NUMERICAL STUDY ON MORPHOLOGY AND SOLIDIFICATION CHARACTERISTICS OF SUCCESSIVE DROPLET DEPOSITIONS ON A SUBSTRATE

by

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Abstract

Numerical Study on Morphology and Solidification Characteristics of Successive Droplet Depositions on a Substrate

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Successive droplet impingement finds extensive applications in additive manufacturing technologies such as 3D printing, Liquid Metal Jetting and Net Form Manufacturing. Deposition, deformation and solidification of droplets are the constitutive stages in the process which determine the final outcome. Detailed knowledge about the flow behaviour, phase transformation and free surface deformation is required to have a complete understanding and optimization of the process parameters. Experimental research in this field is only limited to imaging techniques and post solidification analysis which only provide superficial information while overlooking most of the governing phenomenon. Knowledge of the physics governing the fluid and thermal behaviours can be applied to study the process with real time data pertaining to flow field, temperature profiles and solidification. However, free surface tracking, surface tension modelling, non-isothermal solidification and convection dominant heat transfer pose mathematical challenges in the solution of the governing equations. Moreover, deposition of droplets on pre-solidified splats or non-flat surfaces requires accurate special attention. The objective of the present work is to model the successive droplet impacts and simultaneous solidification and deformation.
The highly non-linear flow field governed by the Navier Stokes equation is solved using a Two Step Projection method. The surface tension effects are accounted for through a Continuum Surface Force technique. One of the crucial elements in the study is the interface tracking algorithm. A Coupled Level Set Volume of Fluid (CLSVOF) method is formulated to give an accurate orientation of the drastically deforming interface and also facilitates generation of multiple droplets in a fixed domain at a user defined frequency, thereby conserving computational resources. The phase change is modelled using an enthalpy formulation of the energy equation with an implicit source term accounting for the latent heat. It is coupled with the flow solver through an Enthalpy-Porosity technique. A modified boundary condition which incorporates the contact resistance has also been implemented.

The case of multiple eutectic solder droplet depositions has been simulated to study the various aspects of splat morphology and solidification characteristics. Effects of impact conditions on single as well as successive droplet depositions have been examined. The role of convection terms in the energy equation has been emphasized and quantitatively analysed. The effect of impact velocity is manifested as surface curvature of the pre-solidified splat and in turn, affects morphology of the subsequent droplets. Initial droplet temperature influences the solidification time of both single and multiple droplets. Under certain conditions, remelting of pre-solidified splat has been observed and its causes have been discussed. Contact resistance has been reported in the literature and has been found to have a strong influence not only on the heat transfer but also the spreading behaviour. Frequency of successive impingements is also an important factor affecting the metallurgical bonding properties.
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Chapter 1

Introduction

Evolution of conventional two-dimensional printing to construct three dimensional objects has brought about a plethora of applications in the field of Additive Manufacturing (AM). Due to its design freedom, enhanced mechanical properties, and lower porosity [1] compared to conventional manufacturing systems, AM is widely applied in fields of aerospace, automobile and biomedical. In recent years, studies are primarily focused on AM’s potential to fabricate intricate and functional parts through metals and alloys [2]. 3D printing, Liquid Metal Jetting (LMJ), Net-Form Manufacturing and Digital Microfabrication are commonly used AM methods for such applications.

Figure 1-1 Example of Droplet Generation
Additive manufacturing of metal and alloys are usually carried out by droplet deposition. Droplet generation for deposition process is a complex phenomenon. Figure 1-1 illustrates an example of a droplet generation process. The metal or alloy is melted in a crucible and the liquid metal is ejected from a nozzle as droplets through the combined action of surface tension, pressure pulse, and gravity. The pressure pulses are generally actuated by electrostatic, thermal or other actuators at specified time intervals. Droplets are generated by two main modes: Continuous Stream (CS) and discrete drops also known as Drop On Demand (DOD) [3]. Latter is widely used due to its placement accuracy, spatial resolution and greater control over temperature, velocity and size of droplets. Figure 1-2 highlights the difference between the two modes. In continuous Stream mode, fluids are continuously ejected from the nozzle and eventually breaks into droplets due to Rayleigh instability or any other perturbing techniques. In (DOD) method, individual droplets are produced directly from the nozzle.
Due to kinetic energy, thermal inertia and the temperature gradient between the droplet and substrate, the droplet spreads continuously. Kinetic energy dissipation of the droplet by solidification at the wetting line and viscous damping arrests the spreading of the droplet. Once the kinetic energy of the droplet is dissipated it recoils due to surface tension force which leads to subsequent oscillation. The various stages of splat dynamics are highlighted in Figure 1-3.

In addition to viscous damping, simultaneous solidification at contact line affects the splat morphology. Droplet impacting on an adiabatic surface at low Reynolds number recoils back due to surface tension and eventually forms a bump. Simultaneous solidification impedes the spreading and affects the recoil and oscillations of the droplet.
Depending on the impact condition and thermal parameters, the droplet either forms a splat, crown or a bump as shown in Figure 1-4.

Figure 1-4 Splat Morphology

A droplet pileup process can be used as a building block for fabricating a complex three-dimensional object. In which molten metal droplet impacts and solidifies on top of a
pre-solidified droplet. An overview of pile up process is shown in Figure 1.5. The objective of this process is to deposit multitude of individual molten droplets at a precise location which solidifies on impact to form a three-dimensional structure. Splat dynamics of a pileup process is similar to that of single droplet deposition but on a non-flat surface of same material rather than a flat substrate.

To fabricate intricate and functional parts through droplet-based Additive Manufacturing system it is essential to achieve a comprehensive understanding of the complex physical phenomena involved in a droplet pileup process. The successive molten droplets experience a drastic change in morphology upon impact due to the curvature of the pre-solidified droplet. Because of which it is important to study spread, recoil and oscillation characteristics and as well free surface deformation of molten droplets impacting on non-flat surfaces of the same material. Formation of satellite droplets due to break off from the main droplet, splat formation, and droplet break off on impact has a negative effect on the conversion of liquid metal to a solid geometry [3]. The above stated challenges are highly dependent on velocity, size and temperature of the droplets. To determine experimentally these quantities are extremely difficult due to the length and time scales involved which are usually in the order of microns and microseconds. Although liquid metal droplet-based manufacturing technologies are widely used still problems like metallurgical bonding, voids, and cold lap exists. To ensure forming accuracy and metallurgical bonding between the droplets, greater understanding of the phase change process involved in droplet pile up is necessary. The imaging techniques used experimentally provides only a real time superficial free surface deformations of the droplets and not accounting for the phase of the droplets deposited. Numerical simulations offers an alternative mean which gives greater insight to droplet deposition and pileup process. The findings of the research and be used to determine the process parameters used for the actual process.
1.1 Literature Review

Over the past two decades, there have been extensive studies on droplet depositions, both experimental and theoretical [5]–[9]. Most of the works focus on impact, spreading, recoil and solidification of a single droplet impacting onto a substrate with very little information reported on droplet pileup process. Till date, most of the available literatures are devoted to droplet generation and on the process of creating objects by droplet deposition. An Initial study on droplet deposition for creating 3D objects was reported by Sonin et al.[10] The study was conducted on columnar wax deposition. Analytical estimates of solidification time and solidification angle were reported. Adhesion effects due to the frequency of droplet were also analyzed. Works of Liu and Orme [11] gave a greater insight to droplet printing technology. The study which includes both experimental and numerical aspects, mostly focused on droplet generation and its application to digital microfabrication. Harfel et al. [12] reported an experimental study on transport and solidification phenomena in microdroplet pileup. The spreading and splat dynamics were analyzed. Various numerical studies on droplet deposition on single droplet deposition were reported. There has been only a few numerical studies reported on droplet impact on a non-flat surface in the literature. Liu et al.[13] numerically investigated the impact of droplets on non-flat surfaces but the energy equation was not taken into account. Harfel et al. [14] also conducted a numerical scheme which was based on an axis symmetric Lagrangian multi-domain Finite Element Model. No front tracking method was used to track the free surface or the interface. The numerical results showed a disagreement at higher substrate temperatures. The literature also highlighted the role of capillary effects at higher temperatures. Du et al. [15] numerically studied pileup process using a commercial code.
The pioneering work in the modeling of phase change was the classical Stefan problem [16]. The model accounted for isothermal solidification in a multi-domain. The works of Brent et al. [17] made it possible to express the phase change phenomenon in a continuum domain. A non-isothermal phase change model was developed. Phase change process occurs over a region called mushy region which is bounded by solidus temperature ($T_s$) and liquidus temperature ($T_l$) as shown in Figure 1-6. The enthalpy formulation was coupled to the flow field through a pseudo porosity method. Tong and Holt [7] used the enthalpy-porosity approach in studying a single copper droplet deposition on a substrate by numerically solving the complete energy equation inclusive of convection terms. The isothermal solidification front was approximated as an infinitesimally small artificial mushy region. The current numerical formulation is based on the work of Tong and Holt [19] with
an improved interface tracking method (Coupled Level Set Volume Of Fluid method) and interface reconstruction scheme (PLIC) for the free surface. Furthermore, the present study introduces a new method of generating multiple droplets successively by re-initialization of the VOF functions which has been a limitation in most of the numerical studies[15]. It has the advantage of having greater control over the frequency of droplets generated thereby reducing computational domain and computational resources. The primary objective of this study is to investigate the effects of important process parameters and material properties on the splat dynamics and solidification behavior of liquid metal droplets sequentially impinging onto a substrate. The numerical formulation is briefly described in Chapter 2 followed by experimental comparison and results and discussion. The scope of further improvements of the present work is also given.
As mentioned in the previous section, the solution for flow field, interface tracking and reconstruction, modeling of phase change and solution of the energy equation are the primary aspects of the numerical algorithm. In general, the continuity equation, Navier-Stokes equation and the energy equation need to be solved simultaneously. However, the presence of multiple interfaces and phase transformation make the process more challenging. A finite volume approach on a fixed grid is used here for the discretization of the governing equations. The formulation of the governing equations on a continuum domain is discussed here along with various aspects of solidification. The variations of the thermo-fluid properties (excluding specific heat) with temperature throughout the scope of the present study have been neglected to emphasize the effects of solidification models discussed later.

2.1 Flow Governing Equations

The classical continuity and Navier-Stokes equations govern the flow field. However, due to the presence of multiple phases within the domain the governing equations need to be modified as follows:

\[ \nabla \cdot \vec{V} = 0 \]  
\[ \frac{\partial \vec{V}}{\partial t} + \nabla \cdot (\vec{V} \vec{V}) = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \vec{r} + \frac{1}{\rho} \vec{F}_b + S_v \]  

Note that the density variation terms from both equations have been dropped because the flow is considered incompressible.
\( \theta \) is a quantity defined as liquid fraction which denotes the volume fraction of liquid within a given control volume. The basic assumption in the formulation is that solid particles are treated as a continuous stationary medium. The region where solid as well as liquid media are present is defined as mushy region. Quantification of the liquid fraction and modeling of mushy region is dependent on the phase change process and will be discussed later. For the purpose of determining the flow field, solid portion is considered as a blockage within a flowing fluid medium. Thus, mushy region can also be modeled as a porous medium where porosity is determined from the solidification model. The term \( S_v \) in Equation 2.2 represents pressure impedance experienced through blockage. The classical Darcy’s theory for flow in a porous medium states that the deceleration due to blockage can be written as:

\[
S_v = -A \vec{V} \quad \text{and} \quad A = \frac{-C (1 - \theta)^2}{(\theta^3 + \epsilon)} \tag{2.3}
\]

The viscous stress for Newtonian fluids in Equation 2.2 is given by

\[
\tau = 2\mu S \quad \text{and} \quad S = \frac{1}{2} \left[ (\nabla \vec{V}) + (\nabla \vec{V})^T \right] \tag{2.4}
\]

where ‘S’ is the rate-of-strain tensor. Taking the fluid-gas interface as a shear-free surface, the scalar boundary condition can be written as

\[
\Delta P_s = \sigma K \tag{2.5}
\]

where \( K \) denotes the local curvature and \( \sigma \) is the surface tension. Note that \( \Delta P_s \) is the jump in fluid pressure across the interface and poses a discontinuity. A continuum surface force method[20] is employed to translate the surface boundary condition into a body force distributed across a finite thickness near the free surface. This body force is mathematically represented as:

\[
\vec{F}_b = \vec{F}_{sv} = \sigma K \vec{\hat{n}} \tag{2.6}
\]
where K is the curvature and \( \hat{n} \) is the unit vector perpendicular to the surface area which will be defined later.

A two-step projection algorithm outlined in [21] is used to solve for the flow field.

Equation 2.2 is discretized in time as

\[
\frac{\theta V^{n+1} - \theta V^n}{\delta t} = - \nabla \cdot (\theta \overline{V})^n + \frac{\theta^n}{\rho^n} \nabla p^{n+1} + \frac{\theta^n}{\rho^n} \nabla \cdot \overline{\tau} + \frac{\theta^n}{\rho^n} F_b^n + \frac{\theta^n}{\rho^n} \overline{S_v}^n
\]  (2.7)

The above equation is then decomposed into two parts.

\[
\frac{\overline{V}' - (\theta \overline{V})^n}{\delta t} = - \nabla \cdot (\theta \overline{V})^n + \frac{\theta^n}{\rho^n} \nabla \cdot \overline{\tau} + \frac{\theta^n}{\rho^n} \overline{F_b}^n + \frac{\theta^n}{\rho^n} \overline{S_v}^n
\]  (2.8)

and

\[
\frac{\theta V^{n+1} - \overline{V}'}{\delta t} = - \frac{\theta^n}{\rho^n} \nabla p^{n+1}
\]  (2.9)

where \( \overline{V}' \) represents an intermediate velocity. In the first step, \( \overline{V}' \) is computed from Equation 2.8 which accounts for the incremental changes resulting from viscosity, advection, gravity, and body forces (\( F_b \) and \( S_v \)). The second step involves taking the divergence of Equation 2.9 while projecting the velocity field, \( (\theta \overline{V})^{n+1} \) onto a zero-divergence vector field for mass conservation. This results in a single Poisson equation for the pressure field given by:

\[
\nabla \cdot \frac{\overline{V}'}{\delta t} = \nabla \cdot \left[ \frac{\theta^n}{\rho^n} \nabla p^{n+1} \right]
\]  (2.10)

Equation 2.10 is solved using an Incomplete Cholesky Conjugate Gradient technique (ICCG) [22].
2.2 Interface Tracking Schemes

The present study employs a Coupled Level Set Volume of Fluid Method (CLSVOF) algorithm for interface tracking and reconstruction. This method uses two classical schemes: Volume of Fluid (VOF) and Level Set (LS). The information from both these methods is incorporated in an interface construction scheme which will be discussed later. A brief introduction of the VOF and LS methods is presented here followed by their integration in a CLSVOF algorithm.

2.2.1 Volume of Fluid Method (VOF)

The volume of fluid (VOF) function, \( F \), defined as:

\[
F = \frac{Volume\ occupied\ by\ fluid}{Total\ volume\ of\ the\ computational\ cell} \tag{2.11}
\]

Following information can be interpreted from this definition:

\[
F = \begin{cases} 
1 & \text{Completely Filled} \\
0 < F < 1 & \text{Partially Filled} \\
0 & \text{Void} 
\end{cases} \tag{2.12}
\]

To better understand the implications of a VOF function, consider a hypothetical circular fluid element as shown in Figure 2-1. The domain is divided into square grids representing a control volumes. The value prescribed in each cell is its corresponding VOF function. The image conforms to the implications mentioned earlier. Once the VOF distribution is acquired in the whole domain, it is advected using

\[
\frac{DF}{Dt} = \frac{\partial F}{\partial t} + \vec{V} \cdot \nabla F = 0 \tag{2.13}
\]

The VOF function has a property of excellent mass conservation.
2.2.2 Level Set Method (LS)

The level set function is defined as a signed function whose magnitude is the shortest distance between the cell center and the interface. Following information can be interpreted from the LS values.

\[ \varphi = \begin{cases} < 0 & \text{Cell center is inside the fluid} \\ = 0 & \text{Cell center is at the interface} \\ > 0 & \text{Cell center is outside the fluid} \end{cases} \quad (2.14) \]

Figure 2-2 demonstrates an example of Level Set function distribution within a domain. The values are then advected using the following equation.

\[ \frac{D\varphi}{Dt} = \frac{\partial \varphi}{\partial t} + \vec{V} \cdot \nabla \varphi = 0 \quad (2.15) \]

After advection, the level set function values do not retain the same physical meaning and need to be re-distanced following the interface reconstruction. The interface orientation is obtained from the function as:

\[ \hat{n} = \nabla \varphi \quad (2.16) \]
The normal vector obtained in this manner gives an accurate orientation of the free surface.

Figure 2-2 Example of LS Distribution

2.2.3 Coupled Level Set Volume of Fluid Method

The coupled level set method was proposed by Tong and Wang [23] with an intention of preserving the mass conservation property of the interface tracking scheme as well as obtaining an accurate interface orientation. This was done through coupling the VOF and LS methods as described in [24] and outlined in Figure 2-3. The VOF and LS functions are individually advected using Equations 2.13 and 2.15. The new interface is reconstructed using a Piecewise Linear Interface Construction scheme [25]. The interface is assumed to be given by a straight line within a computational cell. For example, the interface definition for the case shown in Figure 2-4 is given by:

\[ y = m \cdot s + y_{\text{int}} \]  \hspace{1cm} (2.17)

where ‘m’ is the slope obtained from the normal vector, s is the x-coordinate (x for Cartesian and r for Cylindrical) and \( y_{\text{int}} \) is the intercept.
Figure 2-3 CLSVOF Algorithm

Figure 2-4 Simple PLIC Construction
Note that Figure 2-4 is just one of the sixteen different possibilities in which the interface within a cell could be oriented. The numerical algorithm proposed by Rudman[26] outlines a cell rotation and indexing routines through which each of the orientations can be transformed such that the unit normal always lies in the first quadrant and Equation 2.17 gives the interface. 'y' and 's' are the transformed coordinates corresponding to 'z' and 'r' in cylindrical systems.

2.3 Energy Equation

The conventional energy equation is given in terms of temperature as:

$$\frac{\partial T}{\partial t} + \nabla \cdot (\vec{V}T) - \nabla \cdot (\alpha \nabla T) = 0$$  \hspace{1cm} (2.18)

Phase change problems involve consideration of latent heat addition or dissipation from the system. Therefore, the above equation needs modifications to be applicable in the present work. Voller et al.[27] suggested using the total enthalpy in the energy equation rather than just sensible heat. The total enthalpy \(H\) is given as the sum of sensible heat \(h\) and latent heat \(\delta h\). Equation 2.18 can now be modified as:

$$\frac{\partial H}{\partial t} + \nabla \cdot (\vec{V}H) - \nabla \cdot (\alpha \nabla h) = 0$$  \hspace{1cm} (2.19)

and re-grouped as:

$$\frac{\partial h}{\partial t} + \nabla \cdot (\vec{V}h) - \nabla \cdot (\alpha \nabla h) + \frac{\partial \delta h}{\partial t} + \nabla \cdot (\vec{V}\delta h) = 0$$  \hspace{1cm} (2.20)

Note that diffusion terms in Equation 2.20 remain unchanged as the diffusion flux is only governed by the temperature gradient. Convection flux, on the other hand, involves the total enthalpy.

Pure metals have a unique temperature, called fusion temperature, at which complete latent heat is released (solidification) or absorbed (melting). Such a behavior
poses a discontinuity in Equation 2.20 at the fusion temperature. Therefore it becomes impossible to model isothermal phase change in materials through continuum approach. The method suggested in [19] is to approximate the phase change front as a thin mushy region of finite temperature range over which the latent heat is distributed. A qualitative enthalpy-temperature relation assuming constant specific heat is shown in Figure 1-6. The infinite dh/dT slope for an isothermal enthalpy jump is replaced with a finite slope (having a large value) confined within the temperature range T_s to T_l.

The liquid fraction is defined as the fractional fluid volume in liquid state within a control volume. Mathematically, it can be expressed as the normalized latent heat given by:

\[ \theta = \frac{\delta h}{L} = \frac{T_m - T_s}{T_l - T_s} \]  

(2.21)

which represents a linear distribution of latent heat throughout the mushy region. Following interpretation can be drawn from the value of liquid fraction:

\[ \theta = \begin{cases} 0 & \text{Matter is in solid phase} \\ 0 < \theta < 1 & \text{Matter is in mushy region} \\ 1 & \text{Matter is in liquid phase} \end{cases} \]  

(2.22)

Replacing \( \delta h \) with this definition in Equation 2.20 yields the following:

\[ \frac{\partial h}{\partial t} + \nabla \cdot (\vec{V} h) - \nabla \cdot (\alpha \nabla h) + S_h = 0 \]  

(2.23)

where

\[ S_h = L \left( \frac{\partial \theta}{\partial t} + \nabla \cdot (\vec{V} \theta) \right) \]  

(2.24)

Note that the first three terms are exactly similar to the conventional energy equation while the remaining terms play the role of energy generation or dissipation in the form of latent heat during phase change. It can be understood that the traditional energy equation is regained in pure liquid or pure solid phases. The source terms become active only within
the mushy range. Also note that this is the term appearing in the modified continuity and Navier-Stokes equation representing porosity. If the solid particles are arbitrarily assigned zero velocity, the volume averaged velocity within a control volume can be given by:

\[ \bar{V} = \theta \bar{V}_l \] (2.25)

where \( \bar{V}_l \) is the fluid velocity determined from the flow governing Equation.

A staggered grid arrangement shown in Figure 2-5 is employed to discretize the energy equation.

\[ \frac{\partial (\rho h)}{\partial t} + \frac{1}{r} \frac{\partial J_r}{\partial r} + \frac{\partial J_z}{\partial z} + S_h = 0, \] (2.26)

Where 'J' represents the net flux through a cell face as:

\[ J_r = r \left( \rho u_r h - \alpha \frac{\partial h}{\partial r} \right); J_z = \left( \rho u_z h - \alpha \frac{\partial h}{\partial z} \right) \] (2.27)

and
\[
S_h = \frac{\partial (\rho \delta h)}{\partial t} + \frac{1}{r} \frac{\partial (r \rho u_r \delta h)}{\partial r} + \frac{\partial (\rho u_z \delta h)}{\partial z}
\]  

(2.28)

Integrating the above equation over a control volume by following the notation given in Figure 2-5, the energy equation converts into

\[
\frac{(\rho_p h_p - \rho_p^0 h_p^0) \Delta r \Delta z}{\Delta t} + \frac{1}{r} \left[ (J_e - J_w) + (J_n - J_s) + S_h \Delta r \Delta z \right] = 0
\]  

(2.29)

The continuity equation integrated over the control volume yields

\[
\frac{(\rho_p - \rho_p^0) \Delta r \Delta z}{\Delta t} + \frac{1}{r} \left[ ((\rho u)_e - (\rho u)_w) + ((\rho v)_n - (\rho v)_s) \right] = 0
\]  

(2.30)

Multiplying Equation 2.30 with \( h_p \) and subtracting from Equation 2.29 gives:

\[
\frac{\rho_p (h_p - h_p^0) \Delta r \Delta z}{\Delta t} + \frac{\Delta z}{r_p} \left[ (J_e - r_e (\rho u)_e h_e) - (J_w - r_w (\rho u)_w h_w) \right] + \Delta r \left[ (J_n - (\rho u)_n h_n) - (J_s - (\rho u)_s h_s) \right] + S_h \Delta r \Delta z = 0
\]  

(2.31)

Using the generalized formulation, Equation 2.31 can be written in algebraic form as

\[
a_p h_p = a_e h_e + a_w h_w + a_n h_n + a_s h_s + a_p^0 h_p^0 + b
\]  

(2.32)

with the coefficients given by Equation 2.33. Note that an upwind advection scheme is used to discretize the source term. Introduction of certain degree of underrelaxation may be necessary depending on the thermodynamic properties to ensure stability.

\[
a_e = D_e A(\|P_e\|) + \| - F_e, 0 \|
\]

\[
a_w = D_w A(\|P_w\|) + \| F_w, 0 \|
\]

\[
a_n = D_n A(\|P_n\|) + \| - F_n, 0 \|
\]

\[
a_s = D_s A(\|P_s\|) + \| F_s, 0 \|
\]

\[
a_p^0 = \frac{\rho_p^0 2 \pi r_p \Delta r \Delta z}{\Delta t}
\]

\[
a_p = a_e + a_w + a_n + a_s + a_p^0
\]

\[
b = a_p^0 (\delta h_p - \delta h_p^0) + \text{inflow} - \text{outflow}
\]
outflow = \left[ \|F_n, 0\| (\delta h)_p - \|F_n, 0\| (\delta h)_n \right] \\
\quad + \left[ \|F_e, 0\| (\delta h)_p - \|F_e, 0\| (\delta h)_e \right] \\
inflow = \left[ \|F_e, 0\| (\delta h)_p - \|F_e, 0\| (\delta h)_e \right] \\
\quad + \left[ \|F_w, 0\| (\delta h)_p - \|F_w, 0\| (\delta h)_w \right] \\

Where \\
D_e = \frac{2\pi r_e a \Delta z}{(\Delta r)_e} \quad F_e = 2\pi r_e (\rho u_r)_e \Delta z \quad P_e = \frac{F_e}{D_e} \\
D_w = \frac{2\pi r_w a \Delta z}{(\Delta r)_w} \quad F_w = 2\pi r_w (\rho u_r)_w \Delta z \quad P_w = \frac{F_w}{D_w} \\
D_n = \frac{2\pi r_p a \Delta r}{(\Delta z)_n} \quad F_n = 2\pi r_p (\rho u_r)_n \Delta r \quad P_n = \frac{F_n}{D_n} \\
D_s = \frac{2\pi r_p a \Delta r}{(\Delta r)_s} \quad F_s = 2\pi r_p (\rho u_r)_s \Delta r \quad P_s = \frac{F_s}{D_s} \\

The discretized energy equation is solved iteratively using the definition from Equation 2.21.

3.4.1 Thermal Contact Resistance

Figure 2-6 Thermal Contact Resistance
Attinger et al. [29] and others [29-30] lay importance on the consideration of contact resistance in governing the heat transfer to the substrate. The contact effects are microscopic phenomenon and theoretical evaluation is rather difficult. Experimental findings do prove the importance of such considerations. Holt [7] outlined an indirect method to compute the boundary heat transfer by accounting for the contact resistance which has been adopted in the present model. Similar approach is also found in the works of [30-31]

Contact resistance is incorporated as a modification to the isothermal boundary condition. Imperfect contact (reduced contact area) and entrapment of non-conducting fluids (voids) result into a reduced heat transfer across the contact surface. The resultant effect can be viewed as an increase in the interface temperature. To determine the modified temperature, a steady state one dimensional conduction model is used. The equivalent thermal resistance [34] can be written as

$$ R_{th} = \frac{l}{kA} + \frac{1}{h_c A} $$

where A is the contact area and \( h_c \) is the approximate heat transfer coefficient representing contact conductance per unit area. Attinger [33] suggested a dimensionless approach for evaluating \( h_c \) through the use of Biot number (\( B_i = hl/k \)). The works of [7, 28, 31] suggest a heat transfer coefficient in the range of \( 10^4 \) to \( 10^7 \) W/m²-K for microdroplets while Attinger and Poulikakos [4] suggest a range of \( Bi = 0.01 \) to 2 for accurate thermal resistance modeling through experimental verification. This recommendation is closely followed in the present work.

Using the equivalent resistance from Equation 2.34, the heat transfer from the droplet to the substrate can be calculated as:
\[ q_b = \frac{T_d - T_{sub}}{\frac{l}{kA} + \frac{1}{h_cA}} \]  

(2.35)

Using a half control volume approach, the interface temperature can be calculated by equating the one dimensional (axial) fluxes on both sides of the boundary as shown in Figure 2-7.

Figure 2-7 Thermal Contact Resistance Formulation

\[ \frac{T_d - T_{if}}{\frac{\delta y}{2kA}} = \frac{T_{if} - T_{sub}}{\left(\frac{1}{h_cA}\right)} \]  

(2.36)

gives

\[ T_{if} = \frac{h_c\left(\frac{\delta y}{2}\right)T_{sub}}{1 + \frac{h_c\left(\frac{\delta y}{2}\right)}{k}} \]  

(2.37)
Chapter 3
Results and Discussion

3.1 Problem Setup and Boundary Conditions

3.1.1 Initial Droplet:

A schematic view of the initial free surface shapes and boundary conditions are shown in Figure 3-1. The problem under study is considered to be axis-symmetric. Hence, flow and energy equations are solved only for one half of the droplet. The first step in the problem setup is to define a free surface and geometrical setup which best resembles actual process. Free surface for the droplet is considered to be a circle and is prescribed by defining a VOF function as described in Chapter 2. A rigid free-slip condition is applied to the top and the left boundaries. A rigid no-slip condition is applied to the bottom boundary. A continuative outflow condition is prescribed for the right boundary. In addition to these conditions, an adiabatic boundary condition is applied on all free surfaces. Rigid no-slip or wall boundary condition implies that the velocity at that particular face is zero and there is no flow across that face. Continuous outflow means that the gradient of velocity in the direction perpendicular to the corresponding face is zero. Rigid free-slip boundary condition allows the fluid to move freely over the surface without offering any resistance. The droplet has initial temperature $T_D$ and impact velocity $V_i$. The substrate is replaced by interface temperature $T_{if}$ due to thermal contact resistance. A sample input file is given in the Appendix B.
3.1.2 Successive Droplets:

A schematic view of the problem setup and the boundary conditions for the case of successive droplets is shown in Figure 3-2. After the leading droplet has completely solidified or when the maximum height of the leading droplet falls below solidus temperature a new droplet is generated. The new droplet is generated at an offset distance $R_i + \eta$ and the free surface definition is similar to the initial droplet. The distance $\eta$ corresponds to the final splat height of the pre-solidified droplet and is located
when the temperature of the droplet falls below solidus temperature. The current model of multiple droplet generation has an advantage over other models for it saves computational domain and reduces computational load. Likewise, it should be noted that by this model more than two droplets can be generated. Although present study focuses only on two droplet pileup. The impact velocity, radius, and initial droplet temperature are same as the leading droplet.

Figure 3-2 Successive Droplets
3.1.3 Material Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Solder(liquid)</th>
<th>Solder(solid)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Conductivity, ( k ) (W/m²K)</td>
<td>25</td>
<td>48</td>
</tr>
<tr>
<td>Density, ( \rho ) (kg/m³)</td>
<td>8218</td>
<td>8240</td>
</tr>
<tr>
<td>Surface Tension, ( \sigma ) (N/m)</td>
<td>0.345</td>
<td>-</td>
</tr>
<tr>
<td>Contact Angle, ( \theta_c ) (°)</td>
<td>75</td>
<td>75</td>
</tr>
<tr>
<td>Specific Heat ( C_p ) (J/kg-K)</td>
<td>238</td>
<td>176</td>
</tr>
<tr>
<td>Solidus Temperature, ( T_S ) (K)</td>
<td>457</td>
<td>-</td>
</tr>
<tr>
<td>Liquidus Temperature, ( T_L ) (K)</td>
<td>456</td>
<td>-</td>
</tr>
<tr>
<td>Latent Heat, ( L ) (J/kg)</td>
<td>42000</td>
<td>42000</td>
</tr>
</tbody>
</table>

Since majority of the alloys used in Additive Manufacturing are eutectic in nature, eutectic lead-tin alloy 63Sn-37pb is investigated in present study. It has a sharp melting point at 456K but numerically it is modelled by defining an artificial mushy region over a range which is bounded by liqidus temperature\( (T_L) \) 456K and solidus temperature\( (T_S) \) 457K. The material properties used in all simulations are shown in the Table 3-1.

3.2 Standard Case Simulation

The simulation of standard case for a Sn-Pb alloy is carried out and results are obtained. The grid size and fluid and thermal properties used in the standard case are shown in. A guide to performing the simulation is given in the Appendix B in which an input file is listed.
### Table 3-2

**Standard Case**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>X (mm)</td>
<td>0.066</td>
</tr>
<tr>
<td>Y (mm)</td>
<td>0.128</td>
</tr>
<tr>
<td>Domain size</td>
<td>206x400</td>
</tr>
<tr>
<td>Droplet Diameter (mm)</td>
<td>0.0768</td>
</tr>
<tr>
<td>Droplet density (kg/m³)</td>
<td>8220</td>
</tr>
<tr>
<td>Surface Tension (N/m)</td>
<td>0.345</td>
</tr>
<tr>
<td>Kinematic viscosity ($m²/s$)</td>
<td>3.1*10⁻⁷</td>
</tr>
<tr>
<td>Initial droplet temperature (K)</td>
<td>483</td>
</tr>
<tr>
<td>Substrate Temperature (K)</td>
<td>398</td>
</tr>
<tr>
<td>Specific Heat capacity (J/kg-K)</td>
<td>238</td>
</tr>
<tr>
<td>Latent Heat of phase change (J/kg)</td>
<td>42000</td>
</tr>
<tr>
<td>Melting Temperature of 63Sn-37Pb (K)</td>
<td>456</td>
</tr>
<tr>
<td>Thermal contact resistance (m²K/W)</td>
<td>0.6*10⁶</td>
</tr>
</tbody>
</table>

Figure 3-3 Free Surface evolution of the Leading Droplet (Reference Case) and Figure 3-4 present the free surface evolution and solidification of single and successive droplet depositions respectively. The red contour represents the solidification front. The droplet is completely solidified when the red contour (which represents a temperature of 456 K) disappears. As can be seen from the figures, the first droplet solidifies at 0.19201 ms and the second droplet solidifies at 0.679 ms. Initially, droplet spreads due to kinetic energy and the solidification process start the moment the droplet impacts on the substrate. The onset of solidification and viscous damping impedes spreading of the
droplet. Once the droplet spreading stops, the surface tension of the droplet pulls back the
droplet and recoils at 0.083006 \( m/s \) with subsequent oscillations until complete
solidification.

Once the first droplet has completely solidified successive droplets are generated
as described in Section 3.1.2. The second droplet is generated at 0.19201 \( m/s \) and it goes
through similar splat dynamics as the first droplet but over a non-flat surface of same
material instead of a substrate. From the figures it can be seen that simultaneous
solidification and surface tension of the droplet brings about drastic free surface
deformations and oscillations. It was observed that the number of oscillation cycles for the
second droplet were greater than the first droplet. This is due the slower rate of solidification
of the second droplet. The temperature gradient experienced by presolidified-successive
droplet interface is greater when compared to droplet-substrate interface and also the heat
diffusion process has to take place over a greater length compared to that of first droplet
leading to a slower rate of solidification of successive droplets.
Figure 3-3 Free Surface evolution of the Leading Droplet (Reference Case)
Figure 3-4 Free Surface evolution of the Trailing Droplet (Reference Case)
3.3 Experimental Comparison

The current numerical study is compared with experiments for a substrate temperature of 398 K and with an initial velocity of 1.52 m/s. There was a good agreement between experiment and numerical study for a thermal contact resistance of $1.7 \times 10^{-3} m^2K/W$. Experiments were conducted by Haferl and Poulikakos[12]. They also carried out a Finite Element Method (FEM) based numerical study [35]. However, their numerical result showed a disagreement with the experimental result for a higher substrate temperature and the literature also highlighted that disagreement was due to the capillary effects at higher substrate temperatures. But, the current numerical model employs Continuum Surface Tension (CSF) model which accurately models capillary effects. Figure 3-5 illustrates a comparison between numerical model under study, experimental work and Finite Element Method. The numerical results were compared at exact time instant as the experiment. It can be seen that numerical model has good agreement with experiments. From the figure, it can also be absorbed that solidification time of numerical result is greater compared to the experiment. The reason for the considerable difference in the solidification time is illustrated through Figure 3-6. The figure represents the variation of the centre height of the droplet with time. The figure also explains the overall behaviour of spreading, recoil and oscillations of single as well as multiple droplets. It can be seen that after repeated oscillations droplet comes to rest for few microseconds before complete solidification. According to the numerical data, droplet thickness remains constant from 0.59 m.s until complete solidification. The solidification time in experiments is estimated by using a high-speed camera and other imaging techniques. The moment when the free surface of the droplet is stationary is considered as solidification time. Therefore, imaging techniques provides only superficial real time deformation of droplets and fails to provide
information on the phase of the droplet. Thus above stated reason accounts for the considerable difference in solidification time. This also highlights the need for a numerical model. It should also be noted that numerical results are two-dimensional and only cross section can be viewed.
Figure 3-5 Comparison Present Study with Experiment and FEM method
Figure 3-6 Variation of Center Height with Time
3.4 Parametric Studies

Effect of the key parameters such as impact parameters, thermal parameters and the frequency of the droplets on splat morphology and phase change characteristics of droplets were conducted.

The parameters where kept constant throughout the study:

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>X (mm)</td>
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</tr>
<tr>
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</tr>
<tr>
<td>Kinematic viscosity (m²/s)</td>
<td>3.1x10⁷</td>
</tr>
<tr>
<td>Substrate Temperature (K)</td>
<td>398</td>
</tr>
<tr>
<td>Specific Heat capacity (J/kg-K)</td>
<td>238</td>
</tr>
<tr>
<td>Latent Heat of phase change (J/kg)</td>
<td>42000</td>
</tr>
<tr>
<td>Melting Temperature of 63Sn-37Pb (K)</td>
<td>456</td>
</tr>
</tbody>
</table>

3.4.1 Effect of Impact parameters:

Two key impact parameters which affects the splat morphology are:

- Impact velocity.
- Initial droplet temperature.
3.4.1.1 Effect of Impact Velocity:

The key parameter in the current study is droplet impact velocity. The effect of impact velocity is represented in Figure 3-7. The impact velocity was varied from 1 m/s to 3 m/s. From the figure, it can be observed that impact velocity affects the splat morphology by a considerable amount. At lower velocities droplets forms a bump and at higher velocities droplet forms a splat. At higher impact velocity, the kinetic energy of the droplets overcome the surface tension force and results in a wider spread and faster solidification which in turn arrest the recoil and oscillations of the droplet. Therefore, leading to a splat formation. At lower velocities, the extent of spreading is restricted. The solidification, being comparable to the contact area is also slower in such conditions. The solidification time of droplet varies monotonically with impact velocity. This is due to the fact that increase in
spread factor increases the contact area for heat dissipation resulting in a reduction of solidification time. Droplet height also varies monotonically with impact velocity.

The effect of Impact velocity on successive droplet impacts are presented in Figure 3-8. It can be clearly seen that impact velocity has a greater effect on splat morphology of the pileup. The effect of the impact velocity of successive droplets on the splat morphology is manifested in an implicit manner through the surface curvature of presolidified droplet. The solidification time of the pileup varies monotonically with impact velocity. The second droplet attains maximum thickness at 1 m/s. For greater velocities the final shape of the
second droplet varies and either forms a splat or crown. At $3 \, m/s$ the free surface forms a crown which could lead to void formation with additional successive droplet solidification.

3.4.1.2 Effect of Initial Droplet Temperature

![Figure 3-9 Effect of Initial Droplet Temperature on First Droplet](image)

The effect of initial droplet temperature on Sn-Pb with a melting temperature of 456K was examined. The study included temperature ranges from 463 K to 623 K. A thermal contact resistance of $0.6 \times 10^{-6} \, m^2K/W$ and impact velocity of $1.5 \, m/s$ were used.

As shown in Figure 3-9 the initial droplet temperature has minimal effect on the final spread and splat shape of the droplet. However, it has been found that the solidification time increases with increase in initial droplet temperature. A droplet with a higher initial
temperature possesses a larger value of superheat. The droplet upon impact with the substrate, therefore, has a greater amount of heat energy to transfer to the substrate. Consequently, the time taken to transfer the heat energy to the substrate is longer. Since the process of solidification can begin only after all the superheat is removed from the droplet. Hence, the time taken for solidification is greater when \( T_d \) is increased.

Figure 3-10 Effect of Initial Droplet Temperature on Successive Droplets

Figure 3-10 illustrates the effect of initial droplet temperature on the second droplet and similar trend as the first droplet is seen. However, the solidification time of the second droplet is greater when compared to first. As the first droplet has just solidified when successive droplet impacts it and the temperature of the presolidified droplet is close to melting temperature. Therefore, the successive droplet-pre solidified droplet interface has lower temperature gradient when compared to the gradient experienced by first droplet and
the substrate. Thus, heat transfer occurs at lower rates and successive droplets take a longer time to solidify than the first droplet. It should also be noted that when the droplet temperature is greater or equal to 623 K the pre-solidified droplet remelts and Figure 3-11 shows the remelting behaviour at different time instants. At 0.22801 ms, the convective flux experienced by the presolidified droplet due to the successive droplet is much greater than the conductive flux due to the substrate which causes remelting of the presolidified droplet. From 0.278 ms further remelting effect is due to the conductive flux at the interface of droplets. Since at this point thickness of the droplet reduces leading to a high temperature gradient.

![Figure 3-11 Remelting behavior at 623K](image)

### 3.4.2 Effect of Thermal Parameters

The thermal parameters which has significant effect on the splat morphology are:

- Thermal contact resistance and
- Latent heat of fusion.
3.4.2.1 Effect of Thermal Contact Resistance:

The effect of thermal contact resistance on spreading and phase change process was studied. Thermal contact resistance is varied by changing the interface heat transfer coefficient values in the range $585 \times 10^3 \, W/m^2K$ to $10^{11} \, W/m^2K$. Thermal contact resistance is constant throughout the process and not affected by impact and thermal parameters.

![Figure 3-12 Effect of Thermal Contact Resistance on the First Droplet](image)

Figure 3-12 and Figure 3-13 illustrates the effect of thermal contact on splat morphology of the single as well as successive droplets. It could be seen that thermal contact resistance affects the spreading characteristics drastically. The droplet reaches its maximum spread factor for thermal contact resistance of $585 \, W/m^2K$ and below this value
substrate acts as an adiabatic surface. The substrate acts as isothermal surface for thermal contact resistance value greater than $10^6 \text{ W/m}^2\text{K}$. It was found that spread factor varies monotonically with interface heat transfer coefficient. The influence of thermal contact resistance on the final height is inconclusive due to the fact that oscillations and simultaneous solidification influences the final splat height rather than contact resistance directly.

![Figure 3-13 Effect of Thermal Contact Resistance on the Second Droplet](image)

3.4.2.2 Effect of Latent Heat of Fusion:

Although latent heat is a material property a hypothetical study on effect of latent heat on splat morphology was conducted. Latent heat was varied from 20000 $\text{J/kg}$ to 60000 $\text{J/kg}$. Figure 3-14 and Figure 3-15 outlines the effect of latent heat on splat
morphology on single as well multiple droplets. Latent Heat is the amount of heat required to be added or removed to during phase change of the material. Hence the solidification rate is directly proportional to Latent heat. At the lower latent heat of 20000 J/kg heat transfer occurs rapidly and oscillation effects are damped extremely fast leading to crown formation.

Figure 3-14 Effect of Latent Heat on the First Droplet
3.4.3 Effect of Frequency of Droplets:

The frequency of successive droplets was examined and compared with reference case. At of 33.33 kHz, the first droplet is 25\% solid and at 20 kHz, the first droplet is 50\% solid. When the second droplet comes in contact with the first droplet and at this stage if the first droplet is incompletely solidified, then melt of the first droplet will merge with the incoming droplet. After coalescence, the droplet spreads at contact line due to the momentum of the second droplet. Therefore, the second drop spreads to a greater extent compared to the first one and simultaneous solidification leads to a ripple formation Figure
3-16 and Figure 3-17 outlines the temporal evolution of droplet at various time steps depicting the spreading, coalescence and solidification at frequencies 20 kHz and 33.333 kHz. Figure 3-18 highlights the ripple formation due to the frequency of droplets. The ripples are reduced considerably when the first droplet is completely solid. It was observed that increasing frequency of the droplets reduces the final height of the pileup. It should also be noted that by varying the frequency of the droplets different modes of droplet generation can be achieved: Continuous Stream (CS) or Drop on Demand (DOD). Thus, based on the application, frequency of the droplet can be adjusted. This study also indicates the importance of numerical model for examining the effect of droplet discharge frequency id not possible experimentally.
Figure 3-16  Frequency 20 kHz
Figure 3-17 Frequency 33 kHz
Figure 3-18 Ripple Formation
Chapter 4.
Conclusion and Future Work

4.1 Conclusion

A numerical study on successive droplet deposition has been carried out. The effect of various impact and thermal parameters such as impact velocity, initial droplet temperature, contact resistance and droplet discharge frequency on the splat morphology and solidification characteristics of successive droplet depositions were examined. The numerical model was formulated to solve the highly non-linear flow governing equation and the energy equation to account for the phase change process. The numerical scheme was compared with experimental findings and good agreement was found.

The Continuity and Navier Stokes equations were solved using the two-step projection method. Coupled Level Set-Volume Of Fluid (CLSVOF), was used to accurately model the drastically deforming interface surface. It also facilitates generation of multiple droplets in a continuum domain at specified frequency. The interface reconstruction was carried out using a piecewise Linear Construction (PLIC) scheme. Surface Tension effects were modelled using the Continuum Surface Force method (CSF) where surface tension is calculated as body force in Navier Stokes equation. The non-isothermal phase change is carried out over a region of artificial mushy zone using the enthalpy-porosity technique. Thermal contact resistance was modelled by using a steady one dimensional conduction equation.

The splat morphology and solidification characteristics of a Sn-Pb alloy droplet deposited on a substrate have been examined under varying impact conditions. The splat morphology is highly dependent on the impact velocity and initial droplet temperature. The effect of impact velocity played a major role in formation of splat or bump and the initial
droplet temperature has minimal contribution to it. However, remelting of presolidified droplet at higher droplet temperature due to high thermal inertia, was reported. The monotonically varying droplet height with impact velocity was observed. Effect of impact velocity and droplet temperature on solidification time and extent of spreading was reported. The effect of surface curvature on final shape of the pile up was also studied. The role of convective flux on solidification characteristics, remelting effects and recoil was analysed.

The effect of Thermal contact resistance on spreading and solidification characteristics was examined. Monotonical variation of spread factor and solidification time with contact resistance was observed. Latent heat had little effect on splat morphology but there was considerable increase in solidification time with increase in latent heat.

4.2 Future Work

4.2.1 Moving Substrate and Multiple Nozzle Head

Figure 4-1 Moving Substrate
3D printing a form of additive manufacturing is usually carried out using multiple nozzle head and in most of these process substrate is not stationary[36] Investigating splat dynamics and solidification characteristics of such process becomes challenging for the problem under consideration is not axis symmetric and requires a three dimensional numerical formulation to carry out the simulations. The flow and energy equations must be solve in three dimensional co-ordinate axis. Implementing a three dimensional solver would aid in simulating such intricate cases.

4.2.2 Dynamic Wetting line and Contact Angle

The current numerical study uses static contact angle model. Attinger [37] pointed out the importance of dynamic contact angle variation due to solidification. In the present study, the contact angle is always computed at the bottom wall of the domain with the assumption that the dynamic spreading behaviour of the splat is primarily governed by solidification and that the dynamic contact angle is neglected. At low Re the spreading and recoil effects are clearly visible. However, the difference between the advancing and receding contact angles is quite insignificant. However, Anderson et al. [38] outlines a simple procedure to base the contact angle measurement on the dynamic contact line or the solidification front. Their calculations assumed a simplified horizontal solidification front.
which is physically improbable. Dynamic wetting line and contact angle can be implemented to the current numerical formulation to improve model accuracy.

4.2.3 Liquid Phase 3D printing

Wang and Liu[39] proposed a highly robust and considerably versatile 3D printing technology in a liquid environment. Metals and alloys have very high specific heats and relatively low molten state viscosity in comparison with the polymers used in conventional 3D printing technologies. This makes the problem of stability of the jet or droplet more crucial in applications requiring metal printed parts. This can be implemented by modelling a free surface convection boundary condition.
Appendix A

Grid Refinement
Figure 0-1 Grid Refinement
Appendix B

Program Execution
The current section outlines the various aspects of numerical program executing the model. The program is written in FORTRAN and executed on a High Performance Computing platform operating on UNIX. The High Performance Computing facility at the University of Texas at Arlington and the Texas Advanced Computing Center at The University of Texas at Austin were used for the simulations. Following are the four files required for the execution with their corresponding tasks.

<table>
<thead>
<tr>
<th>File</th>
<th>Task</th>
</tr>
</thead>
<tbody>
<tr>
<td>bjob</td>
<td>A set of instructions for the Load Sharing Facility (LSF) on HPC platform. It is a batch script written to upload a case.</td>
</tr>
<tr>
<td>input</td>
<td>Contains a set of parameters describing a particular case.</td>
</tr>
<tr>
<td>filenam.dat</td>
<td>Contains the total number of output files to be generated and the file name of each.</td>
</tr>
<tr>
<td>ripple.exe</td>
<td>The executable file generated after compiling the program. It contains flow information for the numerical calculations and all the subroutines required. ripple.exe was the basic multiphase flow solver while tcripple.exe includes the phase change module and enhanced interface tracking and construction schemes.</td>
</tr>
</tbody>
</table>

The collection of various subroutines written to perform specific tasks is logically integrated in the main program which upon successful compilation produces the executable called ripple.exe (flow solver coupled with phase transformation). The bjob file is used to submit a case to be run on HPC. The parameters and data required for the numerical experiment are passed from the input file. A set of output files are generated as per the instructions provided in filename.dat. Sample input and output files are shown below with a brief discussion.
Sample Input File:

```
MultiDroplet_impact (pbSn) (d=0.07683mm) [mm,ms,mg,K]
$numparam
  alpha=1.0,
  autot=1.0,
  conserve=.false.,
  delt=1.0e-6,
  dtmax=1.0e-4,
  twfin=200000.0,
  con = 0.3
  fcvlim=0.25,
  idiv=1,
  dmpdt=3000000.0,
  prtdt=1000000.0,
  plttdt=0.001,
  sym=.true.,
  kt=1,
  kb=2,
  kl=1,
  kr=3,
$end
$fldparam
  gy=-9.81e-3,
  icyl=1,
  isurf10=1,
  psat =0.0,
  xnu=3.18e-4,
  rhof=8.22,
  sigma=0.345,
  vi=1.5,
  cangleb=75,
$end
$mesh
  nkx=1,
  xl=0.0,0.06592,
  xc=0.03296,
  nxl=103,
  nxx=103,
  dxmn=0.00032,
  nky=1,
  yl=0.0,0.128,
  yc=0.064,
  nyl=200,
  nyr=200,
  dymn=0.00032,
$end
$obstcl
  nobs=0,
$end
$freesurf
  nfrsr=2,lequib=0,
  fcl(1)=-1.0, ifh(1)=1,
  fa2(2)=1.0,fb1(2)=-0.07811,fb2(2)=1.0,fc1(2)-0.000050,ifh(2)=0,
$end
$graphics
  plots=.true., dump=.false.,
  iout = 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 0, 0, 0, 0, 0, 0, 100, 2, 0, 2,0,0,-1, 0, 1,
  iysymplt=1,
$end
$heateq
  heat = .true.,
  ischeme = 3,
  tid = 483,
```
The first line contains the problem name, following which are nine name lists. Name list is a group of variables containing a specific type of information as shown below.

**Numparam:**  Numerical parameters. Variables defining initial conditions, boundary conditions, initial time steps, plotting frequency etc.

**Fldparam:**  Fluid parameters. Variables defining properties such as density, viscosity, surface tension, contact angle, impact velocity etc.

**Mesh:**  Mesh parameters. Variables defining mesh properties such as convergence point, minimum and maximum domain sizes and sub-meshes for non-uniform grids.

**Obstcl:**  Obstacle parameters. Coefficients defining the conic function representing the surface of obstacles within the domain.

**Freesurf:**  Initial free surface parameters. Coefficients defining the conic function representing the fluid free surface within the domain at t = 0.

**Graphics:**  Originally contained plotting instructions. Currently, post processing is performed using MATLAB. Variables in this list are thus, available for custom user defined operations.
Heateq: Energy Equation Parameters. Variables defining thermal properties such as conductivity, specific heat, mushy range, initial temperatures etc.

Coupled: Logical variables for selecting the interface tracking scheme.

Sample Output File:

```
2.30068E-002  ← Time of plot
2,206  ← First and Last Real Cell # in x or r direction
2,400  ← First and Last Real Cell # in y or z direction
0.00000E+000
3.20000E-004
6.40000E-004
9.60000E-004
1.28000E-003  ← Horizontal or Radial Locations of Cell Faces
. .
0.00000E+000
3.20000E-004
6.40000E-004
9.60000E-004
1.28000E-003  ← Vertical or Axial Locations of Cell Faces
. .
1.28000E+000
. .
. .
0.00000E+000, 0.00000E+000, 1.00000E+000, 1.00000E+000, 9.47240E+004,-4.39726E-003
0.00000E+000, 0.00000E+000, 1.00000E+000, 0.00000E+000, 9.47472E+004,-4.39726E-003
0.00000E+000, 0.00000E+000, 1.00000E+000, 0.00000E+000, 9.47462E+004,-4.39726E-003
0.00000E+000, 0.00000E+000, 1.00000E+000, 0.00000E+000, 9.47455E+004,-4.39726E-003
-1.69022E-005, 0.00000E+000, 1.00000E+000, 0.00000E+000, 9.47413E+004,-4.39726E-003
-2.46812E-005, 0.00000E+000, 6.62553E-001, 1.00000E+000, 9.47285E+004,-4.39726E-003
-2.88858E-005, 0.00000E+000, 7.09506E-001, 1.00000E+000, 9.47292E+004,-4.39726E-003 .
.
U or u_x  V or u_y  F  S  H  L
Velocity Components     VOF Function Liquid Fraction  Enthalpy  Level-set
```
References


Biographical Information

Vimalan Adaikalanathan received his Bachelor of Engineering (BE) Degree in Mechanical Engineering from Anna University, Chennai, Tamilnadu, India. He joined the Department of Mechanical and Aerospace Engineering at the University of Texas at Arlington in August 2014 as a graduate student and earned his Master of Science in Mechanical Engineering in May 2016.