NUMERICAL STUDY OF ELECTRIC REYNOLDS NUMBER ON
ELECTROHYDRODYNAMIC (EHD) ASSISTED ATOMIZATION

by

Patrick John Harper Sheehy

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ABSTRACT

In today’s modern world, nearly all industries utilize the benefits of fast, long distance transportation that burning fossil fuels deliver. However, fluctuating fuel prices has created interest in researching alternatives to fossil fuels. Bio-fuels are one of these alternatives, but they generally have a higher viscosity and water content than diesel. This means high pressures are required to atomize the fuel in the combustion chamber, thus bio-fuels are limited to larger or less efficient engines. A potential method to reduce the pressure requirements is to use Electrohydrodynamic (EHD) assisted atomization.

EHD assisted atomization injects electrical charges into the liquid fuel before spraying, meaning the fuel has an electrical charge distribution before and after atomization. For many relevant engineering flows, including liquid fuel injection, the charge mobility timescale (time it takes the charges to relax to the fluid-gas boundary) is similar in magnitude to the charge convection timescale (relevant flow time), which leads to a non-trivial electric charge distribution. This distribution within the liquid fuel may enhance atomization, the extent to which is dependent on the ratios of the timescales which are known as the electric Reynolds number (Re_e).

In this work, a computational approach for simulating two-phase EHD flows is used to investigate the amount Re_e influences the resulting atomization quality. The computational approach is second-order, conservative, and is used to consistently transport the phase interface along with the discontinuous electric charge density and momentum. The scheme sharply handles the discontinuous electric charge density, allowing robust and accurate simulations. In addition, this method is modified by a work distribution scheme to improve processor utilization on High Performance Computing (HPC) clusters. Using these methods, multiple three-dimensional test cases are simulated with varying Re_e values which highlight the effect of Re_e on the atomization efficiency of a liquid jet. Comparison of these cases shows the importance of Re_e on atomization and suggests that decreasing Re_e (increasing charge mobility) leads to larger concentrations of electric charge density, increased Coulomb force, and ultimately improved break-up during the atomization process.

THESIS INTRODUCTION

The purpose of this work is to elucidate the effect of Re_e on atomization. To that end, a simple analytical analysis of charge distribution inside a spherical droplet was used to assess the effect Re_e has on the Coulomb force. Following this analysis, numerical simulations of EHD flows were used to study the Re_e effects on fluid jets by varying Re_e through three test cases. These cases are ordered by decreasing Re_e value, and highlighted how the flow atomization is related to the Re_e .

This paper is organized into the following format: first a literature review of the relevant research will be covered in Chapter 2. This will be followed by the research submitted to the Atomization and Sprays Journal (AAS) split into chapters. The AAS paper starts with the introduction in Chapter 3, followed by the mathematical governing equations for EHD atomizing flows in Chapter 4. Before running the complex fluid simulations of this research, a simple analytical analysis investigating the relationships between Re_e , electric charge distribution, induced electric field, and Coulomb force on a droplet is provided in Chapter 5. Chapter 6 gives a brief explanation of the numerical methods used to calculate the equations given in Chapter 4, before discussing the fluid parameters of the cases being studied. Chapter 7 covers tangential research into correcting simulation inefficiencies using load balancing methods. Finally Chapters 8 and 9 discuss the results of the simulations, and the conclusions drawn from those results, respectively.

LITERATURE REVIEW

Introduction

In today's modern world, nearly all industries utilize the benefits of fast, long distance transportation that burning fossil fuels deliver. However, over the past few years the cost of fossil fuels has been fluctuating wildly and this fluctuation, along with the tightening of emission legislations (Amine-Eddine and Shrimpton, 2013) has created interest in researching alternatives that are cheaper, renewable, or more efficient as compared to fossil fuels. One of these alternatives are plant based bio-fuels, which are renewable and have properties most similar to diesel fuels as shown in Table 2.1 for a corn based bio-fuel. These bio-fuels are often referred to as bio-oils (Wang et al., 2012).

Table 2.1: Liquid properties for Diesel fuel and a corn based bio-oil (Wang et al., 2012).

	Diesel fuel	Corn oil
Density ρ (kg/m^3)	840	870
Viscosity μ (Ns/m^2)	0.0024	0.054
Surface tension γ (N/m)	0.025	0.031
Conductivity σ ($1/\Omega m$)	1.0×10^{-10}	0.6×10^{-10}
Relative permittivity ϵ_r	2.0-2.2	3.0-3.1
Charge relaxation time τ_C (ms)	1.8-2.0	2.7-2.8

Regular diesel engines require high pressures on fuel injection (Kourmatzis et al., 2012) to achieve the correct fuel to air ratio. As bio-oils are even more viscous than diesel fuels, they require even higher fuel injection pressures than diesel fuels for correct atomization. The required fuel pressures push the limit on what most engines

can handle, which means using bio-oils as the fuel source is limited to larger less efficient engines that can handle the required high pressures (Kourmatzis et al., 2012).

One way to lower the required fuel injection pressure is to use Electrohydrodynamic (EHD) techniques to atomize the injected liquid. A simple definition of EHD is that it is the study of the way fluid mechanics and electrostatics interact (Owkes and Desjardins, 2014b). EHD Atomization potentially allows viscous bio-oils to be atomized at lower pressures, which means they may be usable by small engines as well as large. This method will potentially increase engine efficiency for both regular and bio-fuels, although much work is still required to understand the mechanisms behind EHD atomization and to confirm the theory will work in real engines.

Electrohydrodynamics

As viscosity values for bio-oils are up to 20 times greater than comparable diesel fuels (Malkawi et al., 2010) they do not atomize well at the standard atomization pressures used for fuel injection. Adding to their difficulty as a fuel source is the fact that they also have a high water content as compared to hydrocarbons (Wang et al., 2012). This means they burn less efficiently than diesel fuels as their fuel to air ratio is not at optimal levels, which also increases harmful emissions due to unburnt hydrocarbons (Kourmatzis and Shrimpton, 2011).

EHD atomization holds the possibility to improve liquid fuel breakup at lower pressures (Ryan et al., 2014), which would create acceptable atomization quality without the requirements of high pressure fuel injection. Thus making EHD atomization a viable scheme for use in small combustion engines (Van Poppel et al., 2010a) that cannot handle the high fuel injector pressures required to atomize the more viscous bio-oils. An added benefit of this increased fuel atomization is that complete combustion is more likely to occur during the burn cycle, making a cleaner

burn with less emissions (Amine-Eddine and Shrimpton, 2013). Another advantage of EHD atomization is that the burn residue (soot, NOX) remains charged, meaning electric fields in the engine exhaust could potentially direct the burn residue to easily cleanable containers (Shrimpton and Yule, 2001). This method holds even more potential for bio-oils than diesel fuels due to their higher viscosities because when using this method bio-oils generally produce droplets smaller than the atomizer orifice size and those produced by comparable diesel fuels under the same conditions (Malkawi et al., 2010).

Discussion

Atomization can be split into two main types, Primary and Secondary. Primary atomization occurs when the liquid is broken up into droplets, generally by an atomizer nozzle, while Secondary atomization occurs when the droplets are broken up again into even smaller droplets by perturbations in the spray. Creating a fine atomization can use both Primary and Secondary, and requires the liquid to be made unstable before atomization. This can be achieved by using EHD methods to induce an electric charge on the liquid. Inducing this charge destabilizes the liquid to turbulent flow under pressures that would normally produce laminar flow, meaning a better primary atomization occurs out of the atomizer body than for an uncharged liquid (Kourmatzis et al., 2012).

If EHD atomization methods were used for Primary atomization, Secondary atomization may also occur due to the mutual repulsion of net charges accumulating on each droplet surface as the liquid is atomized. If enough charge accumulated on the droplet surface such that the net force is greater than the opposing surface tension, the droplet will split into smaller droplets. As long as the net charge on each sub-droplet remains larger than the surface tension, the atomizing process will

continue (Wang et al., 2012). The differences between an uncharged and charged flow of an insulated liquid can be seen in Fig 2.1.

The dominant EHD atomization method used for insulated liquids, such as bio-oils and fossil fuels, is electrostatic charge injection. This technique works by injecting an electrical charge into the liquid that, on atomization, promotes smaller droplets to form and disperse than would occur without the charge (Kourmatzis and Shrimpton, 2011). The charge is "injected" by placing an electrode into the flow that is typically maintained at a high negative voltage (Shrimpton and Yule, 2003) while the atomizer body is earthed. Using this technique means atomization can occur for high-flow-rate applications as the spray specific charge, the max amount of charge the spray can hold, increases with flow rate, thus improving the atomization due to increased aerodynamic and electrical forces on the liquid surface (Shrimpton and Yule, 2001).

The main downside to the charge injection technique is that the most popular method utilizes a point-plane setup. A pointed electrode is placed just before the small opening of an atomizer such that the distance from the center of the opening is equal to the diameter of the opening (Shrimpton and Yule, 2001). This setup requires precise alignment to be most efficient, as shown in Figure 2.2. Thus, much time and effort is needed to assemble the setup, and maintain it at optimum efficiency.

Recently Kourmatzis et al. (2010) have suggested a plane-plane type charge injector to help solve some of the point-plane issues. The plane-plane system is similar to the point-plane system except the atomizer body may have several more openings, and the pointed electrode is replaced with a single blunt electrode with a roughened surface. Their results have shown that increasing the number of openings in the atomizer, increases the electrical efficiency of the system. Meaning the atomizer can be run with a much lower voltage while still having the specific charge increase with the flow rate. They conclude by saying: "The [plane-plane] system is very

Figure 2.1: (a) Uncharged (b) Charged flow of Kerosene (Shrimpton and Yule, 2001)

Figure 2.2: General Point-Plane Charge Injection Setup. (Shrimpton and Yule, 2001)

promising since with minimal alignment, high flow rates and thus fine sprays can be achieved.” (Kourmatzis et al., 2010).

Current research has been limited to steady flow, steady voltage (SFSV) experiments so that a better understanding of the underlying principles at work in EHD atomization can be achieved. However, work such as the experimental results of Kourmatzis and Shrimpton (2011) show that charge injection methods with steady flow, pulsed voltage (SFPV) behaves similar to SFSV systems. This means the previous work and results for SFSV can be applied to SFPV, with the eventual goal of using charge injection to improve fuel efficiencies in small engines as well as engines burning bio-oils, both of which will require pulsed flow, pulsed voltages.

Despite the many advancements in understanding how EHD atomization works such as the fact that “the charge injection mechanism is electro chemical in nature.” (Shrimpton and Yule, 2003), and that SFSV results can be applied to SFPV

systems, much still remains to be discovered about these processes. Questions such as how the charge is distributed within the liquid/droplets, and what limits the size distribution of the resulting droplets, still need answers. Thus high-fidelity numerical simulations are needed to help researchers understand the underlying principles of EHD atomization (Van Poppel et al., 2010b) and pave the way for more efficient fuel injection systems.

Review Conclusion

In conclusion, the past decade has seen a great advancement in both the understanding of EHD atomization and interest in utilizing it within fuel injection systems. The current research shows that EHD atomization during fuel injection has the potential to improve engine performance for all types of fuel, with an even greater impact on bio-fuel's efficiency. With the use of ever more powerful computers to simulate even the most complex fluid interactions and the general public's interest in adopting bio-fuels over fossil fuels, EHD atomization seems the most promising method to utilize the full potential of renewable bio-fuels.

ATOMIZATION AND SPRAYS INTRODUCTION

Liquid atomization systems are used in a variety of industries, from food processing and storage, to energy conversion and travel. Thus developing techniques for enhancing spray break-up and control are of great interest. One such method that holds great promise is electrohydrodynamic (EHD) assisted atomization (Shrimpton and Laoonual, 2006).

For fuel atomization applications, EHD provides a mechanism to significantly enhance and control the fuel spray. EHD has been shown to be a viable method to control the distribution of droplets within a combustion chamber under realistic direct injection spark ignition conditions (Shrimpton, 2003). Additionally, the recent interest in using biofuels as an alternative to fossil fuels is hindered by the high viscosity (Malkawi et al., 2010) and significant water content (Wang et al., 2012) of biofuels compared to fossil fuels. EHD has the potential to improve the atomization of these fuels compared with standard atomization methods.

EHD is the science of characterizing the interactions between fluid mechanics and electrostatics (Van Poppel et al., 2010a). Investigation into this branch of science began as early as 1882 with Lord Rayleigh's work demonstrating the dynamics of a liquid drop in an electric field (Rayleigh, 1882). Since then, EHD has successfully been used in a variety of engineering applications including inkjet printing (Yudistira et al., 2010), mass spectrometry analysis of biomolecules (Fenn et al., 1989), Taylor cones (Cloupeau and Prunet-Foch, 1994; Gan-Calvo et al., 1997; Hayati et al., 1986; Kim and Turnbull, 1976; Lopez-Herrera et al., 2003; Smith, 1986), microfluidic devices (Cho et al., 2003; Felten et al., 2008; Kazemi et al., 2009; Laser and Santiago, 2004; Velez et al., 2003; Zeng and Korsmeyer, 2004), agricultural sprays (Edward Law, 2001), and fuel atomization (Kim and Turnbull, 1976; Lehr and Hiller, 1993; Romat

and Badri, 2001; Shrimpton, 2003, 2009; Shrimpton and Kourmatzis, 2010; Shrimpton and Yule, 1999, 2001, 2003, 2004; Shrimpton and Laoonual, 2006; Van Poppel et al., 2010a; Yule et al., 1995).

The most popular method of inducing atomization is electrostatic charge injection. This technique uses a highly negative electrode placed in the flow just before the atomizer opening to inject charge through the insulated liquid into the grounded atomizer body (Kourmatzis and Shrimpton, 2011). As the liquid flows out the opening it strips charge from the electrode, so the resulting spray has a negative charge distribution that generates a self-propagating electric field. This field and the electric charges form the Coulomb force, which promotes better dispersion and droplet formation than would occur without EHD.

The distribution of electric charges within an atomizing flow is governed by two main fluid characteristics: the charge advection and charge mobility timescales. The ratio of these timescales, known as the electric Reynolds number (Re_e) (Van Poppel et al., 2010a), 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.

The impact of the electric charge distribution on the atomizing flow cannot be determined a priori due to competing effects. Electric charges influence the flow through the Coulomb force which is given by $F_c = q\mathbf{E}$, where q is the electric charge density of the flow and $\mathbf{E}$ is the electric field. As electric charges relax towards the surface of the liquid due to repulsion, the electric charge density increases as charges accumulate near the interface, but the electric field will decrease as this is a lower energy state. Therefore, it is unclear what the resulting impact on the Coulomb force will be and ultimately how Re_e helps or hinders the break-up of an atomizing jet.

EHD GOVERNING EQUATIONS

For low Mach number, variable density, multiphase flow, conservation of mass and momentum in both phases can be written as

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}_i) = 0, \quad (4.1)$$

and

$$\frac{\partial \rho_i \mathbf{u}_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i) = -\nabla p_i + \nabla \cdot (\boldsymbol{\sigma}_i^f + \boldsymbol{\sigma}_i^e) + \rho_i \mathbf{g}, \quad (4.2)$$

where ρ_i is the density, $\mathbf{u}_i$ is the velocity field vector, t is time, p_i is the hydrodynamic pressure, and $\mathbf{g}$ is the gravitational acceleration. The subscript i can take values of g or l and indicates variables in the gas or liquid phase, respectively. These equations form the basis of this work, further details can be found in the research of Van Poppel and Desjardins.

Looking at the above equations in more detail $\boldsymbol{\sigma}_i^f$ is the viscous stress tensor given by

$$\boldsymbol{\sigma}_i^f = \mu_i (\nabla \mathbf{u}_i + \nabla \mathbf{u}_i^\top) - \frac{2}{3} \mu_i (\nabla \cdot \mathbf{u}_i) \mathbb{I}, \quad (4.3)$$

where μ_i is the dynamic viscosity and $\mathbb{I}$ is the identity tensor. $\boldsymbol{\sigma}_i^e$ is Maxwell's stress tensor

$$\boldsymbol{\sigma}_i^e = \varepsilon_i \mathbf{E}_i \otimes \mathbf{E}_i - \frac{\varepsilon_i}{2} \mathbf{E}_i \cdot \mathbf{E}_i \left(1 - \frac{\rho_i}{\varepsilon_i} \frac{\partial \varepsilon_i}{\partial \rho_i} \right) \mathbb{I}, \quad (4.4)$$

where ε_i is the electric permittivity and $\mathbf{E}_i$ is the electric field vector.

In the previous equations, magnetic affects have been ignored. This is due to the fact that the EHD timescale is orders of magnitude larger than the magnetic timescale (Saville, 1997). This electrostatic assumption implies the electric field is

only affected by the electric charges distributed in the system not the electric charges velocity (current).

The divergence of Maxwell's stress tensor is a body force that highlights the electric effects on the fluid and can be written as

$$\mathbf{f}_i^e = \nabla \cdot \boldsymbol{\sigma}_i^e = q_i \mathbf{E}_i - \frac{1}{2} \mathbf{E}_i^2 \nabla \varepsilon_i + \nabla \left(\frac{1}{2} \rho_i \frac{\partial \varepsilon_i}{\partial \rho_i} \mathbf{E}_i^2 \right), \quad (4.5)$$

where q_i is the volumetric electric charge density. The three terms in the electric body force are the Coulomb (or Lorentz) force, the dielectric force, and the electrostrictive force. The latter two are only important if a transient electric field exists or if the permittivity is spatially varying and have been shown to be negligible for the relevant timescales in atomization problems (Kourmatzis and Shrimpton, 2009).

The electric field vector is irrotational due to the electrostatic assumption and can be expressed as the gradient of the scalar electric potential ϕ_i , i.e.

$$\mathbf{E}_i = -\nabla \phi_i. \quad (4.6)$$

The electric potential is related to the volumetric charge density by

$$-\nabla \cdot (\varepsilon_i \nabla \phi_i) = q_i, \quad (4.7)$$

which is known as the electric potential Poisson equation.

The dynamics of the electric charge density is described by the conservation equation

$$\frac{\partial q_i}{\partial t} + \nabla \cdot \mathbf{J}_i = 0, \quad (4.8)$$

where $\mathbf{J}_i$ is the current density, which can be written as

$$\mathbf{J}_i = q_i \mathbf{u}_i + q_i \kappa_i \mathbf{E}_i - D_i \nabla q_i, \quad (4.9)$$

where κ_i is the ionic mobility coefficient and D_i is the molecular diffusion coefficient. The three terms that contribute to the current density can be described as advection due to the velocity field, advection due to the electrical velocity $\kappa_i \mathbf{E}_i$, and diffusion.

The equations above have been written in both the gas and liquid phases. They are connected through jump conditions at the phase interface. For example, the jumps in density, viscosity, and permittivity at the interface Γ are written as

$$[\rho]_\Gamma = \rho_l - \rho_g, \quad (4.10)$$

$$[\mu]_\Gamma = \mu_l - \mu_g, \quad (4.11)$$

$$[\varepsilon]_\Gamma = \varepsilon_l - \varepsilon_g. \quad (4.12)$$

In the absence of phase change, the velocity field is continuous in the normal direction, i.e. $[\mathbf{u} \cdot \mathbf{n}]_\Gamma = 0$, where $\mathbf{n}$ is the interface normal vector. Analogously to the no-slip assumption, the tangential velocity at the interface is assumed to be continuous and can be written as $[\mathbf{u} \cdot \mathbf{t}_d]_\Gamma = 0$, for $d = 1, 2$. Combining the two jump conditions for the velocity field, it is clear that the velocity is continuous, i.e.

$$[\mathbf{u}]_\Gamma = 0. \quad (4.13)$$

The pressure is discontinuous due to contributions from surface tension, viscous, and electric forces and can be written as

$$[p]_\Gamma = \gamma \kappa + [\mathbf{n}^\top \cdot (\boldsymbol{\sigma}^f + \boldsymbol{\sigma}^e) \cdot \mathbf{n}]_\Gamma, \quad (4.14)$$

where γ is the surface tension coefficient and κ is the interface curvature. The previous equation can be simplified (Van Poppel et al., 2010a) to

$$[p]_\Gamma - 2[\mu]_\Gamma \mathbf{n}^\top \cdot \nabla \mathbf{u} \cdot \mathbf{n} - \gamma \kappa = \frac{1}{2} [\varepsilon (\mathbf{E} \cdot \mathbf{n})^2 - \varepsilon (\mathbf{E} \cdot \mathbf{t}_1)^2 - \varepsilon (\mathbf{E} \cdot \mathbf{t}_2)^2]_\Gamma. \quad (4.15)$$

The electric field is discontinuous if surface charges are present at the phase interface and can be written as

$$\mathbf{n} \cdot [\varepsilon \mathbf{E}]_\Gamma = q_s, \quad (4.16)$$

where q_s is the surface electric charge density. Due to the electrostatic assumption the electric field remains irrotational and $\mathbf{n} \times [\mathbf{E}]_\Gamma = 0$. A consequence of this relation is the tangential component of the electric field and the electric potential are continuous, i.e.,

$$[\mathbf{E} \cdot \mathbf{t}_d]_\Gamma = 0 \text{ for } d = 1, 2, \quad (4.17)$$

$$[\phi]_\Gamma = 0. \quad (4.18)$$

The balance of shear stress at the interface leads to

$$[\mathbf{n}^\top \cdot (\boldsymbol{\sigma}^f + \boldsymbol{\sigma}^e) \cdot \mathbf{t}_d]_\Gamma = 0 \text{ for } d = 1, 2. \quad (4.19)$$

Conservation of charge at the phase interface is described by

$$[\mathbf{J} \cdot \mathbf{n}]_\Gamma + \nabla_s \mathbf{J}_s = (\mathbf{n} \cdot \mathbf{u})[q]_\Gamma - \frac{\partial q_s}{\partial t} - \mathbf{u}_s \cdot \nabla q_s + q_s \mathbf{n} \cdot (\mathbf{n} \cdot \nabla) \mathbf{u},$$

where ∇_s is the surface gradient operator, $\mathbf{J}_s$ is the surface charge current density, and $\mathbf{u}_s$ is the interface surface velocity. The previous equations describe an EHD

influenced gas-liquid incompressible flow. Details on how they are solved numerically is provided in Chapter 6.

CHARGE DISTRIBUTION ANALYSIS

In this chapter an analytical model is used to assess the effect of the electric Reynolds number (Re_e) on the resulting Coulomb force in a simple fluid droplet. The purpose of this initial analysis is to gain an understanding of what to expect in the more complex simulations that follow. Thus the analysis will show how an electrically charged droplet's Coulomb force will vary based upon its charge distribution, which is controlled by (Re_e). This in turn will highlight how droplets form and disseminate in a large fluid jet.

Electric charges within a droplet migrate or relax to the droplet's surface due to charge repulsion (this effect manifests as $q_i \kappa_i \mathbf{E}_i$ in Eq. 4.9). The degree to which the charges relax is determined by the Re_e , which is defined as

$$\text{Re}_e = \frac{\varepsilon_l U}{d \kappa_e q_l} \quad (5.1)$$

or the ratio of the charge convection timescale to the charge mobility timescale. Depending on this ratio different degrees of non-uniformity within the electric charge density will result.

Development

To understand how the Coulomb force is related to the distribution of electric charges and through that the Re_e , an analytical analysis was performed. The models were defined such that the charge distribution was axisymmetric and that the total electric charge was a constant between different models, only the radial distribution of electric charge was varied inside the droplet.

The three models analyzed were a constant, linear, and Gaussian electric charge distribution. The constant distribution assumes the charge distribution is constant in the radial direction inside the droplet, while the linear distribution lets the charge distribution increase with the radius. The Gaussian distribution varies the charge based on a Gaussian curve in the radial direction of the droplet. These three models replicate the evolution of the charge distribution in time. Assuming a droplet initially has a constant charge distribution, as time progresses the charges will relax towards the surface, which is approximated with the linear and Gaussian distributions.

From Eq. 4.5 and using the assumptions mentioned above, the Coulomb force as a function of radius is given by

$$\mathbf{F}_c(r) = q(r)\mathbf{E}(r), \quad (5.2)$$

where r is the radial coordinate. The electric field $\mathbf{E}$ depends on the electric charge distribution and can be computed using Eqs. 4.6 and 4.7. Note that for an axisymmetric problem, the equations simplify considerably, leading to

$$\frac{1}{r} \frac{\partial(r\epsilon_i \mathbf{E})}{\partial r} = q, \quad (5.3)$$

which can be integrated to obtain $\mathbf{E}$.

For the constant charge distribution case, q was set equal to a constant A within the droplet and zero outside, giving the following equation for the electric field:

$$E = \begin{cases} \frac{A}{2\epsilon_i} r & 0 \leq r \leq R \\ \frac{AR^2}{2\epsilon_i r} & R < r < \infty \end{cases} \quad (5.4)$$

where $A = 1$. R is the radius of the droplet and is also set to 1 for simplicity as was ε_i for all cases. Substituting the results of Eqs. 5.4 back into Eq. 5.2 along with the q for the constant charge density model gives the following Coulomb force:

$$F_c = \frac{A^2}{2\varepsilon_i} r \quad (5.5)$$

for $0 \leq r \leq R$.

The linear charge distribution was given by $q = mr + b$ within the droplet and zero outside, which when substituted into Eq. 5.3 and integrated yields:

$$E = \begin{cases} \frac{m}{3\varepsilon_i} r^2 + \frac{b}{2\varepsilon_i} r & 0 \leq r \leq R \\ \frac{m}{3\varepsilon_i r} R^3 + \frac{b}{2\varepsilon_i r} R^2 & R < r < \infty \end{cases} \quad (5.6)$$

Following the same procedure as was used for the constant case, Eq. 5.6 is substituted back into Eq. 5.2 to produce the linear Coulomb force:

$$F_c = \frac{m^2}{3\varepsilon_i} r^3 + \frac{5mb + 3b^2}{6\varepsilon_i} r^2 \quad (5.7)$$

The constants $m = \frac{1}{2}$ and $b = \frac{2}{3}$ were chosen so that the total electric charge inside the droplet for all distributions were equal.

The Gaussian charge distribution was set to $q = Ce^{-\frac{(x-R)^2}{2d^2}}$. Substituting this into Eq. 5.3 and integrating gives:

$$E = \begin{cases} \frac{1}{r} \left(C d^2 \left(e^{-\frac{R^2}{2d^2}} - e^{\frac{Rr}{d^2} - \frac{r^2}{2d^2} - \frac{R^2}{2d^2}} \right) + \frac{C \sqrt{\pi} R \left(\operatorname{erfi} \left(R \sqrt{-\frac{1}{2d^2}} \right) + \operatorname{erfi} \left(-\sqrt{-\frac{1}{2d^2}} (R - r) \right) \right)}{2 \sqrt{-\frac{1}{2d^2}}} \right) & 0 \leq r \leq R \\ \frac{1}{r} \left(\frac{0.8862 C \operatorname{erfi} \left(\sqrt{-\frac{1}{2d^2}} \right)}{\sqrt{-\frac{1}{2d^2}}} - C d^2 \left(1 + e^{-\frac{1}{2d^2}} \right) \right) & R < r < \infty \end{cases} \quad (5.8)$$

Following the same procedure as was used for the previous cases, Eq. 5.8 was substituted back into Eq. 5.2 to produce the Gaussian Coulomb force:

$$F = \frac{C e^{-\frac{(R-r)^2}{2d^2}}}{r} \left(C d^2 \left(e^{-\frac{R^2}{2d^2}} - e^{\frac{Rr}{d^2} - \frac{r^2}{2d^2} - \frac{R^2}{2d^2}} \right) + \frac{C \sqrt{\pi} R \left(\operatorname{erfi} \left(R \sqrt{-\frac{1}{2d^2}} \right) + \operatorname{erfi} \left(-\sqrt{-\frac{1}{2d^2}} (R - r) \right) \right)}{2 \sqrt{-\frac{1}{2d^2}}} \right) \quad (5.9)$$

For both Eqs. 5.8 and 5.9, erfi is the imaginary error function defined by $\operatorname{erfi}(z) = -i \operatorname{erf}(iz)$ and the constants $C = 1.4614$ and $d = 0.4$ were chosen so that the total electric charge inside the droplet for all distributions were equal.

Results

The results of the analytic analysis are shown below in Fig 5.1. This figure showcases how differences in the electric charge distribution affect both the radial electric field and Coulomb force inside the droplet. From Fig. 5.1(c) we can see

Figure 5.1: Dashed, solid, and dotted lines correspond to the constant, linear, and Gaussian charge distributions, respectively. Plots are of the axisymmetric droplet interior.

that while the constant charge distribution has the largest Coulomb force on the interior of the droplet, the linear and Gaussian charge distributions have a greater magnitude near the droplet interface, with the Gaussian being larger than the linear distribution. Using these three models it can be inferred that the electric charges move into distributions with lower overall energy, as seen by Fig. 5.1(b) where the Gaussian model has the lowest over all electric field. However, the Gaussian model also has the maximum Coulomb forces near the droplet interface. Thus the different charge distributions affect the resultant Coulomb force within the droplet, which in turn will affect the degree of atomization.

As the charge distributions are dependent on the Re_e , through charge mobility, a relationship between the resultant atomization quality and the Re_e of a fluid flow has been demonstrated. This analysis suggests that smaller Re_e will lead to more charge relaxation, larger Coulomb forces near the droplet interface, and potentially enhanced atomization. However, the lower Coulomb force in the center of the droplet may result in a coherent liquid core that remains after the initial dramatic atomization.

NUMERICAL METHODS

The numerical simulations of EHD flows in this paper are conducted using the NGA computational platform (Desjardins et al., 2008a), with the EHD framework based on work by Van Poppel et al. (2010a). Their framework used a bulk electric charge density within the liquid, due to challenges transporting the discontinuous quantity. Here we extend the methods and allow for charge mobility by solving Eq. 4.8. Transport of the discontinuous charge density is performed using a semi-Lagrangian geometric scheme (Owkes and Desjardins, 2014a).

Geometric routines are used to transport the volume-of-fluid (VOF) representation of the phase interface, momentum, and electric charge density near the interface, insuring discrete consistency. Additional details of the application of the geometric method to EHD problems is provided by Owkes and Desjardins (2014b). The spatial discretization away from the interface is performed using second order, fully conservative finite difference operators staggered in both space and time. This approach conserves mass, momentum, and electric charge density and has been shown to be well suited for simulations of turbulent flows (Desjardins et al., 2008b).

The pressure jump and density discontinuity at the interface are handled sharply using the ghost fluid method (GFM) (Fedkiw et al., 1999). The GFM is also used to capture the discontinuous electrostatic properties and electric field jump conditions as described by Van Poppel et al. (2010a). The discontinuity in pressure due to the surface tension force is computed using the mesh-decoupled height function method that is well suited for atomizing flows (Owkes and Desjardins, 2015). The discontinuous viscosity is handled using the height fraction method (Sussman et al., 2007).

The electric field depends on the boundary conditions as well as the distribution of electric charge within the domain. The electric potential Poisson equation, Eq. 4.7, provides a relation between the electric charge density q_i and the electric potential ϕ_i . The potential is related to the electric field by Eq. 4.6, the electric potential equation, which is solved using a parallelized black box multigrid solver (Dendy, 1982). This is the same Poisson solver used to solve the pressure Poisson equation.

Description of Cases

As suggested earlier by the simple droplet analytic models, the atomization quality of an EHD spray is partially dependent on the electric charge distribution within the fluid and spray during atomization, which is influenced by the Re_e . To gain a better understanding of the degree to which the Re_e effects atomization quality for a fluid flow, three different EHD assisted atomization cases were studied where the Re_e was varied and all other properties were held to constants that match experiments run by Shrimpton and Yule (2001). The values of the dimensionless numbers and fluid parameters used to describe the simulated fluid are provided in Tables 6.1 and 6.2. It should be noted that the dimensionless parameters and properties from these tables define the fluid jet before atomization. Table 6.3 lists the specific Re_e values for each case, along with the charge mobility (κ_l) and molecular diffusivity (D_l). The ε_o term from Table 6.2 is the permittivity of free space. In addition, these tables also depict the domain size which was discretized on a 512 x 256 x 256 mesh with the VOF scheme utilizing a twice as fine mesh (1024 x 512 x 512). The domain geometry is shown in Fig. 6.1.

Charging of the liquid was not studied in these simulations as the focus was on the atomization of the spray. The inflow electric charge distribution condition was therefore approximated as a turbulent pipe flow with a constant volumetric charge

Figure 6.1: Geometry for the three-dimensional simulations. Parameters are given in Tables 6.1 and 6.2.

distribution. Thus the varied Re_e value will only effect the flow after the fuel has exited the injector nozzle. This framework was successfully used by Owkes and Desjardins (2014b) who compared their simulation results with experiments by Shrimpton and Yule (2001).

Table 6.1: Dimensionless numbers for simulations (Shrimpton and Yule, 2001).

Number	Sym.	Definition	Value
Bulk Reynolds	Re	$\rho_l U d / \mu_l$	4000
Bulk Weber	We	$\rho_l U^2 d / \gamma$	1700
Electro-inertial	N_{ei}	$q_l^2 d^2 / (\varepsilon_l \rho_l U^2)$	0.04
Electric Reynolds	Re_e	$\varepsilon_l U / (d \kappa_l q_l)$	Varied
Electric Peclet	Pe_e	$q_l \kappa_l d^2 / (D \varepsilon)$	17308
Density ratio	-	ρ_l / ρ_g	664
Viscosity ratio	-	μ_l / μ_g	51
Permittivity ratio	-	$\varepsilon_l / \varepsilon_g$	2.2
Domain length	-	L / d	16
Domain height	-	H / d	8
Domain width	-	W / d	8

While running the simulations described above for this research on High Performance Computer (HPC) clusters, it was discovered that not all the processors assigned to the simulation were being utilized fully during the flux calculations. This instigated a tangential research direction to understand the cause, and potentially address the load imbalance that causes inefficiencies in the NGA code.

Table 6.2: Parameters used in simulations (Shrimpton and Yule, 2001).

Parameter	Def.	Units	Value
Mean velocity	U	m/s	10
Injector diameter	d	μm	500
Liq. density	ρ_l	kg/m^3	800
Gas density	ρ_g	kg/m^3	1.2
Liq. viscosity	μ_l	$\text{kg}/\text{m}\cdot\text{s}$	1.00E-3
Gas viscosity	μ_g	$\text{kg}/\text{m}\cdot\text{s}$	1.98E-7
Surface tension	γ	N/m	0.0235
Bulk electric charge density	q_l	A/m ³	1.35
Liq. rel. permittivity	$\varepsilon_l/\varepsilon_o$	-	2.2
Gas rel. permittivity	$\varepsilon_g/\varepsilon_o$	-	1.0
Liq. molecular diff.	D_l	m ² /s	Varied
Liq. ionic mobility	κ_l	m ² /V·s	Varied

Table 6.3: The Electric Reynolds number and varying parameters for the three test cases.

Case	Re_e	κ_l (m ² /V·s)	D_l (m ² /s)
I	288	1E-9	1E-9
II	28.8	1E-8	1E-8
III	2.88	1E-7	1E-7

LOAD BALANCING

To understand the cause of the simulation inefficiency, the differences in the methods used to calculate the fluxes on the domain mesh must be understood. The NGA code uses two different methods in these calculations, depending on the location of the liquid-gas interface within the mesh. If a mesh cell contains the interface, then that cell will need to use a semi-Lagrangian method (SLF) to calculate the fluxes on that grid, otherwise a finite difference (FD) method is used.

This is where the processor inefficiency is rooted, as the SLF method is computationally expensive while the FD method is not. Thus the time it takes a processor to calculate the fluxes using the SLF method is significantly longer than the time for the same processor using the FD method. To highlight how this inhibits the flux calculations during a simulation, a simple example domain is shown in Fig. 7.1, the red line denotes the interface between the liquid (blue) and gas (gray), while the green lines denote the distribution of the mesh across the assigned four processors. From this figure it can be seen that processors 3 and 4 have no SLF fluxes to calculate, while processors 1 and 2 have three and two respectively. Thus, processors 3 and 4 will finish their flux calculations and then be forced to wait for processors 1 and 2 to catch up. This unbalanced loading of work on the assigned processors is the cause of the simulation inefficiency.

Balancing Method

To address this issue, the amount of work (i.e. SLF needing calculation) can be distributed across all processors such that each processor has approximately the same number of SLF to calculate. This idea is implemented by first predicting the distribution of work across all assigned processors, using the location of the interface,

Figure 7.1: Simple 4x4x1 mesh example domain discretized on 4 processors.

and then ordering the results by the amount of work they need to calculate from least to largest. The resultant array of processors is then used to assign the processors into pairs with one of the pairs having a large amount of work (denoted as Primary) and the other having a lesser amount of work (denoted as Worker). In each of these pairs, the amount of SLF needing to be calculated will be balanced by taking data from the Primary and sending it to the Worker processor such that the Worker can calculate enough of the Primary's SLF to mean both processors have approximately the same amount of work.

To understand how this method works, it can be applied to the example domain of Fig. 7.1, resulting in Fig. 7.2. In this figure the Primary-Worker pairs are processor 1 with processor 3, and processor 2 with processor 4. After balancing the work, all processors have at least one SLF to calculate, with processor 1 having two.

Figure 7.2: Balanced example domain.

Results

In order to test the efficacy of the above balancing method, a simple simulation was created utilizing a domain split across two processors. Half the domain was filled with liquid-gas interface, while the other was left empty as shown in Fig. 7.3. This interface is transported across the domain, so at times load balancing will be beneficial as the interface will be concentrated on one processor, while at other times load balancing will not be needed as the interface is evenly distributed across both processors. The purpose of this non-realistic simulation is to compare the load balancing method with the original unbalanced flux calculations. Thus this ideal test case will highlight the load balancing benefits.

To accurately test all aspects of the load balancing method, three different variations of the flux calculation code were used to calculate the above test simulation.

Figure 7.3: Ideal load balancing simulation on two processors.

These were the regular unmodified code, the new code utilizing the load balancing method, and code comprising of just the framework required to connect the regular code to the load balancing code. The last variation does not contain the load balancing method, and is used to test that the framework will not impact the resultant calculation time. The results of these code variation tests are shown in Fig. 7.4.

From this figure it appears that the load balancing code is slower than the regular code. In addition, the figure also shows that the framework, upon which the load balancing method was connected to the regular code, is significantly slower than the regular and load balanced codes. The reason for this is due to the programming methods used to implement the load balancing method into the flux calculations, i.e. the framework.

To facilitate the calculation of data on the Worker processors, pointer variables were used to distinguish between Worker and Primary data. As pointers can be directed to connect to different variables, the flux calculations would not need to be duplicated for the Worker and Primary data. The calculations could simply be run on

Figure 7.4: Balancing Test results.

the pointer variables, which could be directed towards the Worker and then Primary's data. However, the NGA code is written in the Fortran programming language, and pointers are not efficiently implemented in Fortran, which was not discovered until reviewing the results of Fig. 7.4. This means the framework and load balancing codes' slow calculation time is mostly due to the use of pointers.

With this understanding, a closer examination of Fig. 7.4 shows that while the load balanced code is utilizing the framework, it is still faster at each time step than said framework by about 25 %. This implies that the load balancing method has a significant impact on the calculation time for each iteration, despite the use of pointers. If the framework was improved by optimizing the load balancing functions and removing the need for pointer variables, the load balancing method could potentially speed up the calculation time of the regular code by 25 %, meaning the average calculation time would decrease from 1.7 to 1.3 seconds per

iteration. Thus, the load balancing theory has been shown to be sound, but the author's implementation of it was not. Due to time constraints, correcting the above highlighted issues with the tangential research into work distribution must be left to future investigations.

RESULTS

This section presents the results of the EHD simulations for the three cases discussed in Chapter 6 using the geometry defined in Fig. 6.1. Snapshots of Case II's atomization progression with time are shown in Fig. 8.1 where the PLIC representation of the gas-liquid interface is presented. A comparison of all cases at the analyzation time point of $450 \mu s$ is shown in Fig. 8.2, and Fig. 8.3 provides the three cases at $635 \mu s$.

Figure 8.1 shows how the jet atomizes due to EHD effects. The jet is initially a single coherent structure, then ligament and droplets start forming along the sides of the central core. The ligaments and droplets continue to form until the jet has filled the domain. Figure 8.2 compares the cases at $450 \mu s$ when statistics were computed. Case III has significantly more droplets and ligaments than either Case I or II, which is consistent with the simple droplet analysis of Chapter 5.

Figure 8.3 provides insight into the long time break-up of the central core. At $635 \mu s$, many droplets have interacted with the domain boundaries, but the core dynamics are likely still accurate. We see that Case III still has the most droplets pulling away from the main flow body as compared with with Case I & II. However, both Case I & II are starting to show more break-up effects, with a larger amount of ligaments forming along the jet as well as “holes“ forming where the the core's are pulling apart, as compared to Fig. 8.2.

Atomization Results

Figures 8.4 to 8.7 showcase the effect of Re_e on the droplet statistics, charge distribution, electric field magnitude, and Coulomb force at $450 \mu s$. This time

Figure 8.1: Gas-liquid interface for Case II at different times

Figure 8.2: Gas-liquid interface at 450 μs

was chosen because the jets have undergone significant deformation but have not significantly interacted with the boundary of the simulated domain.

Figure 8.4 compares the mean droplet diameter ($\overline{D}$), mean droplet Weber number ($\overline{We}$), and droplet concentration in the radial direction for each case. For Case III at 450 μs , some of the droplets hit the boundary of the computational domain, these were removed from the analysis. The mean droplet $\overline{We}$ is defined as $\overline{We} = \frac{\rho_l U_r^2 \overline{D}}{\gamma}$, where U_r is the magnitude of the radial droplet velocity ($U_r = \sqrt{v^2 + w^2}$) with v and w being the y and z velocity components. The $\overline{We}$ is a measure of a fluid's, in this case droplet's, inertia to surface tension. Comparing all three cases in Fig. 8.4(a) shows that most droplet diameters are between 10 and 20 μm . Cases I and II have some small deviations from this mean, but the number of droplets recorded for these cases, as shown in Fig. 8.4(c), are quiet low so it is understandable why there is a

Figure 8.3: Gas-liquid interface at 635 μs

small amount of variation. This also explains why Case I has more noise as compared to Cases II and III.

Figure 8.4(b) shows that as the Re_e decreases with each case, the magnitude of the droplet $\overline{We}$ increases. As $\overline{D}$ for each case is approximately the same (Fig. 8.4(a)) as is the surface tension (γ) and fluid density (ρ_l), only the velocity of the droplets changes. This is likely due to Re_e decreasing for each case, meaning more electric charges can concentrate at the boundary before droplets are formed and pulled away from the main jet. These droplet would then have higher charge densities, and feel a larger force, giving them a higher velocity. From these figures it can be seen that the size of the droplets created by EHD is relatively unaffected by Re_e , but the number of droplets created as well as their dissemination and inertia is highly dependent.

Figure 8.4: Solid, dashed, and dotted lines correspond to Cases I-III, respectively.

Charge Distribution Results

The electric charge distribution for the three cases is shown in Fig. 8.5. Comparing these figures shows a definite variation between Cases I and III. In Case III there are significantly more interface corrugations than Case I, with most of Case III's charge being concentrated near the interface and away from the center of the jet. In contrast, Case I seems to have a relatively uniform charge distribution with little to no droplets or ligaments forming. Case II shows similarities to both Case I and III, with a mostly uniform charge distribution along the jets core similar to Case I, but having slightly more charge concentrated near the interface similar to Case III.

Electric Field Results

Looking at the electric field results in Fig. 8.6 we see Case I and II have very similar electric field magnitudes. Case III has a significantly lower magnitude everywhere except near the jet base where it approaches the same values as Case I and II. These results are as expected due to the fact that Case's I and II have significantly more uniform charge distributions than case III, and that a large portion of Case III's charge has been distributed into the droplets surrounding the jet as shown in Fig. 8.5.

Coulomb Force Results

Figure 8.7 shows the effect different Re_e values have on the Coulomb force. As with the charge distribution results of Fig. 8.5, Case III shows much higher concentrations of Coulomb force in Fig. 8.7(c) than what is shown in Fig. 8.7(a) and 8.7(b) for Cases I and II. In addition, the Coulomb force on the interior of Fig. 8.7(c) shows significantly lower magnitudes than what is seen in Fig. 8.7(a) and

Figure 8.5: Plots of the electric charge density (C/m^3) on an x-y plane through the jet center at $450 \mu s$.

Figure 8.6: Plots of the electric field magnitude distribution. (N/C) on an x-y plane through the jet center at $450 \mu s$.

8.7(b), implying that most of the Coulomb force felt by the flow is at the interface. For Cases I and II the distribution of the forces appears very similar except that the interface of Fig. 8.7(b) seems slightly darker, meaning a higher concentration, than seen in Fig. 8.7(a), especially along the main flow body.

Figure 8.7: Plots of the Coulomb force density (N/m^3) on an x-y plane through the jet center at $450 \mu s$.

CONCLUSION

This paper studies the effect Re_e plays on EHD atomization quality. Having a greater understanding of EHD atomization would allow more efficient systems to be designed and utilized in commercial and industrial applications. Thus several numerical simulations were run to study an atomizing EHD jet with varying levels of Re_e .

The results of these simulations show that Re_e has a controlling influence on the resulting Coulomb force of an EHD atomization as well as the droplet concentration and inertia. Specifically, Re_e dictates how the electric charges will be distributed inside the fluid, which in turn dictates how the Coulomb force magnitude will be distributed throughout the atomizing liquid. From comparison of the results we can see that high concentrations of Coulomb force at the interface means the fluid will atomize faster. This takes the form of ligaments and droplets at the interface, which pull the jet apart forming “holes“ through the central core. These high Coulomb force concentrations are the result of low Re_e values. Thus methods for decreasing the Re_e of the fluid to be atomized will be helpful in improving the break-up of an atomizing jet.

Future Work

However, before atomizer designs can be created to utilize the results of this work, the charging mechanisms inside the nozzle must be understood. For example, sufficiently low Re_e may reduce the efficiency of charge injection into the liquid. In the worst case scenario, this could mean electric charges are unable to be injected into a fluid with a low Re_e . Thus future work on this subject will require investigation into the dynamics within the atomizing nozzle.

Once the affects of low Re_e on the charging mechanisms are understood, further work can combine Re_e effects with pulsed flow and voltage to simulate the results of using EHD atomization on an engine fuel injector. The idea being that the Re_e would be used to help predict how the spray will spread after atomization. Thus if the fuel Re_e is known, the injector nozzle can be designed with EHD and atomization affects in mind to produce an optimal spray for achieving the correct fuel to air ratio in an engine.

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