type jet contributes to an earlier onset of primary atomization, and it modifies the interface shape leading to a fuller and wider plume and increased spray cone angle. The charged simulation, Figure 3c, shows the presence of droplets dislodged from the liquid core as well as interface corrugations and ligaments. At this point in the simulation, the charged case, Figure 3c, produced more than 2000 droplets; however, at the same point in the uncharged simulation, Figure 2a, only 50 droplets were created.

Figures 3e and 3f display “bloom” plots from the data stored in a Neo4j database demonstrating how the event data is organized in a logical and accessible format. The nodes are the liquid core and droplets produced from breakup events, which are represented by the lines connecting the nodes. Node colors represent the number of breakup events a structure has undergone, with the ordering (purple (liquid core) → orange → blue → red → gray → green). The liquid core is in the center of the image and the orange droplets represent primary breakup events.

These images illustrate all the droplets produced during the simulation, and all the intermediate droplets between the coherent liquid core and the final droplets. Paths between nodes represent the connections among parent and child droplets. Each node stores the extracted data from the simulation at the location and time at which that droplet separated from the liquid core and became independent. Figure 3f shows many more droplets and breakup events than the uncharged bloom plot in Figure 3e.

6.2. Charged Simulations Comparison

The two cases with highest electro-inertial number, $N_{ei} = 0.1$, exhibit interesting atomization features and a clear pinch-off point. Because of these characteristics, cases Lo.10 and Hi.10 are analyzed and contrasted henceforth, including estimates for the initial onset of primary atomization, breakup and coalescence, charge density distributions in the domain, and estimates for the spray cone angle. Renderings of both cases are shown in Figures 3a and 3c, illustrating a wider spray plume in case Hi.10 attributable to the higher Reynolds number and aerodynamic effects.

Figures 3d and 3f present “bloom” plots generated from the Neo4j database. In these visualizations, nodes represent droplets formed during breakup events, while the lines connecting them signify relationships between parent and child droplets (breakup or coalescence). The colors of the nodes indicate the number of breakup events each droplet has undergone. At the center of each plot lies the liquid core, with all nodes and paths eventually leading back to this core. These visualizations represent the entire droplet breakup cascade. The paths between nodes trace the lineage of droplets as they separate and evolve, while each node stores data about the droplet at the time and location it became independent from its parent droplet. The Lo.10 simulation ultimately produced 269 droplets, whereas the Hi.10 simulation generated 2,014 droplets, reflecting the significant differences in breakup dynamics between the two cases. Table 2 summarizes total droplets and mean diameter for cases Lo.00, Hi.00, and Hi.10, revealing the role of electric effects in jet de-stabilization, droplet production and size.

6.3. Primary Atomization Analysis

Spray cone angle is a useful qualitative description, and in these cases it is an effective parameter to analyze the effects of EHD and Weber and Reynolds numbers. It is clear from these numbers and the jet renderings in Figs. 3a-3c that EHD

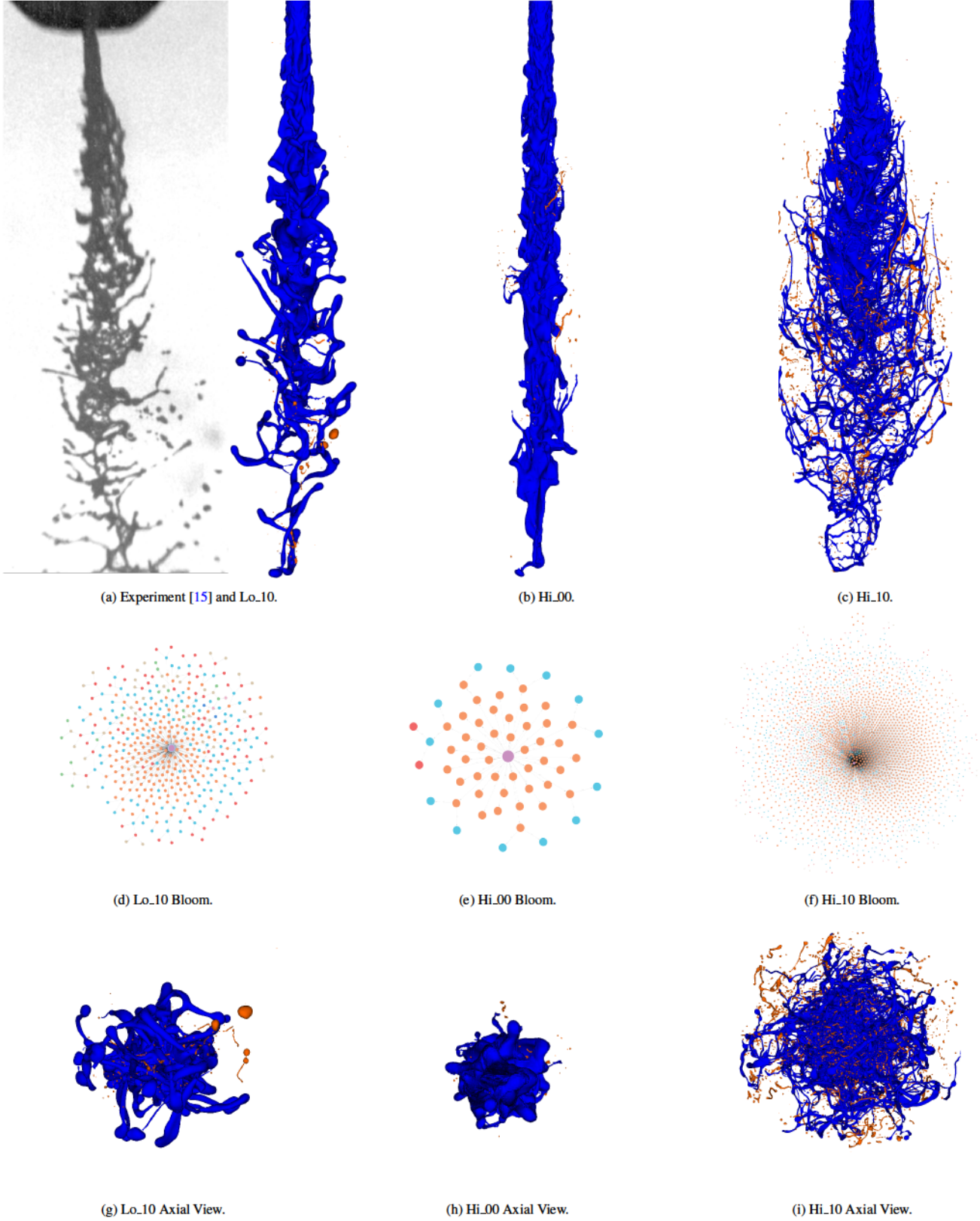
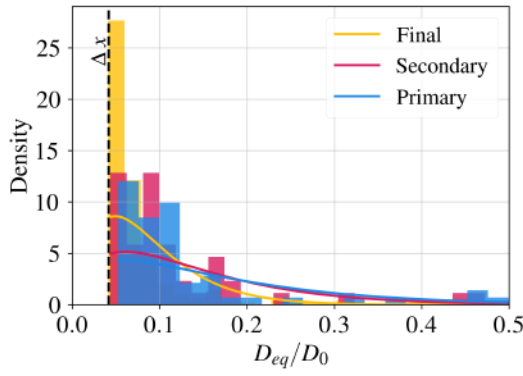


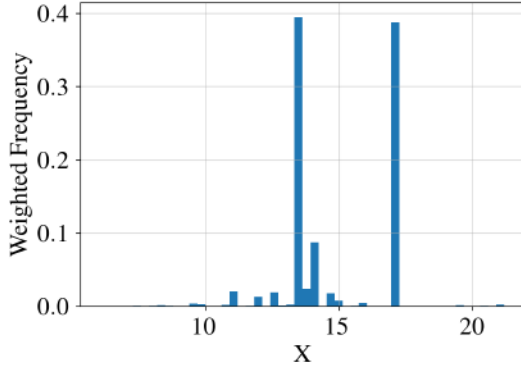
Figure 3: Renderings of experiment reported by Yule and Shrimpton [15] (reproduced with permission) and Lo.10 simulation (a, images not the same scale), Hi.00 (b), and Hi.10 (c) simulations showing contiguous liquid core (blue) and dislodged structures (orange); Bloom plots visualizing breakup events in simulations using ASSET (middle row, (d)-(f)); and axial view of simulations (bottom row, (g)-(i)). Full simulation parameters detailed in Table 1.



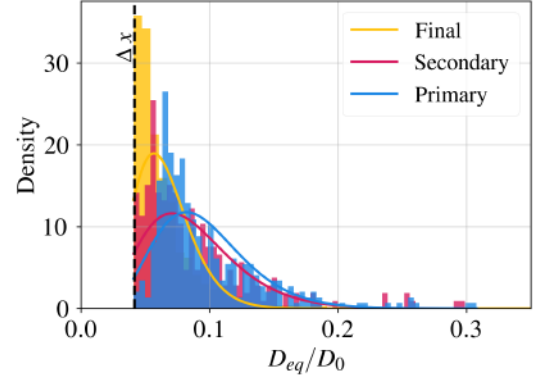
(a) Lo.10 diameter probability density.



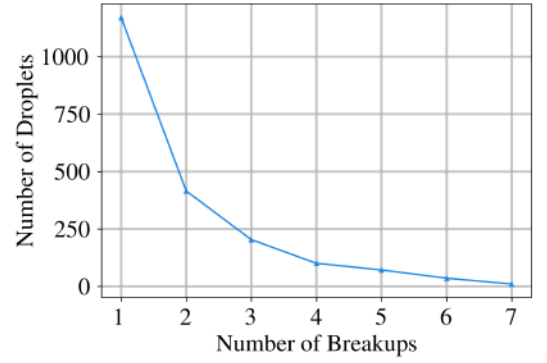
(c) Lo.10 breakup stage of final droplets.



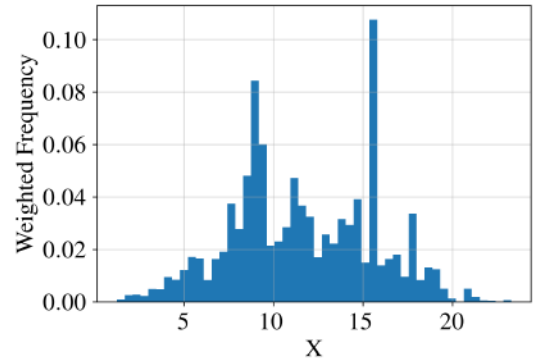
(e) Lo.10 volume-weighted primary breakup locations.



(b) Hi.10 diameter probability density.



(d) Hi.10 breakup stage of final droplets.



(f) Hi.10 volume-weighted primary breakup locations.

Figure 4: Charged simulations statistics for $N_{ei} = 0.1$. Lo.10 (left column) and Hi.10 (right column).

Table 2: Droplet statistics and spray cone angle approximations for select simulations.

Sim ID	Total Droplets	Mean D_{eq}	Spray Cone, $\alpha_{1/2}$
Lo_10	269	$0.2137D_{jet}$	8.6°
Hi_00	50	$0.0749D_{jet}$	$\sim$
Hi_10	2014	$0.0797D_{jet}$	14.0°

has a strong effect on the spray cone angle. The spray cone is defined as a half-angle, $\alpha_{1/2}$, measured from the edge of the nozzle. To determine this angle, a 2D domain is constructed in the radial-axial plane and the volume of liquid at each location is calculated by summing along the corresponding radial

ring. A line is defined on this domain, extending from the outer edge of the nozzle, such that 99% of the total spray volume lies within the resulting conical region. $\alpha_{1/2}$ is calculated using the radial and axial coordinates of this line as the legs of a right triangle. Table 2 reports spray angles measured at the final timestep in each of the five simulations. Both of the uncharged simulations, Lo_00 and Hi_00, experienced negligible radial spread. The plume width increases notably with added charge. Simulations with higher Reynolds and Weber numbers showed greater radial spread, suggesting a strong interaction among inertial, surface tension, aerodynamic, and electric effects, and likely attributable to the relative thinning of liquid structures resulting from higher Reynolds and Weber numbers. These thinner structures are also more susceptible to the effects

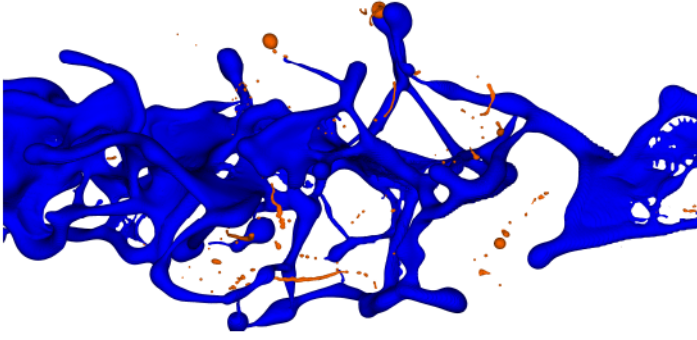


Figure 5: A magnified segment of the Lo_10 simulation, displaying ligaments stretching off of the liquid core (blue) and bulging due to Plateau-Rayleigh instability, ultimately forming large droplets and small satellite droplets (both orange). The VOF resolution for simulations is $60 D_{\text{jet}}/\Delta x$.

of the Coulomb force, thereby increasing their radial dispersion.

Figures 4a and 4b illustrate the droplet size distribution across different stages of the breakup process for both simulations. The data reveals that the Lo_10 simulation generated a greater proportion of larger-diameter droplets compared to the Hi_10 simulation. A clear progression is evident in the plots: larger primary structures give way to smaller secondary structures, culminating in a significant prevalence of small droplets classified as “final” droplets—those that do not undergo further breakup within the simulation. The mean diameter of final droplets was approximately $0.2137D_{\text{jet}}$ in the Lo_10 simulation and $0.0797D_{\text{jet}}$ in the Hi_10 simulation, highlighting a notable difference in the resulting droplet distributions. The sequence of breakup events leading to these final droplets is depicted in Figures 4c and 4d showing the number of breakup events required to reach the final droplet stage, with some structures undergoing as many as seven breakups before stabilizing into their final form.

The ASSET methodology permits the extraction of the locations of primary breakup events. However, sufficient data for meaningful analysis was available only for simulations Lo_10 and Hi_10. Figures 4e and 4f show the total volume of droplets shed at each location along the x -axis. This weighted distribution highlights the regions where the jet becomes most unstable and undergoes significant disintegration. In the Hi_10 simulation, two pronounced peaks appear around $X = 8$ and $X = 16$. The first corresponds to a similar spike in the number of breakup events, indicating both high droplet count and size. The second peak likely represents a large liquid structure detaching from the core, as suggested by a relative decrease in total droplet production seen in Figure 4e. The Lo_10 simulation also shows two peaks, but given its comparatively low droplet output, both peaks are more plausibly linked to large liquid structures separating from the liquid core.

Analyzing the drop size distributions in Figures 4a and 4b confirms the prevalence of small droplets in both simulations. The Lo_10 simulation maintains larger droplets and many fewer droplets total as seen in Table 2. In both cases, there are few large droplets and many small droplets. This distribution is largely due to capillary effects driven by the Plateau-Rayleigh

instability—smooth ligaments are stretched from the liquid core, after which surface tension forces create bulges linked by thinner ligaments, ultimately leading to pinch-off. The resulting thin ligaments formed undergo the same process, producing smaller “satellite” droplets, described in experiments reported by Qian and Law [62] and later in Villiermaux [63]. Figure 5, a magnified segment of the Lo_10 simulation, illustrates this phenomenon, showing several ligaments with bulges and smaller satellite ligaments and droplets. Furthermore, electric effects have been shown to reduce the influence of surface tension, leading to enhanced secondary atomization, more droplets, and a greater number of breakup and coalescence events.

6.4. Electric Charge Density

For completeness, a preliminary assessment of electric charge density is provided here. Figure 6 illustrates x - y cut planes of the Lo_10 and Hi_10 simulations colored by electric charge density showing charge migration through the liquid. The effects of charge mobility even near the issuing nozzle can be observed in both Figure 6a and 6b with higher charge density near the surface resulting from the unipolar charge mutual repulsion. Ligaments and structures dislodged further from the centerline carry higher charge density as both jets disintegrate downstream from primary atomization mechanisms and the interplay among electric stress, inertial forces, and surface tension. Further downstream, structures originating closer to the axial centerline carry lower charge density with levels similar to those nearer jet center prior to initial disintegration.

Using the ASSET tool, values of charge density (L_Q) were extracted for every final droplet in the domains of the Lo_10 and Hi_10 simulations. Electric charge levels are shown as distributions in Figure 7a and 7b, with the initial injected charge value represented as a dashed red line. The distributions are final droplets, meaning droplets that do not experience further breakup in the simulation. Charge density may vary within droplets, but the values reported in Figure 7 are mean charge values within each droplet. Most droplets contain a charge density that is very close to the initial bulk charge. Because charge migration is included in the model, there is a distribution of charge densities in the droplets. Charge migration toward the outer surface of a liquid jet results in higher charge density away from the jet centerline and a higher value of L_Q in structures dislodged near the liquid-gas interface. This trend is more pronounced in the Hi_10 case, illustrated in Figure 7b and the scatter plot in Figure 7c in blue, compared to the charge density distribution for Lo_10 shown in Figure 7a and Figure 7c in orange. The effect of the low electric Reynolds number in these simulations is evident in the prevailing electric charge in the liquid bulk throughout the domain with some migration to the outer surface of the jet.

7. Conclusions

A robust computational framework for simulating electrically charged liquid hydrocarbon jets is developed, tested and demonstrated in this work. First-principles-based numerical

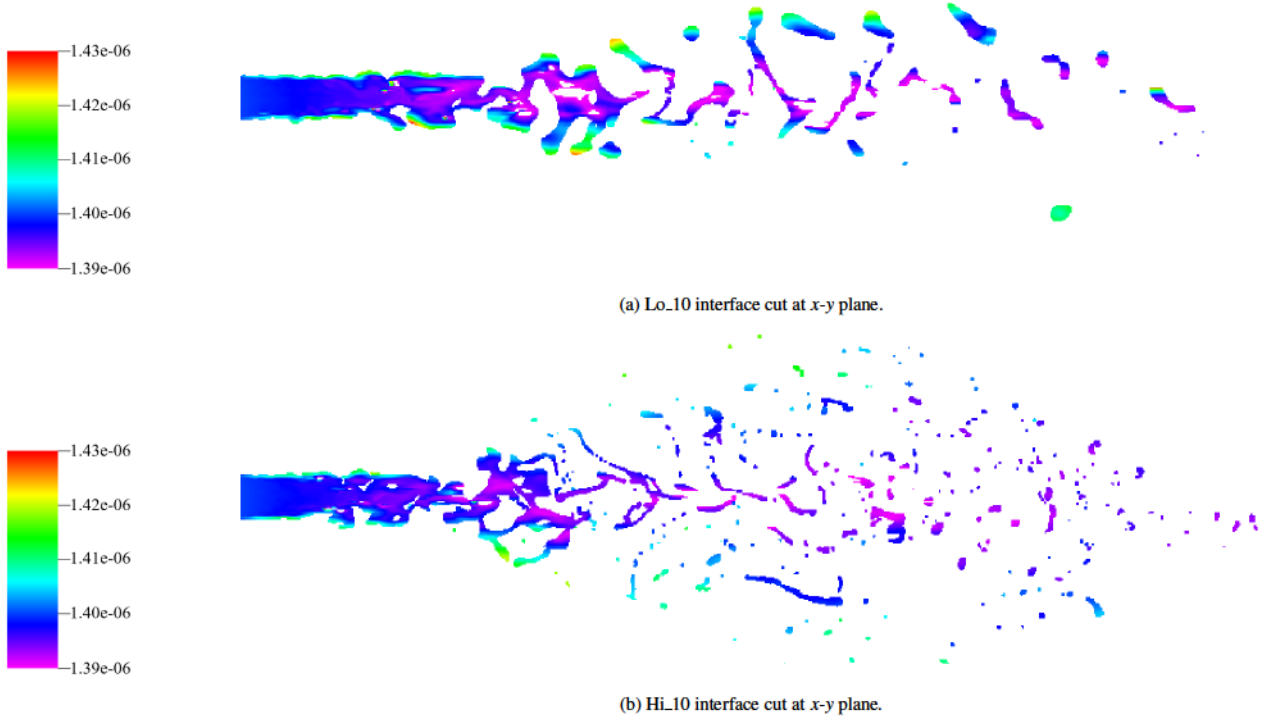


Figure 6: Axial planes $x-y$ colored by charge density.

methods developed specifically for high-fidelity direct numerical simulations of electrohydrodynamic (EHD) flows are implemented within a conservative flow solver using an unsplit, geometric volume-of-fluid transport scheme that includes EHD effects. The numerical framework conserves mass, momentum, and the electric charge density even at the gas-liquid interface where discontinuities exist. A novel approach using a separate mesh is used to obtain accurate boundary conditions of electric potential on the computational domain. Simulations employ a recently developed physics extraction tool that tracks every breakup and coalescence event occurring during an atomizing spray. Data characterizing the atomization processes are stored in a Neo4j graphical database providing an easily accessible format. The framework demonstrated in this work confirms the robustness of the methodology and its tools. The efficient methods for simulating complex atomization of electrically charged jets enable much improved understanding of the effect of the electric field, the interplay between electric and hydrodynamic effects and their influence on atomization processes, and spray characteristics that have proven challenging to obtain experimentally.

Statistics for droplet size, breakup and coalescence events, onset of primary atomization, and spray cone angle are reported for all simulations revealing earlier and enhanced liquid breakup with increasing electric charge. The presence of electric charge de-stabilizes the liquid core, thereby advancing the onset of primary atomization, and increases spray angle and droplet spacing due to the effect of the electric force act-

ing radially outward from the liquid core. Subsequent to initial breakup, a reduction in the effective surface tension in liquid structures due to the presence of electric charge enhances secondary atomization breakup processes in the electrified jet. The effects of charge mobility are evident, resulting from mutual repulsion of the unipolar charge within the liquid and influencing the charge density distribution in droplets and structures dislodged during primary atomization.

The work reported here is an initial step toward a much broader application of DNS for atomizing EHD flows. The simulations reported herein demonstrate extensions to recently developed tools—a physics extraction scheme and the e-Mesh domain solver for electric boundary conditions—to a complex, multi-physics, multi-phase atomization scenario, thereby validating their robustness and the utility of the framework. The integration of these new tools within NGA improves the efficiency and accuracy of EHD simulations and significantly expands the analysis opportunities of primary atomization processes for these types of flows. Analysis of secondary atomization processes and mechanisms is a natural extension of the work reported here. Moreover, continuation of this work will permit the development of DNS databases to support future efforts, both experimental and computational. The methodologies developed in previous work [41, 40, 42, 44, 47] and demonstrated here open new, simulations-based avenues of exploration within a broader category of electrohydrodynamics.

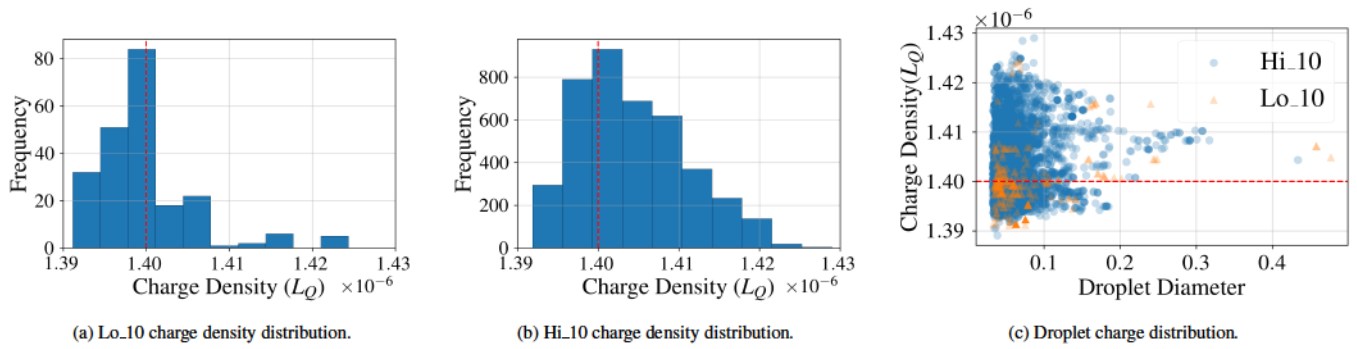


Figure 7: Charge density distributions for droplets in the Lo_10 (a) and Hi_10 simulations (b); scatter plot of droplet charge distribution in Lo_10 (orange) and Hi_10 (blue) simulations (c). Red dashed line shows initial value for L_Q of the injected liquid volume.

Acknowledgments

This work was supported by Advanced Cyberinfrastructure Coordination Ecosystem: Services and Support (ACCESS), National Science Foundation, under a Discovery project allocation. Simulations were performed on Purdue University's Anvil cluster through ACCESS. The authors gratefully acknowledge the contributions of Dr Venkata Krishna implementing e-Mesh. Additional computational efforts were performed on the Tempest High Performance Computing System, operated and supported by University Information Technology Research Cyberinfrastructure (RRID:SCR_026229) at Montana State University. The second author gratefully acknowledges the support provided by the Department of Aerospace Engineering and College of Engineering, Texas A&M University.

References

- [1] L. Rayleigh, On the equilibrium of liquid conducting masses, *Philosophical Magazine, Series 5* 14 (1882) 184–186.
- [2] A. Jaworek, A. Sobczyk, Electro spraying Route To Nanotechnology: An Overview, *Journal of Electrostatics* 66 (2008) 197–219.
- [3] G. Taylor, Disintegration of Water Drops in an Electric Field, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 280 (1964) 383–397. URL: <http://rspa.royalsocietypublishing.org/cgi/doi/10.1098/rspa.1964.0151>. doi:10.1098/rspa.1964.0151.
- [4] G. I. Taylor, Studies in electrohydrodynamics. I. The circulation produced in a drop by an electric field, *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences* 291 (1966) 159–166.
- [5] G. Taylor, P. R. S. L. A., Electrically Driven Jets, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* (1969) (1969) 453–475. doi:10.1098/rspa.1969.0205.
- [6] G. I. Taylor, a. D. McEwan, The stability of a horizontal fluid interface in a vertical electric field, *Journal of Fluid Mechanics* 22 (2006) 1. URL: http://www.journals.cambridge.org/abstract/_/S0022112065000538. doi:10.1017/S0022112065000538.
- [7] J. R. Melcher, Charge relaxation on a moving liquid interface, *The Physics of Fluids* 10 (1967) 325–332.
- [8] J. Melcher, C. Smith, Electrohydrodynamic charge relaxation and interfacial perpendicular-field instability, *Phys. Fluids* (1969).
- [9] D. Saville, Electrohydrodynamic stability: effects of charge relaxation at the interface of a liquid jet, *Journal of Fluid Mechanics* 48 (1971) 815–827.
- [10] K. Kim, R. Turnbull, Generation Of Charged Drops Of Insulating Liquids By Electrostatic Spraying, *Journal of Applied Physics* (1976). URL: http://medcontent.metapress.com/index/A65RM03P4874243N.pdfhttp://ieeexplore.ieee.org/xpls/abs/_/all.jsp?arnumber=5102650.
- [11] A. Kelly, the electrostatic atomization of hydrocarbons, *Journal of the Institute of Energy* (1984). URL: [http://cat.inist.fr/?aModele=afficheN\[&cpsid=9035612](http://cat.inist.fr/?aModele=afficheN[&cpsid=9035612).
- [12] W. Lehr, W. Hiller, Electrostatic atomization of liquid hydrocarbons, *Journal of Electrostatics* 30 (1993) 433–440. URL: <http://www.sciencedirect.com/science/article/pii/030438869390096P>.
- [13] A. Rigit, J. S. Shrimpton, Spray characteristics of charge injection electrostatic atomizers with small-orifice diameters, *Atomization and Sprays* 16 (2006).
- [14] J. Shrimpton, A. Yule, Atomization, combustion, and control of charged hydrocarbon sprays, *Journal of Atomization and Sprays* 11 (2001) 365–396.
- [15] A. Yule, J. Shrimpton, A. Watkins, W. Balachandran, D. Hu, Electrostatically atomized hydrocarbon sprays, *Fuel* 74 (1995) 1094–1103.
- [16] J. S. Shrimpton, Y. Laoonual, Dynamics of electrically charged transient evaporating sprays, *International journal for numerical methods in engineering* 67 (2006) 1063–1081.
- [17] J. Shrimpton, A. Kourmatzis, Direct numerical simulation of forced flow dielectric ehd within charge injection atomizers, *IEEE transactions on dielectrics and electrical insulation* 17 (2010) 1838–1845.
- [18] J. C. Baygents, N. J. Rivette, H. A. Stone, Electrohydrodynamic deformation and interaction of drop pairs, *Journal of Fluid Mechanics* 368 (1998) 359–375.
- [19] R. Collins, M. Harris, O. Basaran, Breakup of Electrified Jets, *Journal of Fluid Mechanics* 588 (2007) 75–129. URL: http://www.journals.cambridge.org/abstract/_/S0022112007007409. doi:10.1017/S0022112007007409.
- [20] G. Tomar, D. Gerlach, G. Biswas, N. Alleborn, A. Sharma, F. Durst, S. Welch, A. Delgado, Two-phase electrohydrodynamic simulations using a volume-of-fluid approach, *Journal of Computational Physics* 227 (2007) 1267–1285.
- [21] J. Feng, T. Scott, A Computational Analysis Of Electrohydrodynamics Of A Leaky Dielectric Drop In An Electric Field, *Journal of Fluid Mechanics* (1996). URL: http://journals.cambridge.org/abstract/_/S0022112096002601.
- [22] J. Feng, Electrohydrodynamic Behaviour Of A Drop Subjected To A Steady Uniform Electric Field At Finite Electric Reynolds Number, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* (1999) 2245–2269. URL: <http://rspa.royalsocietypublishing.org/content/455/1986/2245.short>. doi:10.1098/rspa.1999.0402.
- [23] J. Sherwood, Breakup of fluid droplets in electric and magnetic fields, *Journal of Fluid Mechanics* 188 (1988) 133–146.
- [24] J. Shrimpton, Pulsed charged sprays: application to disi engines during early injection, *International Journal for Numerical Methods in Engineering* 58 (2003) 513–536.
- [25] W.-F. Hu, M.-C. Lai, Y.-N. Young, A hybrid immersed boundary and immersed interface method for electrohydrodynamic simulations, *Journal of Computational Physics* 282 (2015) 47–61. URL: <http://linkinghub.elsevier.com/retrieve/pii/S0021999114007578>. doi:10.1016/j.jcp.2014.11.005.
- [26] H. Paknemat, a. R. Pishevar, P. Pournaderi, Numerical simulation of drop deformations and breakup modes caused by direct current electric

- fields, *Physics of Fluids* 24 (2012) 102101. URL: <http://link.aip.org/link/PHFLE6/v24/i10/p102101/s1?iAgg=doi>. doi:10.1063/1.4754737.
- [27] B. V. Hokmabad, S. Faraji, T. G. Dizajyekan, B. Sadri, E. Esmailzadeh, Electric field-assisted manipulation of liquid jet and emanated droplets, *International journal of multiphase flow* 65 (2014) 127–137.
- [28] W. Du, S. Chaudhuri, A Multiphysics Model For Charged Liquid Droplet Breakup In Electric Fields, *International Journal of Multiphase Flow* 90 (2017) 46–56. URL: <http://www.sciencedirect.com/science/article/pii/S0301932216300465>. doi:10.1016/j.ijmultiphaseflow.2016.11.009.
- [29] Z. Xie, Q. Dong, A. Sau, Z. Wang, Self-propulsion of a Quincke droplet on a superhydrophobic wall under low electric Reynolds number $Re_E \leq 1$, *Physics of Fluids* 36 (2024).
- [30] Q. Dong, A. Sau, Unsteady electrorotation of a viscous drop in a uniform electric field, *Physics of Fluids* 35 (2023).
- [31] J. T. Holgate, M. Coppins, Shapes, Stability, And Hysteresis Of Rotating And Charged Axisymmetric Drops In A Vacuum, *Physics of Fluids* 30 (2018) 064107. URL: <http://aip.scitation.org/doi/10.1063/1.5023437>. doi:10.1063/1.5023437.
- [32] D. Fredrich, E. Weiland, A. Giusti, Electrostatic fields for the control of evaporating charged fuel sprays, *International Journal of Multiphase Flow* 160 (2023) 104312.
- [33] O. Schnitzer, I. Frankel, E. Yariv, Electrokinetic flows about conducting drops, *Journal of Fluid Mechanics* 722 (2013) 394–423. URL: http://www.journals.cambridge.org/abstract/_J5002211201300102X. doi:10.1017/jfm.2013.102.
- [34] O. Schnitzer, E. Yariv, The Taylor–Melcher leaky dielectric model as a macroscale electrokinetic description, *Journal of Fluid Mechanics* 773 (2015) 1–33.
- [35] D. Saville, Electrohydrodynamics: the Taylor–Melcher leaky dielectric model, *Annual review of fluid mechanics* 29 (1997) 27–64.
- [36] J. López-Herrera, M. Herrada, A. Gañán-Calvo, Electrokinetic modelling of cone-jet electrosprays, *Journal of Fluid Mechanics* 964 (2023) A19.
- [37] A. Kourmatzis, J. S. Shrimpton, Electrohydrodynamics and charge injection atomizers: A review of the governing equations and turbulence, *Journal of Atomization and Sprays* 19 (2009) 1045–1063.
- [38] J. M. Crowley, *Electrostatic fundamentals*, 1995.
- [39] O. M. Stuetzer, Magnetohydrodynamics and electrohydrodynamics, *The Physics of Fluids* 5 (1962) 534–544.
- [40] B. Van Poppel, O. Desjardins, J. Daily, A ghost fluid, level set methodology for simulating multiphase electrohydrodynamic flows with application to liquid fuel injection, *Journal of Computational Physics* 229 (2010) 7977–7996.
- [41] P. Sheehy, M. Owkes, Numerical study of electric Reynolds number on electrohydrodynamic (ehd) assisted atomization, *Atomization and Sprays* 27 (2017).
- [42] B. P. Van Poppel, B. Christensen, M. Owkes, V. Krishna, Framework for analyzing atomization in electrically charged diesel-type jets, in: *ILASS Americas 34th Conference on Liquid Atomization and Spray Systems*, 2024, pp. 1–10.
- [43] J. Potyka, K. Schulte, A volume of fluid method for three dimensional direct numerical simulations of immiscible droplet collisions, *International Journal of Multiphase Flow* 170 (2024) 104654.
- [44] V. Krishna, W. Liu, M. Owkes, High-fidelity simulations of a rotary bell atomizer with electrohydrodynamic effects, *International Journal of Multiphase Flow* 168 (2023) 104566.
- [45] V. Krishna, M. Owkes, Investigating atomization characteristics in an electrostatic rotary bell atomizer, *International Journal of Multiphase Flow* (2024) 104814. URL: <https://www.sciencedirect.com/science/article/pii/S0301932224000946>. doi:<https://doi.org/10.1016/j.ijmultiphaseflow.2024.104814>.
- [46] C. Rubel, M. Owkes, Extraction of droplet genealogies from high-fidelity atomization simulations, *Atomization and Sprays* 29 (2019).
- [47] B. Christensen, M. Owkes, Efficient extraction of atomization processes from high-fidelity simulations, *Computers & Fluids* 254 (2023) 105808.
- [48] J. Chang, A. Kelly, J. Crowley, *Handbook of electrostatic processes*, Marcel Dekker, Inc., 1995.
- [49] O. Desjardins, G. Blanquart, G. Balarac, H. Pitsch, High Order Conservative Finite Difference Scheme For Variable Density Low Mach Number Turbulent Flows, *Journal of Computational Physics* 227 (2008) 7125–7159. URL: <http://linkinghub.elsevier.com/retrieve/pii/S0021999108001666>. doi:10.1016/j.jcp.2008.03.027.
- [50] M. Owkes, O. Desjardins, A computational framework for conservative, three-dimensional, unsplit, geometric transport with application to the volume-of-fluid (vof) method, *Journal of Computational Physics* 270 (2014) 587–612.
- [51] M. Owkes, O. Desjardins, A mass and momentum conserving unsplit semi-lagrangian framework for simulating multiphase flows, *Journal of Computational Physics* 332 (2017) 21–46.
- [52] K. W. Morton, M. J. Baines, *Numerical methods for fluid dynamics V*, volume 5, Oxford University Press, 1995.
- [53] J. E. Pilliod Jr, Second-order accurate volume-of-fluid algorithms for tracking material interfaces, *Journal of Computational Physics* 199 (1997).
- [54] M. Owkes, E. Cauble, J. Senecal, R. A. Currie, Importance of curvature evaluation scale for predictive simulations of dynamic gas–liquid interfaces, *Journal of Computational Physics* 365 (2018) 37–55.
- [55] O. Desjardins, H. Pitsch, Detailed numerical investigation of turbulent atomization of liquid jets, *Atomization and Sprays* 1 (2010). URL: <http://www.dl.begellhouse.com/journals/6a7c7e10642258cc,454ec32d683e6c1b,51f20e192293fd90.html>.
- [56] R. D. Falgout, J. E. Jones, U. M. Yang, Pursuing scalability for hypre’s conceptual interfaces, *ACM Transactions on Mathematical Software (TOMS)* 31 (2005) 326–350.
- [57] R. D. Falgout, J. E. Jones, U. M. Yang, The design and implementation of hypre, a library of parallel high performance preconditioners, in: *Numerical solution of partial differential equations on parallel computers*, Springer, 2006, pp. 267–294.
- [58] R. Fedkiw, T. Aslam, B. Merriman, S. Osher, A non-oscillatory eulerian approach to interfaces in multimaterial flows (the ghost fluid method), *Journal of Computational Physics* 152 (1999) 457–492.
- [59] J. Dendy, Black box multigrid, *Journal of Computational Physics* 48 (1982) 366–386.
- [60] M. Herrmann, A Parallel Eulerian Interface Tracking / Lagrangian Point Particle Multi-Scale Coupling Procedure, *Journal of Computational Physics* 229 (2010) 745–759. URL: <http://dx.doi.org/10.1016/j.jcp.2009.10.009>. doi:10.1016/j.jcp.2009.10.009.
- [61] K. Tang, A. Gomez, On the structure of an electrostatic spray of monodisperse droplets, *Physics of Fluids* 6 (1994) 2317–2332.
- [62] J. Qian, C. K. Law, Regimes of coalescence and separation in droplet collision, *Journal of fluid mechanics* 331 (1997) 59–80.
- [63] E. Villermaux, Fragmentation versus cohesion, *Journal of Fluid Mechanics* 898 (2020) P1.