Characterization of Droplet Flight Path and Mass Flux in Droplet-Based Manufacturing

by

Godard Karl Abel

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Submitted to the Department of Mechanical Engineering on May 18, 1994 in partial fulfillment of the requirements for the Degree of Master of Science

ABSTRACT

In this study, the droplet flight path and the mass flux in the Uniform Droplet Spray Forming (UDS) process are characterized through numerical simulation and experiments. In the UDS process electrically charged uniform diameter metal droplet sprays are used to spray form deposits onto stationary and moving substrates. A numerical simulation based on physical models was developed to predict the droplet velocity, the droplet spray cone spreading, the mass flux distribution in the spray, and the cross-sectional shapes of deposits spray formed with a moving substrate.

To verify the numerical simulation results experiments were performed to measure the droplet charging, the droplet velocity, the droplet scattering, and the deposit cross-sectional shapes. The charging and scattering experiments were performed with 200μm diameter Sn droplets. The velocity was measured as a function of flight distance for 95μm and 200μm diameter Sn droplets. The deposit cross-sections were measured for 200μm diameter Sn-40%Pb sprays collected at a flight distance of 300mm and for 200μm diameter Sn-5%Pb droplets at a flight distance of 480mm. The experimental results agreed with the simulation results to within approximately 10% for the charging, velocity, and scattering experiments. There was a larger discrepancy between the shape of cross-sectional deposits due to variations in the process and the impact behavior of the droplets. This numerical simulation can be used to predict droplet flight path and mass flux for single and multiple orifice sprays.

Thesis Supervisor: Jung-Hoon Chun

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Chapter 1
Introduction

This study focuses on the droplet flight path of metal droplets and the resultant mass flux in Droplet Based Manufacturing (DBM). There are many potential applications for DBM processes, and this study concentrates on the Uniform Droplet Spray Forming (UDS) process, which was developed at MIT [Passow, 1992]. UDS is based on uniform metal droplet sprays, in which a laminar jet of molten metal is broken up into electrically charged uniform diameter metal droplets [Passow, 1992]. This study is an extension of the initial work done by Passow. A numerical simulation of the process based on a physical model has been developed. The numerical simulation results are compared to experimental results for the droplet spreading and velocity as a function of flight distance. In addition experimental work to determine the geometry of deposits spray formed on a moving substrate has been completed, using the new UDS spray forming apparatus developed by Bhatia [Bhatia, 1993]. In this introduction the process is described in more detail, the background for studies of charged particle trajectories is given, and the goals and motivation for this study are outlined.

1.1 Uniform Metal Droplet Sprays

The UDS process applies the concept of laminar jet instability commonly used in the continuous ink jet printing process, but it incorporates major modifications to spray molten metals. A basic UDS apparatus is shown schematically in Figure 1.1.
Figure 1.1: Schematic drawing of a basic UDS apparatus used to produce uniform droplet metal sprays [Passow, 1992]
The first step in the UDS process is to melt the metal by applying heat to a crucible containing the metal. Then pressure is applied to the crucible to force molten metal through an orifice at the bottom of the crucible to thereby form a jet of molten metal. The jet is then broken up into uniform droplets by vibrating a disk which is immersed in the molten metal near the orifice. The vibrations are created by a piezo-electric transducer crystal, which vibrates at a set frequency, and the vibrations are transmitted from the piezo-electric transducer to the disk by a shaft. This creates a sufficient disturbance to break up the jet at the desired frequency. This frequency can be used to control droplet diameter. At the point where the jet breaks up into droplets, a negative electric charge is applied to each droplet so that the droplets will repel each other during flight, preventing the droplets from merging further down in the stream.

The primary advantage of the UDS process over conventional spray forming and thermal spray techniques is that the droplets all have the same diameter and therefore have approximately the same velocity and thermal state when they reach the substrate. This makes them much easier to characterize and control than non-uniform droplet sprays.

Currently, we have the ability to create uniform molten metal sprays with droplets with diameters between 75-750\(\mu\)m. The metals and alloys that we can spray include metals with melting points below 1100\(^\circ\)C such as Sn, lead, indium, zinc, aluminum, and bronze [Abel, 1993]. There are many potential industrial applications for Droplet Based Manufacturing processes including the following:
production of uniform diameter metal powders, spray coating, and spray forming three-dimensional parts. This study will be applicable to any of these applications, but it focuses on Uniform Droplet Spray Forming as is shown in Figure 1.2.

**Figure 1.2:** Schematic representation of uniform metal drop spray forming (UDS) on a rotating substrate [Chun, 1992].
1.2 Background on Droplet Flight Path Models

A lot of research has been done in the field of spray forming to characterize the droplet flight path and mass flux of metal droplets in spray forming. Both Mathur et. al. [1988] and Gutierrez-Miravete et. al. [1981] developed models that predict the in-flight behavior of individual droplets. In conventional spray forming gas atomization is used so that the metal droplets have a large variation in diameter and as a result both models are based on an empirically derived distribution of droplet sizes and spray density. The velocity fields of these droplets were then either empirically or computationally determined for a distribution of droplet sizes.

Passow [1992] created a model and numerical simulation for uniform droplet sprays, which takes advantage of their uniform diameter and velocity profiles. This model was used as a starting point for this study.

Other work has been done in characterizing charged droplet sprays in areas outside of metal sprays. For example, Fillmore et al. [1977] studied extensively the behavior of charged droplets in an ink jet printer. Their work focused on the deflection of the droplets using a deflection plate. However, since their work was limited to flight distances of less than 30 mm as is used in ink jet printing, and it did not extensively consider the scattering caused by the electronic repulsion of droplets.

Crowley [1967] derived an analytical expression to characterize the lateral instability in a stream of charged droplets and predicted the growth rate of the transverse disturbance as a function of the initial disturbance. Snarski and Dunn [1991] characterized the
interaction between two sprays of electrically charged liquid droplets in electrically charged ethanol droplet sprays that were generated electrohydrodynamically.

1.3 Motivation and Goals

The motivation for this study is to improve the characterization of uniform droplet flight paths and mass flux, so that the simulation can be used as a design tool for laboratory experiments and industrial spray forming systems. This simulation is one part of the software being developed in our laboratory. Eventually it will be combined with a non-equilibrium droplet solidification model and used as an input for a substrate solidification model. The goal is to have a complete simulation of the uniform droplet spray forming process that will determine the deposit geometry and microstructure. Simulation will allow a quick and inexpensive way to test different spray parameters and to optimize the process.

The droplet flight path is crucial in that it influences many other spray forming parameters which ultimately determine deposit geometry and microstructure. The droplet flight path determines the mass flux in the spray and the velocity of the droplets. The droplet velocity affects the cooling rate of the droplets and their resulting thermal state. The velocity on impact and the droplet thermal state will control the impact behavior of the droplets. By combining the mass flux distribution and the thermal state of the droplets, the enthalpy influx on the substrate can be calculated. The enthalpy influx, when combined with the droplet morphology, determine the microstructure of the deposit. The mass flux distribution in the
spray and the impact behavior of the droplets. When combined with the motion of the substrate predicts, control the geometry of the deposit. By combining this simulation of droplet flight path with a droplet impact and deposit solidification simulation, it is possible to predict both the geometry and microstructure of the uniform droplet spray formed deposits.

The goals for this study are to produce an accurate simulation of the droplet flight path and mass flux based on physical models of the process. The simulation's aim is to accurately predict droplet velocities, droplet spreading, mass flux in the spray, and the shape of deposits on a moving substrate.

1.4 Outline of Study

In the next chapter, the basic physical models of the UDS process used in the simulation are described. In Chapter 3, the numerical simulation is described in more detail, and the results from the simulation are shown. In Chapter 4, the experiments performed to verify the simulation are described, and the experimental data are compared to the simulation. Discrepancies between the model and the simulation are also discussed. In the final chapter, conclusions about this study are made, and recommendations for future work are given.
Chapter 2

Physical Models of Uniform Droplet Sprays

In this chapter the basic physical models of the process are described. The parts of the process that are modeled are the stream break-up, the droplet charging, the droplet flight path, and the thermal state of the droplets.

2.1 Break-up of Laminar Jet into Uniform Droplets

The break-up of a laminar jet into an aligned stream of uniform droplets is shown in Figure 2.1. A laminar jet breaks up into uniform droplets if a perturbation is applied at the correct frequency. The wavelength of the stream break-up, \( \lambda_d \), is equal to the spacing between the droplets. This distance is equal to the initial jet velocity, \( v_j \), divided by the frequency of the disturbance, \( f \), imposed on the jet:

\[
\lambda_d = \frac{v_j}{f}
\]

The Rayleigh frequency for the spontaneous break-up of a laminar jet, \( f_s \), into uniform droplets is given by the following relationship [Passow, 1992]:

\[
f_s = \frac{v_j}{\lambda_m} = \frac{v_j}{4.51 \ d_j}
\]

where \( \lambda_m \) is the wavelength at which the disturbance grows most rapidly and \( d_j \) is the diameter of the laminar jet. This diameter is assumed to be equal to the orifice diameter. When disturbed at this
frequency, a laminar jet should break up into uniform droplets. Passow found that for metal droplets, uniform droplets could be produced over a range of wavelengths from approximately 3.2 to 10.2 times the jet diameter for a 100μm jet, and 5.4 to 10.5 times the jet diameter for a 50μm jet [Passow, 1992].

The initial velocity of the jet is found from the following relationship:

\[ v_j = k_f \sqrt{P_{\text{driving}}} \]  \hspace{1cm} (2.3)

where \( P_{\text{driving}} \) is the pressure differential between the crucible and the spray chamber, and \( k_f \) is an experimentally determined orifice friction coefficient. For a 100μm orifice \( k_f \) equals 9250 Pa·s\(^2\)/m\(^2\), and for 45μm diameter orifice \( k_f \) equals 9500 Pa·s\(^2\)/m\(^2\) [Passow, 1992].

The diameter of the droplets, \( d_d \), is determined by the volume flow rate of the jet and the disturbance frequency. The volume flow rate is equal to the mass flow rate, \( \dot{m} \), divided by the density of the metal, \( \rho_m \):

\[ d_d = \left( \frac{6 \dot{m}}{\pi \rho_m \rho_f} \right)^{1/3} = \left( \frac{6 A_j \lambda_d}{\pi} \right)^{1/3} \]  \hspace{1cm} (2.4)

The droplet diameter can also be found by determining the volume of each drop, which equals the cross-sectional area of the jet, \( A_j \), of the jet break-up wavelength, \( \lambda_d \).
Figure 2.1: Schematic diagram of uniform droplet generation and charging.
2.2 Droplet Charging

2.2.1 Round Charging Cell

In order to prevent the metal droplets from merging in flight, the droplets are all charged electrically, as is shown in Figure 2.1. A charge cell is placed in the region where the droplets break away from the jet and is kept at an electric potential between 250-1000V. The melt is grounded, and the jet is in contact with ground until it breaks into uniform droplets. The grounded jet and the voltage charge cell act as two plates of a capacitor, and as the droplets break off, they all carry an equal induced charge.

To determine the amount of charge per droplet, the jet can be modeled as a continuous line of charge, and one can derive the capacitance per unit length of the jet. The electric field, $E$, around a line of charge is given as [Cheng, 1983]:

$$E = \frac{q'}{2 \pi \varepsilon_0 r}$$  \hspace{1cm} (2.5)

where $q'$ is the charge per unit length, $\varepsilon_0$ is the permittivity of free space, and $r$ is the distance from the line of charge. The potential difference for a cylindrical capacitor can be found by integrating the electric field from the surface of the jet to the electrode. This potential difference, $V$, equals:

$$V = \frac{q'}{2\pi \varepsilon_0} \ln \left( \frac{d_c}{d_j} \right)$$  \hspace{1cm} (2.6)

where $d_c$ and $d_j$ are the diameter of the charge cell and the diameter of the jet, respectively. For any capacitor, the capacitance
equals the charge, \( q \), over the potential difference \( V \). The capacitance per length, \( C' \), is equal to:

\[
C' = \frac{q'}{V}
\]  
(2.7)

The capacitance per unit length for a cylindrical capacitor is therefore equal to:

\[
C' = \frac{2\pi \varepsilon_0}{\ln \left( \frac{d_c}{d_j} \right)}
\]  
(2.8)

The charge per droplet is equal to the charge per length times the wavelength of the droplet break-up:

\[
q_d = C' \lambda_d V = \frac{2\pi \varepsilon_0}{\ln \left( \frac{d_c}{d_j} \right)} \lambda_d V
\]  
(2.9)

As Passow [1992] has shown this is an accurate predictor of the charge per droplet for a cylindrical charging cell.

2.2.2 Parallel Plate Charging

For a parallel plate charging cell, as shown in Figure 2.2, the capacitance and charging per droplet will be different from the cylindrical charging cell. A parallel plate arrangement has the advantage that one can monitor the stream in the charge cell and there is much less chance of the stream hitting the charge cell. For a parallel plate arrangement, the method of images as shown in Appendix A can be used to find the charge per droplet. Assuming an on-center jet, this results in the following correction factor for a parallel plate arrangement if the charge cell width, \( w_c \), is much greater than the jet diameter, \( d_j \).
\[
q_d = C_i \lambda_d V = \frac{2\pi \varepsilon_0}{0.23 + \ln \left( \frac{w_c}{d_j} \right)} \lambda_d V
\] (2.10)

If the jet is off-center by a distance \(x_j\) in a parallel plate charge cell as is shown in Figure 2.3, the method of images used in Appendix A can be utilized to derive the effect on the droplet charge. The calculated effect on the jet misalignment in the charge cell is shown in Figure 2.4 for a 100\(\mu\)m jet that has been broken into 200\(\mu\)m droplets with a charge cell potential and width of 500V and 7.9mm, respectively. As the jet moves toward one of the cell walls the capacitance and charge per droplet increase parabolically and approach infinity as the jet gets infinitely close to the wall. If the jet strikes the wall, the capacitance and the charge of the droplet go to zero. This effect is more important for narrow charge cells as can be seen in the plot, since even a small change in jet position will have a large effect on the charge.
Figure 2.3: Charging of an off-center jet.

Figure 2.4: The calculated charge per droplet as a function of jet misalignment in a 4.7mm and a 7.9mm wide charge cell.
2.3 Droplet Flight Path

The droplet flight path is determined by the initial velocity of the droplets and the forces imposed by gravity, \( F_g \), electrostatic repulsion between droplets, \( F_C \), and the aerodynamic drag force, \( F_d \). A schematic of the forces acting on the droplet is shown in Figure 2.4.

![Diagram of forces acting on droplets](image)

**Figure 2.4:** Forces acting on the droplets in flight.

The basic equation of motion for the droplets can be written as:

\[
m_d \frac{d\vec{v}_d}{dt} = \vec{F}_g + \vec{F}_d + \vec{F}_C
\]

where \( \vec{v}_d \) is the velocity of the droplet.

The drag force acting on the droplets, \( \vec{F}_d \), can be expressed as:

\[
\vec{F}_d = \frac{1}{8} C_d \pi \rho_m d_d^2 |\vec{v}_d| \vec{v}_d
\]

(2.12)
where $C_d$ is the coefficient of drag, $\rho_m$ is the density of the metal, and $\vec{v}_d$ is the velocity of the droplet. For a droplet in free flight, the coefficient of drag, $C_{d_s}$, is equal to [Mathur, 1988]:

$$C_{d_s} = 0.28 + \frac{6}{\sqrt{Re}} + \frac{21}{Re}$$ \hspace{1cm} (2.13)

where $Re$ is the Reynolds number of the droplet, as given by:

$$Re = \frac{\nu_d d_d \rho_g}{\mu_g}$$ \hspace{1cm} (2.14)

The Coulomb force due to the electrostatic repulsion between two droplets with equal charge $q_d$ at distance $r$ is equal to:

$$F_c = \frac{1}{4\pi \varepsilon_o} \frac{q_d^2}{r^2}$$ \hspace{1cm} (2.15)

Therefore the total Coulomb force acting on droplet $i$ due to its $n$ nearest neighboring droplets is given by:

$$\vec{F}_{Ci} = \frac{1}{4\pi \varepsilon_o} \sum_{j=0}^{n} \frac{q_d^2}{r_{ij}}$$ \hspace{1cm} (2.16)

where $r_{ij}$ is the total distance between the droplets $i$ and $j$. The resultant acceleration of the droplet $i$ in the x-direction is equal to the sum of the drag force in the x-direction and the sum of the x-coulomb forces due its $n$ neighboring droplets.

$$m_d \frac{d^2x_i}{dt^2} = -\frac{1}{8} C_d \pi \rho_m d_d \frac{d^2x_i}{dt} \sqrt{\left(\frac{dx_i}{dt}\right)^2 + \left(\frac{dy_i}{dt}\right)^2 + \left(\frac{dz_i}{dt}\right)^2} + \frac{1}{4\pi \varepsilon_o} \frac{q_d^2}{r_{ij}} \sum_{j=0}^{n} \frac{\Delta x_{ij}}{r_{ij}}$$ \hspace{1cm} (2.17)

where $\Delta x_{ij}$ is the x-distance between the droplets $i$ and $j$. The acceleration in the y-direction is of the identical form. The coefficient of drag can be assumed to be the coefficient for a single
sphere, $C_{D_s}$, since the drag in the $x$ and $y$ directions will not be affected by neighboring droplets. The acceleration in $z$ also has the same form with an additional gravity component.

$$m_d \frac{d^2 z_i}{dt^2} = \frac{1}{8} C_d \pi r_m^2 \frac{d^2 z_i}{dt^2} \sqrt{\left( \frac{dx_i}{dt} \right)^2 + \left( \frac{dy_i}{dt} \right)^2 + \left( \frac{dz_i}{dt} \right)^2} + \frac{1}{4 \pi \varepsilon_0} q_d \sum_{j=0}^{n} \frac{\Delta z_{ij}}{r_{ij}} + \frac{g}{m_d}$$

(2.18)

For the acceleration in the $z$-direction the drag coefficient can be corrected as outlined in the next section to adjust for the aerodynamic shielding of droplets in an aligned stream of droplets.

2.3.1 Adjusting the Drag Coefficient for an Aligned Stream of Droplets

In equation 2.13, the drag coefficient for a sphere in free flight was given. However, in the UDS process, the droplets are initially in a continuous stream before the droplets scatter and act as independent spheres. This will reduce the drag force on the droplets flying in an aligned stream, since the droplets will shield each other. According to Mulholland et. al. [1988], the drag coefficient for an aligned stream, $C_{DA}$, of droplets is given by:

$$C_{DA} = \left[ (C_{D1+})^n + (C_{D_y})^{-n} \right]^{1/n}$$

(2.19)

where $n$ is an empirical parameter ($n=0.678+/-.07$), $C_{D_s}$ is the drag coefficient of a sphere as given in Equation 2.13, $C_{D1+}$ is the drag coefficient as ratio of the wavelength and diameter of the droplets approaches one ($\lambda_d/d_d$→1). This drag coefficient, $C_{D1+}$, is equal to:
\[ C_{D_{l+}} = C_{D_1} + \frac{\tilde{a}}{Re} \left( \frac{\lambda_d}{d_d - 1} \right) \quad (2.19) \]

where \( \tilde{a} \) is another empirical parameter \( (\tilde{a}=43.0+/−15.4) \), \( Re \) is the Reynolds number for the droplets, and \( C_{D_1} \) is the drag coefficient when droplet spacing over diameter equals one \( (\lambda_d/d_d=1) \). It is given by:

\[ C_{D_1} = \left[ \left( C_{D_{rod}} \right)^n - \left( C_{D_S} \right)^n \right]^{-1/n} \quad (2.20) \]

and \( C_{D_{rod}} \) is the drag coefficient for a rod and is given by:

\[ C_{D_{rod}} = 0.755 / Re \quad (2.21) \]

Once the droplets have scattered more than one drop radius from the centerline the drag coefficient for a sphere is used. Before that a weighted average, \( C_{D_r} \), of the coefficients \( C_{D_S} \) and \( C_{D_A} \) is used:

\[ C_{D_r} = (1- r/r_d) C_{D_A} + (r/r_d) C_{D_S} \quad (2.22) \]

where \( r \) is the distance from the centerline and \( r_d \) is the radius of the droplets. The effect of this correction factor is shown in the simulation results in Chapter 3.

### 2.4 Equilibrium Model for Droplet Thermal State

The droplet thermal state is defined by the droplet's enthalpy, \( H_d \), temperature, \( T_d \), and liquid fraction, \( x \). According to Passow et. al. [1993] by assuming that equilibrium solidification prevails, the liquid fraction of the droplets can be calculated from:

\[ \Delta H_d = C_p (T_d - 298) + x \Delta H_f \quad (2.23) \]
where $\Delta H_d$ is the enthalpy of a unit mass of uniform droplets referring to the enthalpy of the solid alloy at 298K, $C_p$ is the specific heat of the droplet, and $\Delta H_f$ is the latent heat of fusion of a unit mass of the alloy or metal. If one assumes that there is heterogeneous nucleation (no undercooling) then the droplet temperature and liquid fraction can be calculated directly from the droplet enthalpy. The initial droplet enthalpy is known from the melt temperature and then subsequent thermal states can be determined, since the change in enthalpy will be equal to the heat lost from the droplet in flight.

To predict the rate of heat transfer and solidification of the droplets, a spray deposition model developed by Mathur [1988] and Gutierrez-Miravete et al. [1989] can be utilized. According to this model, the rate of enthalpy loss, $Q$, from the droplets is given by:

$$Q = h \ A_d^s (T_d - T_g) + \sigma \ v \ A_d^s (T_d^4 - T_g^4)$$  \hspace{1cm} (2.24)$$

where $A_d^s$ is the surface area of the droplet, $\sigma$ is the Stefan-Boltzman constant, $v$ is the emissivity, $T_d$ is the droplet temperature and $T_g$ is the gas temperature. The radiation term can be neglected for low melting point metals and alloys such as Sn, lead, and zinc, and only consider the convective term, since it is magnitudes of order less at low temperatures. For high melting point metals and alloys, such as bronze, it becomes important. A uniform droplet temperature can be assumed when the Biot number ($Bi=hd/k_d$) is less than .01, which is the case for 100$\mu$m and 200$\mu$m Sn droplets [Passow, 1992]. Therefore, the heat transfer is interface controlled and the convective heat transfer coefficient, $h$, is given by the following [Levi, 1988]:

26
\[ h = \left( \frac{k_g}{d_d} \right) (2.0 + 0.6 \ Re^{1/2} \ Pr^{1/3}) \left( \frac{C_{g_{\text{avg.}}}}{C_g} \right)^{0.26} \]  

(2.25)

where \( k_g \) is the thermal conductivity of the gas, \( C_g \) is the heat capacity of the gas at the gas temperature, and \( C_{g_{\text{avg.}}} \) is the heat capacity of the gas at the average of the gas and droplet temperatures. \( Re \) is the Reynolds number and \( Pr \) represents the Prandtl number, which equals:

\[ Pr = \frac{\mu_g C_g}{k_g} \]  

(2.26)

To adjust the heat transfer coefficient for an aligned stream of droplets, one can adjust the heat transfer coefficient by the ratio of \( C_{D_r}/C_{D_s} \), where \( C_{D_r} \) is the adjusted drag coefficient for a line of droplets, while \( C_{D_s} \) is the drag coefficient for a single droplet, as was shown in Section 2.3 [Passow, 1992].

\[ h_{\text{aligned}} = \frac{C_{D_r}}{C_{D_s}} h \]  

(2.27)

This gives an adjusted heat transfer coefficient for an aligned stream of droplets. Using this equilibrium solidification model the droplet thermal state can be determined numerically when combined with the simulation of droplet flight path.
Chapter 3: Numerical Simulation of Droplet Flight Path and Mass Flux in the Spray

Using the physical model described in Chapter 3 a numerical simulation software was written to simulate the uniform droplet metal spray process (Appendix B.2). In this chapter the simulation method is briefly outlined, and the results of the simulation are shown. Finally the effect of changing numerical inputs to the simulation, such as the calculation time, step is described.

3.1 Outline of the Simulation

In Figure 3.1, the input to output flow of the simulation is shown. Initially, the inputs are read from an external input file, and the spray parameters, such as droplet diameter, droplet charge, and initial velocity, are calculated from these inputs. Next, the flight path of the droplets is simulated by simultaneously solving the non-linear equations of motion for the droplets' flight paths, using a fourth-order Runge-Kutta numerical integration. The thermal state is also determined by assuming equilibrium solidification of the droplets and using the droplet velocity as an input in determining the rate of heat transfer away from the droplet.

The output data are formatted to create output files that store the key simulation results. The simulation predicts the mass flux in the spray, the velocity profile of the droplets, the scattering of the charged droplets, and the shape of deposits. The simulation can be run for any metal or alloy and can be run for one or more orifices to determine how the interaction between droplets affects deposit
**Figure 3.1:** Droplet flight simulation inputs and outputs.
shape and mass flux. The simulation can also be used to determine the effect of angled orifices or off-center jets.

3.2 Results from the Simulation

3.2.1 Velocity vs. Flight Distance

In Figure 3.2a, the simulated vertical (z-) velocity as a function of flight distance is shown for 200μm diameter Sn droplets, charged in a 7.9mm wide charge cell. In this plot the velocity is calculated using two different models for the drag coefficient for the droplets. The unadjusted plot (solid line) shows the simulation results when the drag coefficient for a sphere in free flight, $C_{D,s}$, is used (Equation 2.13). The other two dashed lines represent the model with the adjusted drag coefficient, $C_{D,r}$, (Equation 2.22), which accounts for the reduced drag experienced by a series of droplets. This adjusted model is applied using two different charge voltages. The change in voltage results in a different droplet charge, determining how rapidly the droplets will spread and determines the adjusted drag coefficient.

These different models will converge to the same terminal velocity as the droplets scatter and act as individual spheres. As the charge per droplet is increased, the adjusted results will approach the unadjusted model.

In Figure 3.2b, the calculated radial velocity of the droplets is plotted for two different levels of droplet charging. As one can see from the plot, an increase in charge will lead to higher radial velocities. Unlike the z-velocity, which will be the same for all droplets at the same flight distance, the radial velocity will vary
Figure 3.2: Calculated 200μm diameter Sn droplet velocity
(a) Z-Velocity vs. flight distance: models using adjusted and unadjusted drag coefficients. (b) Radial droplet velocity vs. flight distance: For two levels of droplet charge the maximum and average radial velocity are plotted versus flight distance.
from droplet to droplet, depending on the Coulomb force acting on the droplet. Therefore, both the average and maximum radial velocities are plotted. One can see that compared to the z-velocity component, the radial velocity component is negligible, even for the maximum radial velocity for the higher level of charge. One can see that the droplets will begin to decelerate in the radial direction as the spray spreads out and the drag force becomes greater than the electrical repulsion. The maximum radial velocity is always less than eight percent of the z-velocity. As a result, the magnitude of the absolute droplet velocity will be within 0.3% of the magnitude of the z-velocity.

3.2.2 Spray Cone Width

The spray cone width is the maximum horizontal distance between any two droplets in the spray at a given flight distance as can be seen in the schematic in Figure 3.3. The spray cone width determines how much area will be covered in one pass of a spray forming experiment. The calculated spray cone width for three different charging voltages is shown in Figure 3.4. The initial jet velocity and diameter are 5.4 m/s and 100μm, respectively. The charge cell is 7.9 mm wide. This calculation is for the same spray parameters as the velocity plots in Section 3.2.1. As one can see from the graph the spray cone will grow more rapidly as the charging voltage is increased. The cone appears to grow almost linearly after the droplets accelerate to the radial velocities shown in Figure 3.2b. These results will be compared to experimental results in Chapter 4.
Figure 3.3: Schematic diagram of UDS process: Definition of the spray cone width, flight distance, and stationary deposit cross-section.
Figure 3.4: Simulated spreading behavior of 200μm diameter Sn droplets charged in a 7.9mm wide charge cell.

3.2.3 Droplet Thermal State

Using the equilibrium solidification model that was outlined in Section 2.4, the simulation predicts droplet thermal state as a function of flight distance. Plots showing the calculated droplet temperature and the equilibrium droplet liquid fraction against flight distance for 200μm diameter Sn droplets are shown in Figures 3.5 and 3.6. The jet diameter was 100μm and the initial velocity was 5.4 m/s. The melt temperature for this calculation was 300°C and the charge cell was 7.9mm wide.

The solid lines on the plots show the results of the simulation using the drag and heat transfer coefficients for a single sphere,
when they are not adjusted for a stream of droplets. The dashed lines on the plots show the results when the drag coefficient and heat transfer coefficients are adjusted for an aligned stream, as was outlined in Chapter 2. In these plots one can see the effect of droplet scattering on the droplet thermal state. In both figures, one can see a significant effect of droplet charging and scattering on the droplet thermal state, as predicted by the adjusted model.

**Figure 3.5:** Calculated droplet temperature vs. flight distance.
Figure 3.6: Calculated droplet equilibrium liquid fraction vs. flight distance for 200μm diameter Sn droplets.

3.2.4 Shape of Stationary Substrate Deposit and Mass Flux Distribution

The shape of the deposit of a droplet spray onto a stationary substrate can also be predicted by the simulation. Figure 3.7 shows how the simulation determines the mass flux in the spray. The coordinates of the droplets when they reach the substrate are recorded by the simulation, and then are grouped into a NxN element grid. The total width of the grid is equal to the spread cone width of the spray on the substrate. The mass flux in each square of the grid is determined by dividing the mass of the droplets deposited in each during the simulation by the simulation run time. Figure 3.8 shows
the mass flux grid for a simulated UDS spray. The number in each square represents the fraction out of one thousand of the total mass flux deposited in each grid during a simulation.

The three-dimensional shape of a deposit on a stationary substrate is determined by the mass flux distribution. The height in an element of the grid is proportional to the mass flux. Figure 3.9 shows the predicted three-dimensional shape for 200μm diameter Sn-40%Pb droplet deposit at a flight distance of 300mm. Figure 3.10 shows a contour map of the corresponding mass flux. These figures represent the mass flux distribution of a typical UDS spray. The mass flux is concentrated in a circle at some distance from the center, and the resulting shape is a cone with a hollow center. The shape is caused by the electrostatic repulsion of the droplets in flight.
Figure 3.7: Schematic diagram that shows how the simulation quantifies the mass flux distribution of a UDS spray.

Fraction (/1000) of Total Mass Flux Per Grid

Figure 3.8: Simulated grid of mass flux distribution.
Figure 3.9: Simulated 3D Shape of stationary substrate UDS deposit.

Figure 3.10: Contour map of stationary substrate UDS deposit.
3.2.5 Shape of Deposit on Sprayed onto Moving Substrates

To spray form parts of varied geometry and to control the enthalpy flux a substrate can be moved through the uniform droplet spray cone as shown in Figure 3.11. The substrate can be moved through the spray cone at different speeds and at varying time intervals to vary the deposit geometry and enthalpy flux. This will lead to the formation of a deposit on the substrate. If the substrate is moved along only one axis, the result is a deposit with a uniform cross-section. The speed of the substrate, $v_{\text{sub}}$, the mass flux distribution in the spray, and the number of passes through the spray will determine the shape of the deposit cross-section.

![Diagram of spray forming with moving substrate.]

**Figure 3.11:** Uniform droplet spray forming with moving substrate.
If the substrate is moving along the y-axis then the cross-sectional shape of the deposit can be found by calculating the average amount of mass flux in each column of the mass flux grid. The average mass flux for any column i of the grid will determine the height for that portion of the deposit. The height for section i of the deposit cross-section can be found by determining the total amount of material deposited on that section of the substrate. The amount of material deposited is equal to the amount of time in the spray area, $t_s$, times the average mass flux, $m_{avg_i}$. The amount of time spent in the spray area is equal to the spray cone width, $w_s$, divided by the substrate velocity $v_{sub}$. By dividing the amount of material deposited by the area of a grid element, $A_{ij}$, and the density of the metal one can find the normalized height of the deposit in that column. This assumes that the deposit is fully dense and ignores the splattering behavior of the droplets. If more than one pass is made the amount of material is multiplied by the number of passes under the substrate made by the spray, $n_p$. The resulting height of the deposit for a columns of the grid is normalized using the following expression:

$$h_i = \frac{t_s}{A_{ij} \rho_m} m_{avg_i} n_p = \frac{w_s}{v_{sub}} \frac{m_{avg_i}}{A_{ij} \rho_m} n_p$$

This will give $N$ discrete points that define the shape of the moving deposit cross section. A simulated cross-section for a 200$\mu$m diameter Sn-40\%Pb deposit at a flight distance of 300mm is shown in Figure 3.12. In this simulation, the substrate is moving along the
y-axis at a speed 38.1 mm/s, and the normalized height is calculated for 140 passes of the substrate through the spray.

![Graph showing height vs. x-position](image)

**Figure 3.12:** Calculated cross-section shape of 200\(\mu\)m diameter Sn-40%Pb deposit spray formed onto a moving substrate at a flight distance of 300mm.

3.2.6 Multiple Orifice Sprays

To achieve a high mass flux and to vary the geometry of spray deposits, multiple orifice systems that generate multiple jets of molten metal can be used. The droplets from different nozzles will interact due to the electrostatic repulsion between the droplets. To design such a system, it is critical to know how the droplets from the different jets will interact, and how this will affect the mass flux and deposit geometry. The simulation can predict the mass flux and deposit geometry resulting from multiple orifice sprays.
One possible arrangement of the orifices is to arrange them in an equilateral triangle, as shown in Figure 3.13. The calculation is for a 100μm Sn-40%Pb jet broken into 200μm diameter droplets with an initial jet velocity of 5.4 m/s. In this calculation, the deposit height is normalized for a substrate that is moving along the y-axis at a speed 380 mm/s. The normalized height is for 140 passes under the spray at this speed. The resultant moving deposit cross-section is shown for three different levels of droplet charge. As the charge is increased, the interaction between the droplets from the different jets will increase. Using the simulation different orifice spacing and droplet charging amounts can be tried to determine the best arrangement to achieve a desired mass flux.

In Figure 3.14, the simulation results are shown for an in line orifice arrangement. Again the simulated cross-section on a moving substrate is shown. From these figures, one can see that the deposit shape is very sensitive to the droplet charging amount. The lowest charge cases have six individual peaks corresponding to the peaks created by the individual nozzles. The outer peaks look more like the angled jet case shown in Figure 3.15. The center peak also appears more narrow than it was in the single orifice case. This is because the outer two jets apply an inward radial force on the center jet. As the droplet charge is increased, the interaction between the jets increases and the three nozzle spray begins to resemble a single orifice spray. The initial orifice positions do not seem to have much effect on the deposit geometry, although for the case where the orifices are in a line 2.5mm apart, the interaction between the sprays is increased and there is a larger total spread width.
Figure 3.13: Simulated cross-section of three orifice spray deposited onto a moving substrate. The resultant cross-section is shown for three different droplet charges.
Figure 3.14: Simulated cross-section of three-orifice spray deposited onto a moving substrate. The resultant cross-section is shown for three different droplet charges.
The deposit cross-section for the highest charge level looks much like the single nozzle cross-section in Figure 3.12 for both orifice arrangements, but the overall spread width is much greater and the distribution is more uniform.

3.2.7 Uniform Droplet Sprays with an Initial Jet Angle

In our UDS system, the jets are not always perpendicular to the substrate plane. If the orifice is mounted at some angle or the orifice is partially blocked, this will result in a jet with an initial angle, as shown in Figure 3.15. This will affect the mass flux distribution on the substrate and the resulting shape of a moving deposit. In Figure 3.16, one can see the simulated effect of an angled jet on the moving deposit cross-section. In the calculation, it is assumed that the angle is in the x-direction, so the initial y-velocity component is not affected by the angle. The angled jet will lead to an asymmetric mass flux distribution and cross-section shape. The cross-section still has two peaks, but they have different heights. The center of the distribution is also shifted on the x-axis. If the angle, α, is large enough, the charging of the droplets will also be affected, since the jet break-up will occur away from the center of the charge. This will increase the droplet charge, as was shown in Section 2.3, and will lead to additional scattering of the droplets.
Figure 3.15: Jet with an initial angle, \( \alpha \), due to a slanted orifice

Figure 3.16: Simulated cross-section of moving substrate with a 3° and a 5° initial jet angle, \( \alpha \).
3.3 Effect of Numerical Inputs Used in the Simulation

Numerical inputs used in the simulation affected the outputs from the simulation. Several key simulation parameters had to be determined in order to assure that the simulation would run efficiently and accurately. The pattern and magnitude of the initial perturbation is discussed first. The accuracy computation time of the simulation is determined primarily by the number of droplets simulated and the size of the time step used in the calculation. Therefore these inputs are also discussed in this section.

3.3.1 Initial Perturbation

In order for the stream of droplets to begin scattering, there has to be some radial perturbation that displaces the droplets in the horizontal plane. Since the physical cause of the perturbation is not known, a perturbation pattern was assumed in the simulation. A random initial displacement in both x and y was selected to initially perturb the droplet stream and cause the initial instability that leads to the scattering. To find the correct magnitude for this displacement, several simulations over a range of perturbation magnitudes were performed and compared to the experimental data. In Figure 3.17, the droplet spread cone width is plotted for three different perturbation levels. The spreading is plotted for perturbation magnitudes of 1x10^{-3}, 5x10^{-4}, 1x10^{-4}, and 1x10^{-5} times the droplet diameter, \( d_d \). This is for 200\( \mu \)m diameter Sn-5\%Pb droplets with an electrical charge of 3.8x10^{-12} C/droplet. The droplet scattering is not nearly as sensitive to the perturbation amplitude as it is to droplet charging. The magnitude of the random perturbation determines the point where the jet begins to scatter,
but the slope for all three curves is the same, since they will have
the same radial velocity profile due to equal levels of droplet charge.
Based on the experimental data the amplitude of $5 \times 10^{-4}$ times the
droplet diameter, $d_d$ was selected.

![Graph showing spread cone width vs. flight distance]

**Figure 3.17:** The effect of the initial perturbation magnitude on droplet spreading simulation.

### 3.3.2 Number of Calculations per Droplet Creation

The number of calculations that were performed between the
creation of each droplet will determine the numerical time step. As
one increases the number of calculations per unit of time, the
accuracy of the simulation increases, but so does the simulation time
and cost. Therefore, the minimum number of calculation steps was
found where the accuracy of the simulation is not significantly affected.

As the time step is decreased, the results of the simulation should approach an asymptotic limit. In order to find the minimum number of calculations, where the simulation was sufficiently accurate, the number of calculations was increased until the solution approached the asymptote. In Figure 3.18, the maximum spread width of a 200μm diameter Sn droplet spray is plotted as a function of the number of calculation steps. From this, it was concluded that six calculations steps per droplet calculation was sufficiently close to the asymptote, since improved accuracy due to more calculations is small, and the calculation time and cost increase linearly with the number of calculations. The resulting simulation time step, $h_{sim}$, is equal to:

$$h_{sim} = \frac{1}{6f}$$

(3.2)

Figure 3.18: Maximum spray cone width vs. number of calculations.
3.3.2 Number of nearest neighbors in Coulomb force Calculation

Another critical simulation input is the number of a droplet's neighbors, \( n \), that is included in the calculation to determine the total Coulomb force acting on a droplet. If the interaction between all the droplets is considered, the simulation time and cost will be very high. The Coulomb force is reduced by the distance between droplets squared, as is shown below:

\[
\vec{F}_{Ci} = \frac{1}{4 \pi \varepsilon_0} \sum_{j=0}^{n} \frac{q_d^2}{r_{ij}^2}
\]  

(2.16)

The point where the solution was no longer significantly affected by including more neighboring droplets, \( n \), in the Coulomb force calculation was found. Again, the solution should approach an asymptotic limit as the number of neighboring droplets is increased. In Figure 3.19, the maximum spread width of a 200\( \mu \)m diameter Sn droplet spray is plotted as a function of the number of nearest neighbors. This plot is for a flight distance of 200mm with a droplet charge of 7.6\( \times 10^{-12} \) C/droplet. From the figure, it was concluded that considering more than the twenty nearest neighboring droplets has a negligible effect on the simulation results. Therefore to minimize the simulation time and cost, only the twenty nearest neighbors are included for single orifice sprays. For multiple orifice sprays, twenty of the nearest neighboring droplets from each different jet are included.
Figure 3.19: Effect of number of droplets, n, included in Coulomb force calculation on spray cone width.
Chapter 4
Experimental Results

To verify the simulation results, several experiments were performed to determine the droplet charging amount, the spreading of the droplets, the velocity profile of droplets in flight, and the shape of deposits on a substrate. In this chapter, these experiments are described, the results of these experiments compared to the simulation results, and the discrepancies discussed.

4.1 Charging Experiment

The amount of charge per droplet determines how rapidly the droplets will scatter, which affects the velocity, mass flux, and thermal state of the droplets. Therefore, it is important to verify the charging model that was described in Section 2.3. The experimental apparatus shown in Figure 4.1 was used to measure the amount of charge per droplet. As can be seen in the figure, the current flow from a collection crucible inside the spray chamber which was electrically isolated to insure that all the charge from the droplets would discharge through the circuit. The amount of current was measured using a resistor in parallel with the capacitor, and the signal was amplified using a small Op-amp. The amount of charge per droplet, $q_d$, can be calculated from the measured voltage using the following relationship:

$$q_d = \frac{(V_o/R)}{f}$$  \hspace{1cm} (4.1)
Figure 4.1: Experimental setup for droplet charge measurement.
where $V_o$ is the measured voltage, $R$ is the resistance, and $f$ is the disturbance frequency. The experiments were performed for 200µm diameter Sn droplets using a 7.9mm wide parallel plate charge cell. The charging voltage was varied between 375 and 875 Volts, which are our normal operating voltages. The charge per droplet was measured at 125 Volt intervals and the results are shown in Figure 4.2. The measurements were taken using an oscilloscope, which contained a significant amount of noise. The measurements were taken at the midpoint of the noise amplitude. The experimental results are compared to the parallel plate and cylindrical capacitor models which were described in Section 2.3. A curve fit to the data shows that the charge per droplet varies linearly with the voltage as would be expected from the model.

The data agree well with the parallel plate model for droplet charging. The uncertainty in the data is due to the amount of noise in the measurement and a slight drift in the DC gain of the amplifier. The uncertainty in these measurements is within about 12%, due to noise and possible errors in reading the voltage from the oscilloscope. These data confirm that it is reasonable to use the parallel plate model to predict droplet charging.
Figure 4.2: Charge per droplet for 200\(\mu\)m diameter Sn droplets with 7.94mm wide charge dell. Experimental results are compared to the two charging models.
4.2 Spreading Experiments

Experiments were performed to determine the maximum spreading of the jet as a function of flight distance and droplet charging. The spread width of the jet is critical for coating and spray forming applications, since it determines how much surface area will be covered by one pass of the spray. The spread width is the maximum width of the spray at a given flight distance.

The experiments were performed using 200 μm Sn drops for a range of flight distances. The experimental setup shown in Figure 4.3 was used to perform these experiments. The spray was monitored inside the boro-silicate glass chamber with a Micro-Mac CCD video camera (Techni-Quip: Hollywood, CA) with a Unimac 0.7x to 4.5x power microscopic zoom lens (Meiji Techno: Woburn, MA), and a 1538-A Stroboscope (Quadtech: Bolton, MA). The camera and strobelight were mounted on a linear table, which was attached to the chamber support frame. The linear table was controlled by a computer using TermWorks software, so that the camera and strobelight could easily be moved in precise increments. Experiments were performed for flight distances between 5-450mm for three levels of droplet charge. The spreading amount was measured on the screen and the measurements were calibrated by moving a ruler into the screen. The maximum spread width that could be measured was 40mm due to the field of view of the camera. The results of the experiments are compared to the results of the numerical simulation for three different levels of charge.

The uncertainty in these experiments is caused by the calibration of the measurements. A scale of known dimension was
held in the field of view of the camera, and its size was measured on
the screen to calibrate the measurements. The droplet spreading
would also change from frame to frame, and the maximum width
measured at a flight distance and charge was used as the spread cone
width. In addition to this uncertainty there was some variation in
the droplet spray scattering due to physical changes in the process.
The stream initial jet angle changed during the experiments, which
led to a small change in droplet charging and changed the distance
from the stream to the camera. This led to measurement errors since
the calibration was performed for a set distance between the camera
and the jet. The total uncertainty in the measurements is
approximately 10% of the measured values as is indicated by the
error bars on the graph.

From Figure 4.4, it appears that this uncertainty in the
measurements when combined with possible variation in droplet
charging explains most of the discrepancy between the calculation
and the experiment. The flight distance, where the jet begins to
spread significantly (spread width>1mm), is predicted to within
20mm in all three cases, and most of the data points lie within their
uncertainty of the calculated spreading. The discrepancy is greatest
for the lowest charge level, because the small spread widths were
most difficult to measure. Overall, it appears that the simulation
provides a good approximation of the droplet scattering.
Figure 4.3: UDS Apparatus used in Experiments
Figure 4.4: Comparison of experiment and simulation for spread cone width versus flight distance for 200μm diameter Sn droplets at three levels of charge.
4.3 Droplet Velocity Experiments

Experiments were also performed to measure the droplet velocity as a function of flight distance. The droplet velocity is important for determining the thermal state of the droplet, as well as predicting its behavior on impact on the substrate. These experiments were performed at Sandia National Laboratory using the UDS system, which was shown in Figure 4.3. The experiments were performed with pure Sn for a range of droplet diameters from 95-205\(\mu\)m. The droplet charges were also varied to determine the effect of droplet charging and scattering on the droplet velocities as a function of flight distance.

To perform these experiments, we used a Kodak EKTAPRO high speed video system to take pictures at a rate of 3000 frames/second with a shudder speed of 20\(\mu\)s. The pictures were downloaded to an IBM PC, and EKTAPRO motion analysis software was used to determine the droplet velocities. For each experimental point the velocity was determined by tracking a droplet for at least five frames using the software. The velocity between each of these five frames was calculated, and the average of these five points was taken to determine the measured velocity at that flight distance. The system was calibrated by moving a scale of known size into the field of view of the camera at the point where the spray was being recorded. The number of pixels on the screen could thereby be converted to a length scale. Two sets of experiments were performed using a 100\(\mu\)m and a 45\(\mu\)m diameter orifice, and the results are described in this section.
4.3.1 100μm Orifice Experiments

Using a 100μm diameter orifice, experiments were performed to measure the droplet velocity at flight distances between 75mm and 500mm. The results for two different levels of droplet charge are shown in Figure 4.5. The driving pressure for the experiments was 136KPa (20psi) and the disturbance frequency was 10KHz. The width of the charge cell was 7.9mm. The droplet diameters were approximately 203μm, as measured from the scanning electron microscope (SEM) picture, shown in the Figure 4.6. The dashed lines in Figure 4.5 represent the calculated results for the model with a drag coefficient adjusted for an aligned stream of droplets, and the solid line represents an unadjusted drag coefficient for a single sphere.

It appears from this plot that the adjustment model in Section 2.3 overestimates the effect of the droplets being aligned in a stream as opposed to being in free flight. The difference between the 500V and 1000V experiments is not as large as would be predicted in the model, and the data appear to lie in between the adjusted model and the single sphere model.

The uncertainty in the data comes primarily from possible errors in calibrating the velocity measurements. Since the stream of droplets had some initial angle, the distance of the droplets from the camera changed as the flight distance was increased. Also, in moving the camera up and down using a tripod system, there may have been some horizontal movement of the camera, which would affect the focal length of the camera. We performed several calibrations that varied in magnitude by approximately 10%, and this led to an
uncertainty of about ten percent in the data as shown by the error bars in Figure 4.5.

All of the experimental data lie between the calculations for the two models, indicating that both provide a reasonable estimate of droplet velocity. The reason that the data does not agree well with the adjusted 500V data could be caused by an overestimate of the effect on the drag coefficient of the drops being in an aligned stream of droplets or due to an error in estimating the initial droplet velocity based on the empirical orifice friction coefficient.

![Graph showing velocity vs. flight distance](image)

**Figure 4.5:** Velocity vs. Flight Distance for 203µm diameter Sn droplets sprayed with a 100µm diameter orifice.
Figure 4.6: SEM picture of 203μm diameter Sn droplets.

Figure 4.7: SEM picture of 96μm diameter Sn droplets.
4.3.2 45μm Orifice Velocity Data

A similar set of experiments was performed with a 45μm diameter orifice. The driving pressure for these experiments was 204KPa (30psi) and the frequency was 22.8 KHz. The charge cell was 7.9 mm wide and the material was electrolytic grade Sn. The droplet diameter was approximately 96μm as measured from the SEM picture shown in Figure 4.7. The results are plotted in Figure 4.8.

Initially, the data follows the adjusted model more closely than in the 100μm diameter orifice experiments, but further down in flight, the data points move toward the single sphere model. Four of the five 500V experimental data points lie on the line of the adjusted 500V mode, but the last data point lies on the unadjusted model line. Initially, the difference between the 500V and 1000V charge is not as large as predicted by the model, but at a flight distance of 300mm, there appears to be a significant difference between the velocities measured for the two different levels of charge. The uncertainty is as large as it was in the 100μm diameter orifice case, due to the same measurement uncertainties. Therefore, it is not clear from the experimental results which model calculates the droplet velocity more accurately.
Figure 4.8: Velocity vs. flight distance for 96\(\mu\)m diameter Sn droplets.
4.4 Cross-Section Shape of Moving Substrate Deposits

In this section, the results from deposition experiments on a moving substrate are described and compared to the simulation results that were outlined in Section 3.3. A linear table, as shown in Figure 4.9, is used to move the substrate under the spray in the y-direction. In these experiments, one nozzle was used. Many passes are made underneath the spray until the desired part thickness is achieved. For the experiments in this section, the substrate was moved along the y-axis at a speed of 38.1 mm/s and 136 passes were made through the uniform droplet metal spray. Two sets of experiments were performed with different alloys at different flight distances and charges. The first set of experiments was performed with Sn-40%Pb at a flight distance of 300mm and the second set of experiments was performed with Sn-5%Pb at a flight distance of 480mm.

4.4.1 Sn-40%Pb Deposits at Flight Distance of 300mm

For this set of experiments, the driving pressure was 136KPa (20 psi) and a 100μm diameter orifice was used. The disturbance frequency was 10KHz, and the resulting droplet diameter is approximately 200μm. In this case, the charge cell was a 6.3mm wide slot and the charging voltage was 850V. The resulting charge per droplet is 5.84x10^-12 C. A cut was made through the deposits perpendicular to the substrate motion (along the x-axis) so that the cross-section of the deposit could be measured. The deposit cross-section was measured at intervals of 1mm, and these measurements are accurate to within +/-1mm. The measured results are plotted in gray lines in Figure 4.10 as experiments #7-12, which were all
performed at the same spray parameters, with varying droplet thermal states. This accounts for the difference in deposit height.

In the simulation, 1000 droplets were deposited and the mass flux was divided into a 30x30 grid. The simulation parameters were the same as those used in the experiment. The cross-section height is normalized for the total experimental mass flux and plotted in the black line in Figure 4.10 for comparison to the experimental results.

**Figure 4.9:** Schematic of X-Y table UDS System.
The calculated shape of the deposit is similar to the experimental shapes. Both exhibit a two peak shape. There is some variation between the experimental shapes due to factors such as angled sprays, different deposit densities due to different thermal conditions, and the wandering of the jets during the experiments. The simulation also ignored the impact behavior of the droplets. When the droplets hit the substrate they may splatter, bounce, or splash, depending on their thermal state. This will change the geometry of the deposit. The reasons for the discrepancy between the model and simulation are discussed further in Section 4.5.

**Figure 4.10:** Sn-40\%Pb deposit cross-sections. These samples were collected at a flight distance of 300mm.
4.4.2 Sn-5%Pb Deposits at a Flight Distance of 480mm

Experiments were also performed on a moving substrate using 200μmSn-5% Pb diameter at a flight distance of 480mm. The initial jet velocity and diameter were 5.4m/s and 100μm, and the disturbance frequency was 10.3 KHz. The charge plate was 7.9mm wide and the charging voltage was 600V. The resulting charge on each droplet was 3.8 x10^{-12} C. The substrate was moved at a rate of 38.1mm/s and 136 passes were made through the spray cone. The experimental cross-sections for experiments 1-4 are plotted as gray lines and compared to the normalized simulation result plotted in the dark line in Figure 4.11. The experimental results represent deposits of varying porosity, and therefore have different cross-sectional areas.

Again, the basic shape of the deposits agrees with the simulation results, although these deposits all had high porosity so the overall height does not agree well. The discrepancy is greater for these deposits which were collected at a flight distance of 480mm than for the samples collected at 300mm, due to the additional flight distance, since the effects of physical changes, such as varying jet angle and charging amount, will be greater at a longer flight distance.

The samples collected in the experiments #5 and #8 had a very skewed or asymmetric geometry, as can be seen in Figure 4.12. The spray parameters for these two experiments were the same as for experiments #1-#4, which were plotted in Figure 4.11. These skewed shapes were most likely caused an initial angle in the jet. In Figure 3.10, the skewed results are compared to the normalized cross-sections predicted by the simulation for a spray with initial
angles of 3° and 5°. These shapes have the same skewed form with one hump higher than the other, so it is likely that these were caused by jets with an initial angle. The reasons for the discrepancies between the simulation and experiment are discussed in detail in the next section.

![Graph showing cross-section of 200μm diameter Sn-5%Pb droplet deposits on a moving substrate at a flight distance of 480mm.](image)

**Figure 4.11:** Cross-Section of 200μm diameter Sn-5%Pb droplet deposits on a moving substrate at a flight distance of 480mm.
Figure 4.12 Asymmetric cross-section shape compared with 3° and 5° initial jet angle simulations.
4.5 Discussion of the Discrepancy between the Experiment and Simulation Results

For the charging, spreading, and velocity experiments, described in Sections 4.1-4.3, it appears that the difference between the model and experiments is primarily caused by the uncertainty in the measurements. For the cross-section shape of the deposits, the discrepancy is much larger than the uncertainty of the measurements. As was discussed earlier, this may be caused by physical changes in the experiment such as a changing initial jet angle. In this section, this variation in the experiments is discussed in more detail.

There is a large variation in the shape of the experimental deposit cross-sections, as can be seen in Figures 4.10-4.12. All of these samples were collected for the same spray parameters and flight distance. The expected mass flux distribution would be the same for all these experiments. The thermal state and substrate temperature were varied, leading to a variety of deposit morphology, which explains the difference in height of the deposit cross-sections. As was mentioned earlier, the impact behavior of the droplets was also ignored in the simulation model. The droplets spread, splattered, bounced, splashed, or flowed on the substrate, and this will also change the geometry of the deposits. However, these factors do not explain the large change in the cross-sectional shape of the experimental deposits.

The first factor that may lead to this variation is that the orifices that were mounted at an angle, due to a rough surface finish in the orifice pocket and imperfections in the orifice jewel. The
resulting jet will have an the initial velocity with both a radial and a vertical component. An angled jet will skew the distribution of the mass flux, as was shown in Section 3.2.6, but in the simulation, it was assumed that the angle only changed the initial x-velocity of the droplets. This case shows the maximum effect on the moving deposit cross-section for a substrate moving in the y-direction. In the experiments, this angle may have been in any direction, and this would have varying effects on the mass flux distribution. The cross-section will still be skewed, but to varying amounts. Also, if the angle is large enough the droplet charging amount will increase, as was shown in Section 2.3. Although it requires a large amount of misalignment to change the droplet charge significantly, the spreading and deposit shapes are very sensitive to the charging amount, so that a small change in the charge will have a real effect on the spreading of the spray and the deposit cross-section.

For each experiment, a new orifice was used and the geometry of these orifices varied. The orifice diameters were measured for the nominal 100μm diameter orifices and were found to have a size distribution of 100+/−5μm. This variation in jet diameter leads to changes in the total mass flux and droplet diameter. Also, other dimensions on the orifices may have changed and led to changes in the wetting angle, which affects the stability of the droplet break-up [Bredt, 1992]. Changes in this wetting angle of the orifice can also cause changes in the initial angle of the jet. The wetting angle can also change due to changing material properties of the metal, such as its viscosity or density. This variation in the experiments can be
partially explained by these changes in the orifice geometry and the wetting angle.

During the experiments, the jet usually wavered so that the initial angle of the jet was always changing. This may be caused by impurities in the molten metal in the crucible or by the changes in the wetting angle described above. This leads to a less bimodal distribution than would be predicted by the simulation, since the centerline of the mass flux distribution is constantly changing. It would also explain why the experimental shapes are wider than the simulated shapes. In some cases, the jet also jumped due to partial blockages in the melt. This caused a permanent shift in the centerline of the distribution and will affect the shape of deposit. In this case, the resulting deposit cross-section will be a superposition of two different mass flux distributions. Because of the large variation in the experimental cross-sections, it was difficult to compare the simulation to the experiments.
Chapter 5

Conclusion

In this chapter, the study is summarized and conclusions are made about the accuracy of the numerical simulation and the validity of the assumptions made in the modeling. Finally recommendations are made for future work and for improving control of the UDS process.

The goal for this study was to produce an accurate simulation of the droplet flight path and mass flux based on physical models of the process. To achieve this goal, the charging of metal droplets, the droplet flight path, and the droplet thermal state were physically modeled. Next, a numerical simulation was developed, based on these physical models, that determines the cone spread width of UDS sprays, the velocity of the droplets as a function of flight distance, the mass flux distribution on the spray, the shape of stationary substrate deposits, and the cross-sectional shape of deposits sprayed onto a moving substrate. The simulation results were shown and the simulation was used to predict the mass flux and cross-sectional shape for multiple orifice sprays.

Experiments were performed to verify the simulation model for droplet charging, the spray cone width, the velocity profile of the droplets, and the cross-sectional shape of deposits sprayed onto a moving substrate. These experiments for droplet charging and spray cone width were performed using 200μm diameter Sn droplets and the velocity profile was measured for 95μm and 200μm diameter Sn droplets. The cross-sectional deposit shapes were determined for
200\(\mu\)m diameter Sn-40\%PB droplets at a flight distance of 300mm, and for 200\(\mu\)m diameter Sn-5\% Pb droplets at a flight distance of 480mm.

From the results given in Chapter 4, it appears that the simulation is a useful tool that can be used to predict the droplet charging, droplet spreading, droplet velocity, and moving deposit cross-section. The agreement of the simulation and experiments is limited to approximately \(\pm 10\%\) for the droplet spreading and velocity profiles. For the shape of the moving deposits, there is still some significant discrepancy between the experimental and simulation results cause by variations in the process and by the impact behavior of the droplets, which is ignored in the simulation. The causes of this discrepancy were discussed in detail in Section 4.5.

The simulation can also predict droplet thermal state and multiple orifice interaction, but these results still have to be experimentally confirmed. Since the simulation appears to be an accurate tool for predicting the interaction of droplets in a single orifice spray, it is likely that it can be used for multiple orifice sprays as well.

To improve the consistency of the UDS process, some design modifications should be made to the existing apparatus. Filtering the molten metal before it is sprayed through the orifice could reduce the wavering of the jets and eliminate the jumping of the stream caused by partial blockages. Instead of allowing the droplets to scatter randomly based on an unknown disturbance, the droplets could be charged to varying amounts and then deflected to create a more predictable mass flux distribution. The simulation could be
improved by including the impact behavior of the droplets, which will affect the shape of the spray deposits.

The simulation created in this study can be used to predict the effects of varying droplet parameters on the droplet velocities, spray cone width, and moving substrate deposit cross-sections. The simulation can be combined with a droplet solidification and droplet impact model to produce a complete simulation of the UDS process, which will be a tool that can be used to design experimental and industrial UDS systems.
References


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Appendix A
Method of Images

The droplet charging amount for a Parallel plate capacitor and an off-center jet in a Parallel capacitor were derived using the method of images. This method can be used to solve electrostatic problems with boundary conditions that appear difficult to satisfy if Laplace's equation is solved directly [Cheng, 1983]. This method is based on the fact that a grounded conducting plane affects the electric field near a charged body in the same way as a mirror image of the body with an opposite charge. A point charge casts an electric field around a grounded plane in the same pattern as though there were an oppositely charged particle on the opposite side of the wall. At the surface of the plane the electric field will always be perpendicular to the wall [Bredt, 1993].

Figure A.1: Images of Line Charge for a Parallel Plate Charge Cell
In Figure A.1 one can see the jet represented as an infinite line of charge off center in the charge cell. The two cell walls act as two mirrors creating an infinite number of images all at distance $w_c$.

By integrating the electric field from point b on the edge of the jet to point a on the cell wall the potential difference between the charge cell and the wall can be found. This expression shows the first few terms of this potential.

$$V = \frac{q}{2\pi\varepsilon_0} \int_{x_1}^{r} \frac{dr}{r} + \int_{x_1}^{2x_1-r} \frac{dr}{r} - \int_{2x_2-x_1}^{2x_2+2x_1-r} \frac{dr}{r} - \ldots \quad (A.1)$$

Evaluating this integral leads to the following expression.

$$V = \frac{q}{2\pi\varepsilon_0} \ln \left( \frac{r}{x_1} \right) + \ln \left( \frac{2x_1}{x_1} \right) + \ln \left( \frac{2x_1-r}{2x_2+x_1} \right) - \ln \left( \frac{2x_2+2x_1-r}{2x_2+x_1} \right) - \ldots \quad (A.2)$$

Using the code called "charge.c" in Appendix B the convergence of this series can be found. This code can be used to find the charge for an off-center jet in any charge cell. For an on-center jet this expression were the cell width was much larger than the jet diameter, the solution was found to converge to Equation 2.10:

$$q_d = C \lambda_d V = \frac{2\pi\varepsilon_0}{.23 + \ln (w_c/d_j)} \lambda_d V \quad (A.3)$$

The result for an off-center jet was shown in Figure 2.4. The charge per droplet increases parabolically and goes to infinity as the jet approaches the wall. This same effect of jet misalignment was found by Fillmore et al. for a 35μm jet [Fillmore, 1977].
Appendix B

Numerical Code used for Simulation

B.1 Droplet Charging Code

/*charge.c-Goddard K Abel-program to predict droplet charging*/
/*in a parallel plate charge cell for on and off-center jets*/

#include<stdio.h>
#include<math.h>
#include<stdlib.h>

FILE *plo;

/*global constants*/
double e0=8.85e-12; /*permittivity of free space*/
double pi=3.142; /*pi*/

main()
{
    double width,x1,x2,r,V,q,qtotal,off,qd;
    double v0,freq,length;
    int a,b,c,d,e,f,s,
    int i,j,k,terms,points;
    terms =100; /*number of terms in integration*/
    points=20; /*number of samples across charge plate gap*/
    /*get inputs from user*/
    printf("Enter the number of terms in integral: ");
    scanf("%d",&terms);
    printf("Enter the jet radius (m): ");
    scanf("%lf", &r);
    printf("Enter the initial jet Velocity(m/s): ");
    scanf("%lf", &v0);
    printf("Enter the frequency (Hz): ");
    scanf("%lf", &freq);
    printf("Enter charge plate width (inches): ");
    scanf("%lf", &width);
    printf("Enter number of data points on plot: ");
    scanf("%d", &points);
    printf("Enter the charge plate Voltage (V): ");
    scanf("%lf", &V);

    length=v0/freq; /*wavelength of jet break-up*/

    width/=0.254*width; /*convert inches to metric*/
    /*in .0254*r;*/
    plo=fopen("charge.out", "w"); /*open output file*/

    for(j=1;j<points;j++) /*loop to calculate charge across the charge cell*/
        x2=width/i/2.0*points;
    x1=width-x2;
    off=((x1-x2)/2)/0.254; /*distance from center in inches*/
    if(x2>3*r) /*check to make sure there is no contact to charge plate*/
        a=1;b=0;c=0;d=0:e=0:f=1;k=0:s=1:qtotal=0;
    for(i=0;i<terms;i++) /*loop to calculate charge at one point*/
    {if(k=11)
        a=1;c=-1:d=1;f=-1;s=1;
    }if(k=21)
        a=1;b=2;c=1;d=1:e=2;f=1;s=(-1);
    }if(k=31)
        a=1;c=1:d=1:f=1;s=(-1);
    }if(k=41)
        a=1;c=1:d=1:f=1;s=1;
    }k=1;
    if(k>4)
        k=1;
    qtotal+=s*log(((a*x2)+(b*x1)+(c*r))/((d*x2)+(e*x1)+(f*r)));
\begin{verbatim}
}
q=2*pi*e0*V/qtotal;
qd=q*length;
fprintf(plo,"%lf\t%lf\t%lf\t%e\t%lf\t%e\n",x1,x2,off,q,qtot,qd);
}
}
close(plo);
}
\end{verbatim}
B.2 Droplet Flight and Mass Flux Code

/*19.c-Godard K Abel-uniform charged metal droplet trajectories*/
/*program to predict single and multiple orifice droplet flight path*/
/*and mass flux in the spray*/

#include<stdio.h>
#include<math.h>
#include<stlib.h>
FILE *inp; /*open file for inputs*/
FILE *dro; /*file to store drop velocity,temperature.enthality*/
FILE *res; /*open file for results*/
FILE *his; /*open file for histogram*/
FILE *cut; /*file for radial heigh distribution*/
FILE *gra; /*file for 3d mesh plot*/
FILE *nhr; /*file for numerical distribution grid*/
FILE *nrd; /*file for number of drops per section*/
FILE *spr; /*file to find spread angle of spray*/
FILE *mov; /*file to record shape of moving deposit*/
FILE *amv; /*file to record averaged shape of moving deposit*/

/*constants defined as global variables*/
double g=9.81; /*gravity (m/s^2)*/
double knitrogen=.0259; /*conductivity at 300K (W/m-K)*/
double pnitrogen=1.1233; /*density of nitrogen at 300K (kg/m^3)*/
double unitrogen=17.34e-6; /*viscosity of nitrogen at 300K (kg/ m-s)*/
double cnitrogen=1041; /*specific heat of nitrogen at 300K (J/kgK)*/
double Pr=.715; /*Prandtl number for Nitrogen at 300K*/
double Tgas=27; /*chamber gas temperature (Celsius)*/
double e0=8.85e-12; /*permittivity of free space*/
double cmoliquid.cmolid.Ts.pmetal.hof; /*metal/alloy properties*/
double xmin,xmax,ymin,ymax,rmax;
double *current;

/*initialize calculated constants as global variables*/
double distance.md.cl.cre.ccould.f;
double e.temp;
int dif=0; /*number of droplets in flight*/
int nd=0; /*number of droplets created*/
int count=0; /*flag for when first drop reaches substrate*/
int mn.norf.old.mp.N.deposited;

/*function prototypes*/
void runge_kutta(int.double **.
double*).(double,double,double,int.double **,double).
double*).(double,double,double,double,double,int.double **,double).
double*).(double.double,double,double,double,double,int.double **,double.double,double).
double;

double uprime(double.double,double,double,double,double,int.double **,double);
double vprime(double.double,double,double,double,double,int.double **,double);
double wprime(double.double,double,double,double,double,int.double **,double.double,double)
);

void thermal_state(double **,double.double);
void spread(double **,int);

void output(int.double **);
void histogram(int.double **);
void rcut(int.double **);
void grid(int.double **,int.double.double);

main()
{
    double x=0; double y=0;double z,u,v,w;
    double pressure.od.runtime.volt, width, l; /*initialize inputs*/
double qd, capacitance, v0, level;
double steps, h;
double t=0;
double kj;
int td, dr, alloy, step;
int spd, i, j, k, n, c, ii, jj, max;
double **a;
double **orf;
int passes;
double disturbance;
double totalmass, speed;
double timed=0; /*time droplets depositing on substrate*/

/*dynamically allocate memory for array to store orifice positions*/
orf=calloc(norf, sizeof(double *));
for(i=0; i<norf; i++){
  orf[i]=calloc(2, sizeof(double));
}

/*read inputs here from "inputs" file*/
inp=fopen("inputs", "r");
fscanf(inp, "%d
", &alloy);        /*alloy number*/
fscanf(inp, "%lf
", &temp);     /*melt temperature*/
fscanf(inp, "%lf
", &pressure); /*driving pressure (psi)*/
fscanf(inp, "%lf
", &d);        /*orifice diameter (m)*/
fscanf(inp, "%lf
", &f);        /*piezo-electric frequency (Hz)*/
fscanf(inp, "%lf
", &width);    /*width of charging slot (inches)*/
fscanf(inp, "%lf
", &volt);     /*charging plate voltage (V)*/
fscanf(inp, "%lf
", &distance); /*distance from nozzle to substrate (m)*/
fscanf(inp, "%d
", &td);        /*total drops deposited*/
fscanf(inp, "%d
", &spd);       /*calculation steps per drop creation*/
fscanf(inp, "%d
", &passes);    /*number of passes depositing onto substrate*/
fscanf(inp, "%lf
", &speed);    /*speed of substrate (m/s)*/
fscanf(inp, "%e
", &disturbance); /*magnitude of disturbance*/
fscanf(inp, "%d
", &nn);        /*# of droplets in Coulomb force calculation*/
fscanf(inp, "%d
", &N);         /*# of elements in mass flux grid*/
fscanf(inp, "%d
", &norf);      /*# of orifices*/
nn=nn*norf;

/*dynamically allocate memory for array to store orifice positions*/
orf=calloc(norf, sizeof(double *));
for(i=0; i<norf; i++){
  orf[i]=calloc(3, sizeof(double));
}

/*read orifice positions from file*/
for(i=0; i<norf; i++){
  fscanf(inp, "%lf
", &orf[i][0]);    /*x-position of orifice*/
  fscanf(inp, "%lf
", &orf[i][1]);    /*y-position of orifice*/
  fscanf(inp, "%lf
", &orf[i][2]);    /*angle of orifice*/
}
fclose(inp);

/*print orifice positions*/
printf("\nORIFICE POSITIONS\n");
for(i=0; i<norf; i++){
  j=i+1;
  printf("\nx-position of orifice # %d= %lf (m)\ty-position of orifice # %d= %lf (m)\n",
    j, orf[i][0], j, orf[i][1]);
  if(orf[i][2]==0)
    printf("\angle of orifice # %d= %lf degrees\n", j, orf[i][2]);
}

for(i=0; i<norf; i++){
  orf[i][2]=orf[i][2]/180*3.142;    /*convert degrees to radians*/
}
dro=fopen("drop.m","w"); /*create files to be appended*/
close(dro);
spr=fopen("spread.m","w");
close(spr);

if((td<(20*norf)) /*make sure there are enough drops to track velocity and thermal stat*/
    td=20*norf;
if(norf>1)
    td=((td/norf)+1)*norf;
mp=td/2; /*track around this particle*/

/*print inputs to simulation*/
printf("\n\nTHE INPUTS TO THE SIMULATION:\n\n");
printf("\nmelt temperature = %f degrees Celsius\n\n",tmp,alloy);
printf("\nreduced temperature = %f psi\n\n",pressure,od);
printf("\npiezo-electric frequency = %f (Hz)\n\n",f,charge_plate_width);
printf("\ncharging voltage = %f V\n\n",volt,distance);
printf("\ntotal # of drops = %d \n\n\ntotal calculation steps per drop = %d\n\n",td,spd);
printf("\nnumber of passes = %d\n\n\nsubstrate speed = %f m/s\n\n",passes.speed);
printf("\nsize of disturbance = %e x droplet diameter\n\n",disturbance);
printf("\nnumber of neighbors in coulomb force calculation = %d\n\n",nn);

if(alloy==1){
pmetal=9114; /*density of eutectic tin-73%/lead (kg/m^3)*/
    Ts=184; /*solidification temperature (Celsius)*/
    cmliq=216.7; /*specific heat of molten metal (J/kgK)*/
    cmsold=203.8; /*specific heat of solid metal (J/kgK)*/
    hof=46054; /*heat of fusion of metal (J/kg)*/
}

if(alloy==2){
pmetal=7800; /*density of pure tin (kg/m^3)*/
    Ts=232; /*solidification temperature (Celsius)*/
    cmliq=257.3; /*specific heat of molten metal (J/kgK)*/
    cmsgo=244.4; /*specific heat of solid metal (J/kgK)*/
    hof=59570; /*heat of fusion of metal (J/kg)*/
}

if(alloy==3){
pmetal=11350; /*density of pure lead (kg/m^3)*/
    Ts=327.5; /*solidification temperature (Celsius)*/
    cmliq=147.5; /*specific heat of molten metal (J/kgK)*/
    cmsgo=134.6; /*specific heat of solid metal (J/kgK)*/
    hof=23040; /*heat of fusion of metal (J/kg)*/
}

if(alloy==4){
pmetal=7978; /*density of tin-5%lead (kg/m^3)*/
    Ts=200; /*solidification temperature (Celsius)*/
    cmliq=251.8; /*specific heat of molten metal (J/kgK)*/
    cmsgo=238.9; /*specific heat of solid metal (J/kgK)*/
    hof=58894; /*heat of fusion of metal (J/kg)*/
}

if(alloy==5){
pmetal=9220; /*density of tin-40%lead (kg/m^3)*/
    Ts=190; /*solidification temperature (Celsius)*/
    cmliq=213.4; /*specific heat of molten metal (J/kgK)*/
    cmsgo=200.48; /*specific heat of solid metal (J/kgK)*/
    hof=44958; /*heat of fusion of metal (J/kg)*/
}

/*calculate initial jet velocity*/
if(od>375e-6&&od<425e-6)
k=1.5; /*estimated orifice coefficient*/
if(od>90e-6&&od<110e-6)
k=1.1547*sqrt(1.1); /*orifice coefficient for nominal 100um orifice*/
if(od<60e-6&&od>40e-6)
k=1.1859; /*orifice coefficient for nominal 50um orifice*/
v0=kvj*sqrt(pressure);

/*calculate droplet diameter*/
d=pow(1.5*pow(od,2.0)*v0/f),(1.0/3.0));

/*calculate droplet mass*/
m=1.0/6.0*3.1421*pow(d,3.0)*pmetal;

/*calculate initial droplet enthalpy*/
e=m*{(temp-Ts)*cmliquid)+(h0f)+(Ts-Tgas)*cmsolid});
/*constant for calculating drag force*/
c1=1.25*3.14*pnitrogen*d*d;
cre=pnitrogen*d/unitrogen; /*constant for calculating the reynold’s number*/

/*calculate charge per droplet*/
l=v0/f; /*length of jet that forms each droplet=jet velocity/frequency*/
/*capacitance between jet and charging plate*/
width=width*.0254; /*convert inches to meters*/
capacitance=2.0*3.1416*60*1/(.23+log(width/od));
qd=capacittance*volt; /*charge per droplet*/

/*constant for calculating the coulomb force between droplets*/
coulu=4*3.14*e0);

/*calculate integration increment in seconds*/
h=1/(f*spd);

/*print calculated constants here*/
printf("nTHE PARAMETERS AND CONSTANTS CALCULATED FROM THE INPUTS

droplet diameter = %e (m) \n",v0,d);
printf("initial jet velocity= %f (m/s) droplet mass = %e (kg)\n",v0,f);
printf("drag constant cl = %e Reynolds constant= %f\n",cl,cre);
printf("jet length/drop= %e (m) capacitance= %e (F)\n",l,capacittance);
printf("charge per drop= %e (C) coulomb force constant= %e\n",qd,coulu);
printf("integration step size= %e\n",h);

/*dynamically allocate memory for array to store droplet position+velocity*/
a=calloc(td.sizeof(double *));
for(i=0;i<td;i++){
  a[i]=calloc(6.sizeof(double));
}
current=calloc(td.sizeof(double *));
for(i=0;i<td;i++){
  current[i]=calloc(6.sizeof(double));
}

/*loop to create droplets and calculate droplet trajectories*/
dif=0;
while(deposited<td){ /*continue running until all drops reach substrate*/
  if(n<0&&n<1){ /*create drops until all are created*/
    for(k=0;k<norf;k++) { /*create droplets with random disturbance in this loop*/
      a[0][0]=orf[k][0]+disturbance*d*(.5-rand()*1.0/RAND_MAX); /*x-position*/
      a[0][1]=orf[k][1]+disturbance*d*(.5-rand()*1.0/RAND_MAX); /*y-position*/
      a[0][2]=0; /*initial z-position*/
      a[0][3]=sin(orf[k][2])*v0; /*initial x-velocity*/
      a[0][4]=0; /*initial y-velocity*/
      a[0][5]=cos(orf[k][2])*v0; /*initial z-velocity*/
      nd=1; /*keep track of total droplets created*/
    }
  }
}
dif++1;       /*keep track of number of droplets in flight*/
}
)
for(j=0;j<spd;j++){ /*do this many calculations between droplet creations*/
    if(count==1)
        timed+=h;
    for(i=nd;i>nd-dif;i--){ /*store current position of droplets before*/
        for(k=0;k<6;k++)
            /*runge-kutta steps*/
            current[i][k]=a[i][k];
    }
    if(a[mp][2]>level){
        spread(a,td);
        level+=distance/50;
    }
    if(nd>mp+1)
        thermal_state(a,h,Tgas);
    for(c=1;c<(dif+1);c++)
        /*for each drop in flight use runge kutta*/
        n=nd-c;
        runge_kutta(n,a,uprime,vprime,wprime,h);
    }
    step+=1;
    printf("nstep= %d",step);
}

/*call output formatting functions here after completing simulation*/
output(td,a);       /*print results to output file*/
if(norf==1)
    rcut(td,a);       /*radial cross-section of deposit*/
grid(td,a,passes.speed,timed); /*3D shape of deposit and moving cross-section*/

/*print important simulation results*/
printf("nnSIMULATION RESULTS

time=spd*step*h;
printf("Simulation time= %lf\n",runtime);
printf("nxmin= %lf\n",xmin.xmax);
printf("nxmax= %lf\n",xmax.xmin);
printf("nymax= %lf\n",ymin.ymax);
printf("nmax= %lf\n",rmax);

deposited=td-dif;     /*total number of droplets that reach substrate*/
printf("nnumber of droplets deposited= %d\t",deposited);
totalmass=deposited*md*1000; /*total mass deposited in grams*/
printf("ntotal mass deposited= %e (g)\n",totalmass);
printf("ntotal time depositing droplets= %e\n",timed);
}

/*fourth-order runge-kutta function*/
void runge_kutta(int n, double **a,
    double (*uprime)(double, double, double, double, double, double, int, double **, double),
    double (*vprime)(double, double, double, double, double, double, int, double **, double),
    double (*wprime)(double, double, double, double, double, double, int, double **, double, double, double)
    ,double h)
{
    double u,v,w,x,y,z;
    double xa,ya,za,xb,yb,zb,xc,yc,zc,xd,yd,zd;
    double va,ub,uc,ud,va,vb,vc,vd,wa,wb,wc,wd;
    double ul,vl,wx,yl,zl;
    double vel,rc,cd,c2;
    double radius;
    /*loop to perform runge-kutta steps*/
    u=a[n][3];
v=a[n][4];
w=a[n][5];
x=a[n][0];
y=a[n][1];
z=a[n][2];

vel=sqrt((u*u)+(v*v)+(w*w)); /*find absolute velocity*/
re=cre*vel; /*find Reynolds number*/

cd=.28+(6/sqrt(re))*(21/re); /*find drag coefficient*/
c2=(c1*cd*vel); /*drag force constant*/

ua= h * uprime(u,v,w,x,y,z,n,a,c2);
xu= h * u;
va= h * vprime(u,v,w,x,y,z,n,a,c2);
yu= h * v;
wa= h * wprime(u,v,w,x,y,z,n,a,c2, re, cd);
zu= h * w;

ul=u+ua/2;vl=v+va/2;wl=w+wa/2;
xl=x+xu/2;yl=y+yu/2;zl=z+zu/2;
vel=sqrt((ul*ul)+(vl*vl)+(wl*wl));
re=cre*vel;

cd=.28+(6/sqrt(re))*(21/re);
c2=(c1*cd*vel);

ub= h * uprime(ul,vl,ul,yl,zl,n,a,c2);
xb= h * ul;
vb= h * vprime(ul,vl,ul,yl,zl,n,a,c2);
ymb= h * vl;
wb= h * wprime(vl,ul,yl,yl,zl,n,a,c2, re, cd);
zb= h * wl;

ul=u+ub/2;vl=v+vb/2;wl=w+wb/2;
xl=x+xb/2;yl=y+yb/2;zl=z+zb/2;
vel=sqrt((ul*ul)+(vl*vl)+(wl*wl));
re=cre*vel;

cd=.28+(6/sqrt(re))*(21/re);
c2=(c1*cd*vel);

uc= h * uprime(ul,vl,ul,xl,yl,zl,n,a,c2);
xc= h * ul;
vc= h * vprime(ul,vl,ul,xl,yl,zl,n,a,c2);
yc= h * vl;
wc= h * wprime(ul,vl,ul,xl,yl,zl,n,a,c2, re, cd);
zc= h * wl;

ul=u+uc/2;vl=v+vc/2;wl=w+wc/2;
xl=x+xc/2;yl=y+yc/2;zl=z+zg/2;
vel=sqrt((ul*ul)+(vl*vl)+(wl*wl));
re=cre*vel;

cd=.28+(6/sqrt(re))*(21/re);
c2=(c1*cd*vel);

ud= h * uprime(ul,vl,ul,xl,yl,zl,n,a,c2);
xd= h * ul;
vd= h * vprime(ul,vl,ul,xl,yl,zl,n,a,c2);
xd= h * vl;
wd= h * wprime(ul,vl,ul,xl,yl,zl,zl,n,a,c2, re, cd);
zd= h * wl;

/*updates position and velocity for each increment*/
a[n][3]= u + ua/6+ ub/3+ uc/3+ ud/6;
a[n][0]= x + xa/6+ xb/3+ xc/3+ xd/6;
a[n][4]= v + va/6+ vb/3+ vc/3+ vd/6;
a[n][1]= y + ya/6+ yb/3+ yc/3+ yd/6;
a[n][5] = w + wa/6 + wb/3 + wc/3 + wd/6;
a[n][2] = z + za/6 + zb/3 + zc/3 + zd/6;

if((a[n][2])>distance) {/*check to see if droplet has reached substrate*/
    dif=1;  /*reduce number of droplets in flight*/
    count=1;  /*flag to indicate when first drop lands*/
    deposited+=1;
}
x=a[n][0];
y=a[n][1];
if(x>xmax)  /*keep track of minimum and maximum of parameters*/
    xmax=x;
if(x<xmin)
    xmin=x;
if(y>ymax)
    ymax=y;
if(y<ymin)
    ymin=y;
radius=sqrt((x*x)+(y*y));
if(radius>rmax)
    rmax=radius;
}

"uprime function to find acceleration in x"/
double uprime(double u, double v, double w, double x, double y, double z, int n, double **a, double c2)
{
    int k;
    double dx,dy,dz,r;
    double fcoul,totalfcoul,prime;
    totalfcoul=0;
    /*find coulomb force acting on drop n from nn*2 nearest neighbors in this loop*/
    for(k=(n-nn);k<(n+nn);k++)
        if((k<n)&&(k>(n-dif)))
            if(k!=n)
                /*don't calculate for same droplet*/
                dx=x-current[k][0];  /*x-distance between the droplets*/
                dy=y-current[k][1];  /*y-distance between the droplets*/
                dz=z-current[k][2];  /*z-distance between the droplets*/
                r=sqrt((dx*dx)+(dy*dy)+(dz*dz));  /*absolute distance between the drops*/
                fcoul=ccoul*(dx/pow(r,3.0));  /*calculate force between the drops*/
                totalfcoul+=fcoul;  /*sum coulomb forces*/
}

"drag force acting in x-direction=c2*u"/
prime=(1/md)*(totalfcoul-(c2*u));  /*find total acceleration*/
return(prime);
}

"vprime function to find acceleration in y"/
double vprime(double u, double v, double w, double x, double y, double z, int n, double **a, double c2)
{
    int k;
    double dx,dy,dz,r;
    double fcoul,totalfcoul,prime;
    totalfcoul=0;
    for(k=(n-nn);k<(n+nn);k++)
        if((k<n)&&(k>(n-dif)))
            if(k!=n)
                /*don't calculate for same droplet*/
                dx=x-current[k][0];  /*x-distance between the droplets*/
dy=y-current[k][1]; /*y-distance between the droplets*/
dz=z-current[k][2]; /*z-distance between the droplets*/
r=sqrt((dx*dx)+(dy*dy)+(dz*dz)); /*absolute distance between the drops*/
f Coul=ccoul*(dy/pow(r,3.0)); /*calculate force between the drops*/
totallfcoul+=f Coul;
}

/*drag force acting in y-direction=c2*v*/
prime=(1/md)*(totallfcoul-(c2*v)); /*find total acceleration*/
return(prime);
}

/*wprime function to find acceleration in z*/
double wprime(double u, double v, double w, double x, double y, double z,
int n, double **a, double c2, double re, double cd)
{
    int k;
    double dx,dy,dz,r;
    double f Coul,totallfcoul,prime;
    double clearance,cd_rod,cd_one,cd_one_plus,cd_stream,cd_combined;
    totallfcoul=0;
    for(k=(n-nn):k<(n+nn):k++) {
        /*find coulomb force acting on drop n from nearest neighbor.*/
        if((k<n)d&& (k>(nd-dif))){
            /*check to make sure drop exists and is in flight*/
            if(k!=n){
                /*don't calculate for same droplet*/
                dx=x-current[k][0]; /*x-distance between the droplets*/
                dy=y-current[k][1]; /*y-distance between the droplets*/
                dz=z-current[k][2]; /*z-distance between the droplets*/
                r=sqrt((dx*dx)+(dy*dy)+(dz*dz)); /*absolute distance between the drops*/
                f Coul=ccoul*(dz/pow(r,3.0)); /*calculate force between the drops*/
                totallfcoul+=f Coul;
            }
        }
    }

    /*drag force acting in z-direction=c2*w*/
    clearance=sqrt(x*x+y*y);
    if(clearance>(d/2)||n<0)
    prime=9.81*(1/md)*(totallfcoul-(c2*w)); /*find total acceleration if drop in free flight*/
    else{
        /*correct drag for effects of neighboring droplets*/
        cd_rod=.755/re;
        cd_one= pow(pow(cd_rod,-.678)-pow(cd,-.678),(-1.0/.678));
        cd_one_plus= cd_one+((43/re)*((w/f)/d)-1);
        cd_stream= pow(pow(cd_one_plus,-.678)+pow(cd,-.678),(-1.0/.678));
        cd_combined= ((1-clearance/(d/2))^cd_stream+((clearance/(d/2))^cd);
        prime=9.81*(1/md)*(totallfcoul-cd_combined*p nitrogen*d*d*.125*3.142));
    }
    return(prime);
}

/*function to create enthalpy and velocity plots for drops*/
void thermal_state(double **a, double h, double Tgas)
{
    double re,ht,q,vel,emelt,liqfrac,as,zvel,rvel;
    double clearance,cd_rod,cd_one,cd_one_plus,cd_stream,cd_combined;
    int i,j;reduce;
    emelt=md*(T-Tgas)*cnsolid; /*enthalpy required to begin melting a drop*/
    if((a[mp][5]>0)&&(a[mp][2]<distance)){
        vel=sqrt((a[mp][3]*a[mp][3])+(a[mp][4]*a[mp][4])+(a[mp][5]*a[mp][5]));
        re=cre*vel;
        /*calculate Reynolds's number*/
    }
}

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ht=(knitrogen/d)*(2.0+ (6*(sqrt(re)*pow(Pr,(1.0/3.0)))))
clearance=sqrt((a[m][0]*a[m][0])+(a[m][1]*a[m][1])); /*find distance from center*

if (clearance<(d/2) & & norf=1) { /*find adjustment factor for h*/
  cd=2.28*(6/sqrt(re))+(21/re); /*find drag coefficient*/
  cd_rod=7.75/re;
  cd_one= pow((pow(cd_rod,-.678)-pow(cd,-.678)),(-1.0/.678));
  cd_one_plus= cd_one+(43/re)*(((a[m][5]/f)/d)-1);
  cd_stream= pow((pow(cd_one_plus,-.678)+pow(cd, -.678)), (1.0/.678));
  cd_combined= ((1-(clearance/(d/2)))*cd_stream+((clearance/(d/2))*cd);
  ht=(cd_combined/cd)*ht; /*adjusted heat transfer for a series of droplets*/
}

as=4/3.142*(pow((d/2.0),2.0)); /*surface area of the droplet*/
q=ht*as*(temp-Tgas); /*rate of heat transfer from one drop W/(J/s)*/
e=e-(q*h);
if(temp>Ts){
  temp=temp-(((q*h)/cmliquid)/md); /*droplet temperature if above melting point*/
  liqfrac=1.0;
}
else{
  if(e<emelt){
    temp=temp-(((q*h)/cmsolid)/md); /*droplet temperature if below melting point*/
    liqfrac=0;
  }
  else
    liqfrac=(e-emelt)/(hof/md); /*liquid fraction during solidification*/
}

reduce=(a[m][2]*200); /*only write to data file after each half mm*/
if(reduce>old){
  for(i=mp-5;i<mp+5;i++){
    zvel=a[i][5]; /*average z-velocity*/
    rvel=sqrt(pow(a[i][3],2)+pow(a[i][4],2)); /*average radial velocity*/
  }
  zvel=zvel/10;
  rvel=rvel/10;
  dro=fopen("drop.m","a");
  fprintf(dro,"%lf %lf %lf %lf %lf %lf %e\n",a[m][2],zvel,rvel,term,liqfrac,e);
  fclose(dro);
  old=reduce;
}
}

/*/function to find maximum spread of spray cone and radial velocity*/
void spread(double **a, int td)
{
  int i,j;
double r, maximum, width;
double rvel, rvelmax;
for(i=0;i<td;i++){
  r=sqrt(pow(a[i][0],2)+pow(a[i][1],2)); /*spread cone radius*/
  rvel=sqrt(pow(a[i][3],2)+pow(a[i][4],2)); /*radial velocity*/
  if(r>maximum){
    maximum=r;
    j=i;
  }
  if(rvel>rvelmax){
    rvelmax=rvel;
    j=i;
  }
}
width=2*maximum; /*convert maximum radius to spray width*/
spr=fopen("spread.m","a");
fprintf(spr,"%lf\t%lf\t%lf\n",a[j][2],width,rvelmax);
fclose(spr);
}

/*output function to print results to data file*/
void output(int td,double **a)
{
    double x,y,z,u,v,w;
    int m;
    /*print droplet impact positions and velocities*/
    res=fopen("results.m","w");
    for(m=0;m<td;m++){
        x=a[m][0];
        y=a[m][1];
        z=a[m][2];
        u=a[m][3];
        v=a[m][4];
        w=a[m][5];
        fprintf(res,"%lf %lf %lf %lf %lf %lf\n",x,y,z,u,v,w);
    }
    fclose(res);
}

/*function to create histogram of x-position*/
void histogram(int td, double **a)
{
    double range,size,xaxis,normalf;
    int num,p,i,j;
    int *f;
    range=xmax-xmin;
    size=5*d; /*size of intervals in histogram*/
    num=range/25; /*number of intervals on histogram*/
    /*dynamically allocate memory for array to store frequency*/
    f=malloc(num,sizeof(int));
    for(i=0;i<td-dif;i++){
        p=((a[i][0]-xmin)/size);
        f[p]++;
    }
    his=fopen("histogram.m","w");
    for(j=0;j<num;j++){
        xaxis=xmin+j*size+size/2;
        normalf=(1.0*f[j])/(td-dif);
        fprintf(his,"%lf %lf\n",xaxis,normalf);
    }
    fclose(his);
}

/*function to create histogram across radius*/
void rcut(int td, double **a)
{
    double size,range,r,xaxis,ro,ri,area,volume,heigth;
    int num,p,i,);
    int *f;
    range=rmax;
    size=rmax/4;
    fprintf(spr,"%lf\t%lf\t%lf\n",a[j][2],width,rvelmax);
    fclose(spr);
}
num=range/size; /*number of intervals on histogram*/

/*dynamically allocate memory for array to store frequency*/
f=callloc((num+5).sizeof(int));
for(i=(2*nn);i<(td-2*nn);i++){
    r=sgt(pow(a[i][0],2.0)+pow(a[i][1],2.0));
    p=r/size;
    f[p]=f[p]+1;
}
cut=fopen("cut.m", "w");
for(j=(num-1);j>=0;j--){
    xaxis=-1.0*(j*size+size/2);
    ro=(j+1)*size; /*outer radius of area*/
    ri=j*size; /*inner radius of area*/
    area=3.142*(ro*ro-ri*ri);
    volume=(1.0*f[j])*3.142*(1.0/6.0)*pow(d,3.0);
    height=volume/area;
    fprintf(cut,"%lf %e\n",xaxis,height);
}
for(j=0;j<num;j++){
    xaxis=j*size+size/2;
    ro=(j+1)*size; /*outer radius of area*/
    ri=j*size; /*inner radius of area*/
    area=3.142*(ro*ro-ri*ri);
    volume=(1.0*f[j])*3.142*(1.0/6.0)*pow(d,3.0);
    height=volume/area;
    fprintf(cut,"%lf %e\n",xaxis,height);
}
fclose(cut);

/*function to create grid of x and y locations*/
void grid(int td, double **a, int int passes, double speed, double timed)
{
    double x,y,size,range,area,volume,heigh,flux,heigt,pos;
    double min;
    int fraction;
    int num, xl, yl;
    int j, k;
    int **pm; /*array for stationary deposition pattern*/
    int **mv; /*array for moving substrate shape*/
    
    range=rmax*2;
    size=range/(N*norf);
    area=size*size;
    N=(range/size)+2;
    N=(N/2)*2; /*convert to an even number*/
    num=N*N; /*number of sections on grid*/
    min=(N/2)*size;
    printf("\nThe grid size for the mesh is %e (m) \t N= %d\n",size,N);

    /*dynamically allocate memory for array to store frequency*/
    m=callloc(N,sizeof(int *))
    for(i=0;i<N;i++){
        m[i]=callloc(N,sizeof(int));
    }

    for(i=(2*nn);i<nd-(2*nn);i++){
        x=a[i][0];
        y=a[i][1];
        xl=1*(x+min)/size;
    }
}
yl=1*(y+min)/size;
if((x1<0)||(y1<0)){
x1=0;
y1=0;
}
m[y1][x1]+=1.0;
}
gri=fopen("grid.m","w");
for(j=0;j<N/2;j++){
for(k=0;k<N/2;k++){
    volume=(1.0*m[j][k])*3.142*(1.0/6.0)*pow(d, 3.0);
    height=volume/area;
    fprintf(gri,"%e\t","heigth");
}
fprintf(gri,"\n");
}
fclose(gri);
/*print out a grid of fraction of mass flux per square*/
ngr=fopen("ngrid.m","w");
fprintf(ngr,"\n\nFraction (/1000) of Total Mass Flux Per Grid\n\n");
fprintf(ngr,"\n\n y-axis\n");
for(j=0;j<N/2;j++){
for(k=0;k<N/2;k++){
    fraction=((1.0*m[j][k])/(td-4*nn))*1000;
    fprintf(ngr,"%d ",fraction);
    if(fraction<10)
        fprintf(ngr," ");
}
fprintf(ngr,"\n");
for(k=0;k<N/2;k++){
    fraction=((1.0*m[j][k])/(td-4*nn))*1000;
    fprintf(ngr,"%d ",fraction);
    if(fraction<10)
        fprintf(ngr," ");
}
fprintf(ngr,"\n");
}
for(i=0;i<N;i++)
    fprintf(ngr, "---");
fprintf(ngr,"\n\nx-axis\n");
for(j=N/2;j<N;j++){
for(k=0;k<(N/2);k++){
    fraction=((1.0*m[j][k])/(td-4*nn))*1000;
    fprintf(ngr,"%d ",fraction);
    if(fraction<10)
        fprintf(ngr," ");
}
fprintf(ngr,"\n");
for(k=0;k<N/2;k++){
    fraction=((1.0*m[j][k])/(td-4*nn))*1000;
    fprintf(ngr,"%d ",fraction);
    if(fraction<10)
        fprintf(ngr," ");
}
fprintf(ngr,"\n");
}
fclose(ngr);

ndr=fopen("dgrid.m","w");
for(j=0;j<N;j++){
for(k=0;k<N;k++){
    fprintf(ndr,"%d ",m[j][k]);
    if(m[j][k]<10)
        fprintf(ndr," ");
}
fprintf(ndr, "\n");
}
fclose(ndr);

/*find shape when substrate is moving along y-axis*/
mv=calloc((N+3).sizeof(double));
for(i=0;i<N;i++) {
    /*sum drops in each mesh line along y-axis*/
    for(j=0;j<N;j++) {
        mv[i]+=m[j][i];
    }
}

mv=fopen("moving.m","w");
for(i=0;i<N;i++) {
    /*volume flux per second*/
    flux=(1.0*mv[i]*3.142*(1.0/6.0)*pow(d,3.0))/((td-4*nn)/f);
    height=size*N/speed*(flux/(area*N))*passes;
    pos=-min+(i*size)-(size/2.0);
    fprintf(mv,"%e %e
",pos,height);
}
fclose(mv);

amv=fopen("movingavg.m","w");
for(i=0;i<N/2;i++) {
    flux=(1.0*(mv[i]+mv((N-i-1)))*3.142*(1.0/6.0)*pow(d,3.0))/(2*((td-4*nn)/f));
    /*volume flux per second*/
    height=size*N/speed*(flux/(area*N))*passes;
    pos=-min+(i*size)-(size/2.0);
    fprintf(amv,"%e %e
",pos,height);
}
for(i=((N/2)-1);i>-1;i--){
    flux=(1.0*(mv[i]+mv((N-i-1)))*3.142*(1.0/6.0)*pow(d,3.0))/(2*((td-4*nn)/f));
    /*volume flux per second*/
    height=size*N/speed*(flux/(area*N))*passes;
    pos=-1.0*(min+(i*size)+(size/2.0));
    fprintf(amv,"%e %e
",pos,height);
}
fclose(amv);