A Numerical Study of Supersonic Rectangular Jet Impingement and
Applications to Cold Spray Technology

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(ABSTRACT)

Particle-laden supersonic jets impinging on a flat surface are of interest to cold gasdynamic spray technology. Solid particles are propelled to a high velocity through a convergent-divergent nozzle, and upon impact on a substrate surface, they undergo plastic deformation and adhere to the surface. For given particle and substrate materials, particle velocity and temperature at impact are the primary parameters that determine the success of particle deposition. Depending on the particle diameter and density, interactions of particles with the turbulent supersonic jet and the compressed gas region near the substrate surface can have significant effects on particle velocity and temperature. Unlike previous numerical simulations of cold spray, in this dissertation we track solid particles in the instantaneous turbulent fluctuating flow field from the nozzle exit to the substrate surface. Thus, we capture the effects of particle-turbulence interactions on particle velocity and temperature at impact.

The flow field is obtained by direct numerical simulations of a supersonic rectangular particle-laden air jet impinging on a flat substrate. An Eulerian-Lagrangian approach with two-way coupling between solid particles and gas phase is used. Unsteady three-dimensional Navier-Stokes equations are solved using a six-order compact scheme with a tenth-order compact filter combined with WENO dissipation, almost everywhere except in a region around the bow shock where a fifth-order WENO scheme is used. A fourth-order low-storage Runge-Kutta scheme is used for time integration of gas dynamics equations simultaneously with solid particles equations of motion and energy equation for particle temperature. Particles are tracked in instantaneous turbulent jet flow rather than in a mean flow that is commonly used in the previous studies. Supersonic jets for air and helium at Mach number 2.5 and 2.8, respectively, are simulated for two cases for the standoff distance between the nozzle exit and the substrate. Flow structures, mean flow properties, particles impact velocity and particles deposition efficiency on a flat substrate surface are presented. Different grid resolutions are
tested using 2, 4 and 8 million points. Good agreement between DNS results and experimental data is obtained for the pressure distribution on the wall and the maximum Mach number profile in wall jet. Probability density functions for particle velocity and temperature at impact are presented. Deposition efficiency for aluminum and copper particles of diameter in the range $1 \mu m \leq d_p \leq 40 \mu m$ is calculated.

Instantaneous flow fields for the two standoff distances considered exhibit different flow characteristics. For large standoff distance, the jet is unsteady and flaps both for air (Mach number 2.5) and for helium (Mach number 2.8), in the direction normal to the large cross-section of the jet. Linear stability analysis of the mean jet profile validates the oscillation frequency observed in the present numerical study. Available experimental data also validate oscillation frequency. After impingement, the flow re-expands from the compressed gas region into a supersonic wall jet. The pressure on the wall in the expansion region is locally lower than ambient pressure. Strong bow shock only occurs for small standoff distance. For large standoff distance multiple/oblique shocks are observed due to the flapping of the jet.

The one-dimensional model based on isentropic flow calculations produces reliable results for particle velocity and temperature. It is found that the low efficiency in the low-pressure cold spray (LPCS) compared to high-pressure cold spray (HPCS) is mainly due to low temperature of the particles at the exit of the nozzle. Three-dimensional simulations show that small particles are readily influenced by the large-scale turbulent structures developing on jet shear layers, and they drift sideways. However, large particles are less influenced by the turbulent flow. Particles velocity and temperature are affected by the compressed gas layer and remain fairly constant in the jet region. With a small increase in the particles initial temperature, the deposition efficiency in LPCS can be maximized. There is an optimum particle diameter range for maximum deposition efficiency.
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Chapter 1

Introduction

Cold spray is a material deposition process discovered in 1980s at the Institute of Theoretical and Applied Mechanics of Siberian Branch of the Russian Academy of Sciences (ITAM of RAS), as a spin-off of studying models subjected to a supersonic two-phase flow in a wind-tunnel (6–13). Earlier, it was believed that formation of coatings due to particles flux can only be achieved when particles incident on the substrate have a temperature close to the melting temperature of the particles. Alkimov et al. (6; 7) obtained experimentally for the first time the deposition of aluminum particles at room temperature at Mach number 2.6 using a mixture of helium and air. In cold spray, particles ranging in size from 1 to 50 microns are heated and accelerated to a high velocity through a converging-diverging (de Laval) nozzle. Spray particles travel at high speed and after passing through the shock (in front of the substrate) impact on the substrate. The solid ductile particles, plastically deform on impact, and consolidate to create coatings (7; 14). Cold spray means a coating process where the temperature of sprayed particles at the time of injection into the nozzle is typically much lower than the melting temperature. In other words, in cold spray particles are not necessarily heated separately before injection into the nozzle.

Based on particles injection method into the nozzle, cold spray can be categorized into two methods, namely high-pressure cold spray (HPCS) and low-pressure cold spray (LPCS). In high-pressure cold spray, shown schematically in figure 1.1, solid particles are injected at the nozzle inlet by applying high pressure (15). The working gas which is usually nitrogen,
air, helium or mixture of air and helium at high pressure is preheated to a high temperature. Expansion of the gas in the divergent section of the nozzle results in supersonic exit velocity in the range of (1200-1500 m/s) (16). Spray particles in fine powder form are fed into the gas stream axially, upstream in the nozzle convergent section. To avoid back flow of the gas into the powder feeder; the pressure in the powder feeder is higher than the gas pressure at the injection section. Particles deposition efficiency is higher in HPCS compared to LPCS. Due to high pressure requirements and sophisticated equipments for particles injection, HPCS is more expensive than LPCS.

Figure 1.1: Operational principle of high-pressure cold spray (1; 2)

In low-pressure cold spray (LPCS), shown in figure 1.2, spray particles are injected into the diverging section of the nozzle from a low-pressure gas supply (17). The gas pressure is in the range of 5 – 10 bars. In order to increase particle deposition efficiency, the gas is heated before injecting into the nozzle. Both air and Nitrogen are used in LPCS. Low pressure requirement makes this process safer, portable and less expensive. In LPCS, nozzle life is longer because particles are injected into the divergent part of the nozzle which eliminates wear at the nozzle throat. However, the deposition efficiency in LPCS is low. LPCS is suitable for short runs.
There are many theories associated with the bonding mechanism in cold spray (4; 18–22). The widely accepted bonding theory in cold spray is based on adiabatic shear instability. The adiabatic shear instability occurs at the particle/substrate interface beyond a certain velocity. This velocity is called critical velocity. When a spherical particle impacts a substrate at critical velocity, a strong pressure field is generated at the point of contact. This pressure field propagates into the particle and substrate from the point of contact. Due to this pressure field, a shear load is generated, which accelerates the material laterally and causes localized shear straining. The shear loading leads to adiabatic shear instability, which leads to a discontinuous jump in strain and temperature and breakdown of flow stresses (4; 18–22).

When a metal particle impacts on a metallic surface, there are three possibilities. The particle may rebound, stick or penetrate the surface. If particle velocity is low, the particle will rebound and small erosion will occur. If particle velocity is very high, particle will penetrate and strong erosion will occur. However, if particle velocity is not very high nor very low, but between the lower-bound and upper-bound, the particle will stick to the surface. This velocity range is narrow and varies with temperature and velocity at impact. This width (range) is commonly known as to “windows for cold spray” (3; 4).
showing the deposition windows for cold spray is shown in figure 1.3.

After the discovery made in ITAM of RAS, cold spray became very popular in late 90s and henceforth due to its low cost compared to other available coatings and spray techniques. Figure 1.4 shows combinations of gas temperature and velocity for different thermal spray processes. The temperature required for the cold spray is lowest. It is important to mention that in the cold spray process, the substrate is also not heated. Low thermal requirement makes it a low cost, quick, and efficient coating process. Since particle melting is eliminated in this process; the entire setup can be made compact and amenable to field applications. Also many problems associated with other conventional thermal spray processes, e.g. oxidation, evaporation, melting, crystallization, residual stresses, gas release, and other common problems are easily avoided in cold spray (5; 23). Since cold spray is an impact-fusion phenomenon, ductile materials, e.g. Zn, Ag, Cu, Al, Ti, Nb, Mo, NiCr, CuAl etc. can easily be used for spray (5; 7; 23; 24). The overall success of cold spray is due to the following process characteristics:
1. Temperature requirement in cold spray is very low compared to all conventional metal deposition processes. Metal particles are not required to be heated before injection. Furthermore, substrate is not heated. No cooling is used in cold spray. Cold spray can be used for temperature-sensitive materials.

2. Cold spray process is operated through a converging-diverging nozzle. The beam of spray can be targeted and moved with a precise control. Metal particles flow rate and oxide level in the feedstock can be controlled. This feature of cold spray extends its application to small cracks and cavity filling in complex geometry, where targeted and controlled deposition is required.

3. Dense, uniform coatings that exhibit identical micro structures can easily be achieved. The oxidation level in cold spray coating is low compared to other processes.

4. Low thermal requirement, elimination of substrate heating and elimination of cooling equipments make cold spray setup very compact. This extends cold spray applications to the on-field jobs e.g. parts repairing, cavity and filling etc.

Although there are many advantages of cold spray. However, more research is needed to overcome the difficulties and limitations of cold spray. The deposition window in cold spray is narrow and material dependent. Coatings of brittle materials like ceramics are hard to achieve without secondary ductile material, which works as a binder. With the use of helium, high deposition efficiency can be achieved easily. However, helium is expensive and recycling is necessary. Still more research is needed to over-come these limitations.

Cold spray process has many operating parameters. Among most important parameters in cold spray are the particle temperature and velocity at impact. Other important parameters, especially for materials with low density are particles and gas densities, gas stagnation pressure and temperature, nozzle stand-off distance from the substrate, nature of the shock (oblique or normal), spray angle, nozzle length, stability of jet and substrate material and temperature, etc.

Initially, research was focused on how to create coatings using different materials and to investigate the quality of the coatings. Alkhimov et al. (6) showed a successful deposition
of micro size aluminum particles at room temperature using a mixture of air and helium. Later successful deposition of Cu, Ti, Ni, Ni alloys were achieved, and subsequently cermet, ceramic (7; 25) and other materials were also successfully deposited. Particle impact velocity, which depends on gas velocity, is an important parameter in cold spray. Hence, the nozzle design and jet flow are important parameters (26). Research has been done to optimize nozzle shape and dimensions. Almikov et al. (6) investigated particle velocities and the effects of nozzle wall boundary in different types of rectangular nozzles. Almikov et al. (27) studied experimentally particle strain due to impact velocity. Assadi et al. (28) presented a method for the construction of the window of deposition and the selection of optimum process parameters, and demonstrated the method for copper, aluminum and titanium. The analysis is based on one-dimensional gas-dynamics formulation in combination with experimental data. Further assessment of the proposed method and extension to other materials requires new experimental data and high-fidelity simulations.

Computational fluid dynamics (CFD) is a viable tool for in-depth understanding and optimization of cold spray. From the discovery of cold spray, efforts are being made to use
CFD to explore features of cold spray dynamics and to develop and generalize the parametric study for the cold spray. Dynamically the process involves expansion of the gas inside nozzle, particle dynamic and thermal interactions with the carrier gas and shock development outside the nozzle and its effects on the gas and particles. Other features like oscillations and instability of jet, nozzle cross sections, etc. also play an important role in the cold spray process.

Initially, numerical studies were focused to investigate important parameters of cold spray, e.g. critical velocity, temperature and impact angle, etc. Park et al. (29) used a commercial code (FLUENT) to examine characteristics of supersonic flow in de Laval nozzle and jet impingement on a substrate. They found that nozzle geometry optimization is required because shock-wave-induced fluctuations in flow properties can yield non-uniform coating. Optimal operating conditions correspond to the isobaric nozzle in which the exit pressure is equal to the ambient pressure. Yin et al. (30) also used FLUENT to study the effects of substrate size on supersonic flow characteristics and temperature distribution within the substrate in cold spraying. Champagne et al. (31) used CFD to predict velocity of aluminum particles accelerated in nitrogen gas in a de Laval nozzle, and obtained good comparison with experimental data. In cold spray, deposition efficiency depends on the impact angle. Gang et al (32) showed that the contact area between the deformed particle and substrate decreases with increasing the tilting angle at the same impact velocity. In their simulations, they showed that for maximum deposition efficiency, the tilt angle should be less than 30 degrees. Earlier, it was believed that the efficiency will be maximum only when the impact is normal to the plane. However, recent studies suggest that deposition efficiency is maximum over a small range of angles (33). The interaction of solid particles with bow shock and subsequent deceleration in the compressed gas layer makes this region a strongly coupled two-phase flow region. Using CFD, Jodian, B. (34) showed that shock-particle interactions pose limits on the nozzle exit Mach number. The dynamics of the gas motion and solid particles in this region determine the magnitude and direction of the particle velocity just before impact. It is the normal component of the particle velocity that matters for deposition efficiency. The particle normal velocity must exceed a critical value, and ideally should be uniformly distributed over the substrate area for high-quality deposition. Lower-than-critical normal
velocity causes particle rebound and erosion. In addition to the particle velocity, the particle size and temperature distributions before impact must also be determined. The compressed gas region is dominated by viscous and heat transfer effects. Flow unsteadiness is caused by impingement of large-scale turbulent fluctuations of the jet shear layers and oscillations of bow shock.

High-order accurate numerical schemes are necessary for the accurate numerical simulations of turbulent supersonic flow with shocks. For unsteady problems having embedded shock waves, numerical schemes must be less dissipative in order to accurately predict small scales in smooth regions. At the same time, the numerical schemes must robustly capture shock waves without any non-physical oscillations. Higher-order numerical schemes such as ENO, WENO and high-order compact schemes are widely used for numerical simulations (35–39). Compact schemes give spectral like resolutions for linear problems but will develop spurious oscillations and will lead to instabilities when applied to a problem having discontinuities or sharp gradients. Numerical schemes like ENO and WENO give good solution for a problem having shocks, but are more dissipative and less accurate for turbulence prediction. Different high-order filter based numerical schemes have been developed (40–42). These schemes use high order spatial and temporal schemes such as compact schemes to resolve the turbulence in smooth regions and dissipative schemes like ENO, WENO and TVD as a filter. Hybrid schemes in which two schemes are combined is another approach (26; 43–45). High-order schemes such as the compact scheme are used in smooth region and dissipative schemes such as ENO or WENO are used in the region (domain) where shock occurs. Hybrid schemes are computationally efficient, give high resolutions for turbulent scales and accurately capture shocks. Supersonic flows with high Mach number involving large gradients are hard to resolve computationally. For such flows, hybrid scheme may fail especially when applied on large three-dimensional structures.

1.1 Motivation

Despite the progress made in experimental research in the field of cold spray for deposition of different materials using different conditions, less work has been done so far in the numerical
simulation of the cold spray process. Most of the numerical work done so far are based on
Reynolds-Averaged Navier-Stokes (RANS) calculations. Such simulations ignore the effects
of instantaneous unsteady flow properties. Simulating multiphase flow involving turbulence
and shocks poses significant challenges. Numerical schemes must be capable of capturing
shock as well resolve small-scale turbulence. At the same time, it must be time efficient.
Combination of dissipative numerical schemes (e.g. ENO, WENO) with the non-dissipative
schemes (e.g. central difference schemes) will be required for such simulations.

Our aim is to resolve the turbulent two-phase compressible flow by direct numerical
simulations (DNS). In DNS, all turbulence scales are accurately resolved in space and time,
and no turbulence model is needed. Resolving all the turbulence scale will predict more
realistic velocity and temperature at impact. Accurate scheme for shock will explore particle-
shock interactions; another important parameter of cold spray not studied so far. We will use
a Lagrangian approach to track solid particles from nozzle exit to impact on the substrate
surface.

1.2 Contributions

1. This dissertation is the first attempt to simulate the cold spray process with three-
dimensional supersonic rectangular jet at high Mach number (2.5 and 2.80) by direct
numerical simulation approach using high-order numerical schemes.

2. The development and validation of a parallel CFD code based on unsteady compressible
flow equations coupled with particles equations of motion are solved using a fifth-order
WENO scheme (35–37) to capture shock and six-order compact scheme(39) with 10th
order filter to resolve small-scale turbulence.

3. It is shown that the instantaneous three-dimensional turbulent velocity field is essential
for tracking small particles in cold spray. The mean flow field that is obtained by solving
Reynolds-averaged Navier-Stokes equations is irrelevant for tracking small particles on
the size encountered in cold spray.

4. Effect of particle temperature on deposition efficiency is investigated. Traditionally,
the critical velocity is considered the single most important parameter for successful deposition.

5. Effects of other important parameters, e.g. particle shock interaction, shock standoff distance from the substrate and particle diameter, etc. have been explored for cold spray.

6. Simple one-dimensional model for predicting particle velocity and temperature at impact is also presented. The model can also predict deposition efficiency.
Chapter 2

Mathematical Formulation

This chapter presents the governing equations, and the assumptions involved in deriving these equations. The non-dimensional and the transformed forms of these equations are also defined.

2.1 Governing Equations

At time $t^*$, let $u_i^*$, $\rho^*$, $p^*$, $T^*$, $e^*$, $\mu^*$, and $\kappa^*$ represent, respectively, Cartesian velocity components, density, pressure, temperature, specific internal energy, dynamic viscosity, and thermal conductivity of the fluid at position $x_i^*$. The field equations are:

Continuity Equation:

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial \left( \rho^* u_j^* \right)}{\partial x_j^*} = 0,$$

(2.1)

Momentum Equation:

$$\frac{\partial \left( \rho^* u_i^* \right)}{\partial t^*} + \frac{\partial \left( \rho^* u_i^* u_j^* + p^* \delta_{ij} \right)}{\partial x_j^*} = \frac{\partial \sigma_{ji}^*}{\partial x_j^*} - f_i^*,$$

(2.2)

where $-f_i^*$ is the force per unit volume transferred from the solid particles to the carrier gas.
Energy Equation:
\[
\frac{\partial (\rho^* E^*)}{\partial t^*} + \frac{\partial \left[ (\rho^* E^* + p^*) u_j^* \right]}{\partial x_j^*} = \frac{\partial \left( \sigma_{ji}^* u_i^* - q_j^* \right)}{\partial x_j^*} - q^*,
\tag{2.3}
\]

where \( E^* = e^* + \frac{1}{2} u_i^* u_i^* \) is the total energy per unit mass, and \(-q^*\) is the rate of heat per unit volume transferred from the solid particles to the carrier gas. The fluid is assumed to be a perfect gas.

Equation of State:

\[
p^* = \rho^* R^* T^*,
\tag{2.4}
\]

\[
E^* = \frac{p^*}{(\gamma - 1) \rho^*} + \frac{1}{2} u_i^* u_i^* \tag{2.5}
\]

We also assume a Newtonian fluid, and write the viscous stress tensor as

\[
\sigma_{ij}^* = \lambda^* e_{kk}^* + 2 \mu^* e_{ij}^*,
\tag{2.6}
\]

where the rate of strain tensor is

\[
e_{ij}^* = \frac{1}{2} \left( \frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} \right),
\tag{2.7}
\]

In this work; we we adopted Stokes hypothesis (bulk viscosity is zero), \( \lambda^* = -\frac{2}{3} \mu^* \).

\[
\sigma_{ij}^* = \mu^* \left( \frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} - \frac{2}{3} \frac{\partial u_k^*}{\partial x_k^*} \delta_{ij} \right),
\tag{2.8}
\]

The heat flux vector is given by Fourier law,

\[
q_j^* = -\kappa^* \frac{\partial T^*}{\partial x_j^*},
\tag{2.9}
\]
where $\kappa^*$ is the gas thermal conductivity. In this dissertation, simulations are presented for air and helium. The gas constant $R^*$ and the ratio of specific heats $\gamma$ for air are given by

$$\gamma = \frac{c_p^*}{c_v^*} = \frac{7}{5},$$

and

$$R^* = c_p^* - c_v^* = 287.06 \text{ Jkg}^{-1}\text{K}^{-1},$$

and for helium,

$$\gamma = \frac{c_p^*}{c_v^*} = \frac{5}{3},$$

and

$$R^* = c_p^* - c_v^* = 2077 \text{ Jkg}^{-1}\text{K}^{-1},$$

Here the specific heat at constant pressure $c_p^*$ and the specific heat at constant volume $c_v^*$ are assumed to be constants. The dynamic viscosity and thermal conductivity are determined by the Sutherland law (46)

$$\mu^* = \mu_0^* \left(\frac{T^*}{T_0^*}\right)^{3/2} \left(\frac{T_0^* + S_\mu^*}{T^* + S_\mu^*}\right),$$

$$\kappa^* = \kappa_0^* \left(\frac{T^*}{T_0^*}\right)^{3/2} \left(\frac{T_0^* + S_\kappa^*}{T^* + S_\kappa^*}\right),$$

For air, we used the parameters $T_0^* = 273K$, $\mu_0^* = 1.716 \times 10^{-5} \text{N.s/m}^2$, $\kappa_0^* = 0.0244 \text{W/m.K}$, $S_\mu^* = 111K$ and $S_\kappa^* = 194K$. For helium, we used $T_0^* = 273K$, $\mu_0^* = 1.8618 \times 10^{-5} \text{N.s/m}^2$, $\kappa_0^* = 0.14151 \text{W/m.K}$, $S_\mu^* = 80K$. 
2.2 Governing Equations in Non-dimensional Form

Using reference length $L^*$, velocity $W^*$, density $\rho^*$, temperature $T^*$, specific heat at constant pressure $c_{pr}^*$, thermal conductivity $\kappa^*$ and dynamic viscosity $\mu^*$, we introduce non-dimensional variables

$$
\frac{t}{L^*} = \frac{t^* W^*}{L^*}, \quad \frac{T}{T^*} = \frac{T^*}{T^*}, \quad \frac{u_i}{W^*} = \frac{u_i^*}{W^*}, \quad \frac{\rho}{\rho^*} = \frac{\rho^*}{\rho^*}, \quad \frac{p}{p^*} = \frac{p^*}{\rho^* W^*^2},
$$

$$
\frac{T}{T^*} = \frac{T^*}{T^*}, \quad E = \frac{E^*}{W^*^2}, \quad \frac{\mu}{\mu^*} = \frac{\mu^*}{\mu^*}, \quad \frac{\kappa}{\kappa^*} = \frac{\kappa^*}{\kappa^*}, \quad \frac{c_p}{c_{pr}^*}
$$

Using the above dimensionless variables, we write the governing equations in non-dimensional form as follows:

Continuity Equation:

$$
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0,
$$

Momentum Equation:

$$
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j + p \delta_{ij})}{\partial x_j} = \frac{\partial \sigma_{ji}}{\partial x_j} - f_i,
$$

where

$$
f_i = \frac{f_i^* L^*}{\rho^* W^*^2},
$$

Energy Equation:

$$
\frac{\partial (\rho E)}{\partial t} + \frac{\partial [(\rho E + p) u_j]}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \sigma_{ji} u_i - \frac{1}{(\gamma - 1)} \frac{M^2 Re Pr}{q_j} q_j \right] - q,
$$

where
\[ q = \frac{q^* L^*_r}{\rho^*_r W^*_r}, \]  

(2.22)

**Equation of State:**

\[ p = \rho RT, \]  

(2.23)

**with**

\[ E = \frac{p}{(\gamma - 1) \rho} + \frac{1}{2} u_i u_i, \]  

(2.24)

\[ \sigma_{ij} = \frac{\mu}{Re} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right), \]  

(2.25)

\[ q_j = -\kappa \frac{\partial T}{\partial x_j}, \]  

(2.26)

The Reynolds number \( Re \), the Mach number \( M \) and the Prandtl number \( Pr \) are given by

\[ Re = \frac{\rho^*_r W^*_r L^*_r}{\mu^*_r}, \]  

(2.27)

\[ M = \frac{W^*_r}{\sqrt{\gamma R^*_r T^*_r}}, \]  

(2.28)

\[ Pr = \frac{\mu^*_r c^*_{pr}}{\kappa^*_r}, \]  

(2.29)
The non-dimensional gas constant is given by

\[ R = \frac{R^* T_i^*}{W_r^2} = \frac{1}{\gamma M^2} \]  

(2.30)

### 2.3 Equations of Motion and Thermal Energy Equation for Solid Particles

In this dissertation, solid particles are treated as point masses. Particles trajectories are calculated by integrating the equations of motion for the particles simultaneously with the field equations of the carrier gas. In this study only the drag force is considered, hence the equations of motion of a particle are given by

\[ m_p \frac{dv_i^*}{dt^*} = F_i^* \]  

(2.31)

\[ \frac{dy_i^*}{dt^*} = v_i^* \]  

(2.32)

where \( y_i^* \) and \( v_i^* \) are the particle position and velocity vectors.

The drag is given by

\[ F_i^* = \frac{1}{2} A_p^* \rho^* C_D (u_i^* - v_i^*) | u^* - v^* | \]  

(2.33)

where \( A_p^* = \pi d_p^2 / 4 \) is the projected area of the particle, \( C_D \) is the drag coefficient, and \( u_i^* \) and \( \rho^* \) are the carrier gas velocity and density at the instantaneous particle position \( y_i^* \), respectively. We assume a spherical particle with diameter \( d_p^* \). In this study, the drag coefficient of a spherical particle including compressibility and rarefied gas effects is adopted (47). A formula for the drag coefficient is given in Appendix A.

The particle temperature \( T_p^* \) is determined by integrating the thermal energy equation for the particle simultaneously with the carrier gas field equations. A small Biot number
is assumed and hence the temperature gradient within the particle is neglected. Only heat transfer by convection is considered.

Thermal energy equation for a particle is given by

$$m_p^* c_{pp}^* \frac{dT_p^*}{dt^*} = h^* (T^* - T_p^*) S_p^*$$  \hspace{1cm} (2.34)

where $S_p^* = \pi d_p^{*2}$ is the surface area of a spherical particle, $m_p^* = \rho_p^* \pi d_p^{*3}/6$ is the particle mass, $c_{pp}^*$ is the particle’s material coefficient of heat capacity and $h^*$ is the coefficient of convection.

We note that $T^*$ is the carrier gas local temperature at the instantaneous particle position $y_i^*$.

We introduce non-dimensional particle variables by using the same reference length, velocity, density, and temperature as used to non-dimensionalize the gas variables.

$$y_i = \frac{y_i^*}{L_r^*}, \quad T_p = \frac{T_p^*}{T_r^*}, \quad v_i = \frac{v_i^*}{W_r}, \quad \rho_p = \frac{\rho_p^*}{\rho_r^*}, \quad c_{pp} = \frac{c_{pp}^*}{c_{pp}^{*r}}.$$ \hspace{1cm} (2.35)

The non-dimensional particle equations are

$$ \frac{dv_i}{dt} = \frac{3}{4} \frac{1}{d_p^* \rho_p^*} C_D (u_i - v_i) |\mathbf{u} - \mathbf{v}| $$ \hspace{1cm} (2.36)

$$ \frac{dy_i}{dt} = v_i $$ \hspace{1cm} (2.37)

$$ \frac{dT_p}{dt} = \frac{1}{c_{pp}^* Pr Re \rho_p^* d_p^{*2}} \frac{6Nu}{(T - T_p^*)} $$ \hspace{1cm} (2.38)

where the Nusselt number $Nu$ is defined by

$$Nu = \frac{h^* d_p^*}{\kappa^*}$$ \hspace{1cm} (2.39)

We use a formula for the Nusselt number given by Carlson and Hoglund (48) and is shown in Appendix A.
Chapter 3

Numerical Methods

Numerical methods presented in this chapter include a five-stage fourth-order Runge-Kutta method (49), a fifth-order WENO finite-volume scheme (36; 50) and a compact sixth-order finite-difference scheme (39) with the tenth-order spatial filter (51). These numerical schemes are well documented in publications by respective authors. However, the way we combined the schemes to simulate a supersonic jet impingement problem and two-way coupling of solid particles is new. Because we developed our own computer code, we felt that it is important to describe the details of numerical methods and their implementation in our code and give specific parameters.

3.1 Nonuniform Cartesian Mesh

The Navier-Stokes equations in Cartesian coordinates are written as

$$\frac{\partial U}{\partial t} + \frac{\partial (\tilde{F} - \tilde{F}_v)}{\partial x} + \frac{\partial (\tilde{G} - \tilde{G}_v)}{\partial y} + \frac{\partial (\tilde{H} - \tilde{H}_v)}{\partial z} = -\tilde{S}$$

(3.1)

A nonuniform Cartesian mesh in the \((x, y, z)\) space is mapped by a smooth transformation to a uniform mesh in the computational domain \((\xi, \eta, \zeta)\).

$$x = x(\xi)$$

$$y = y(\eta)$$

$$z = z(\zeta)$$

(3.2)
Introducing the notation

\[ x_\xi = \frac{dx(\xi)}{d\xi} \]
\[ y_\eta = \frac{dy(\eta)}{d\eta} \]
\[ z_\zeta = \frac{dz(\zeta)}{d\zeta} \]
\[ J = \frac{1}{x_\xi y_\eta z_\zeta} \]

we transform Eq(3.1) to

\[ \frac{\partial Q}{\partial t} + \frac{\partial (F - F_v)}{\partial \xi} + \frac{\partial (G - G_v)}{\partial \eta} + \frac{\partial (H - H_v)}{\partial \zeta} = -S \]

where

\[ Q = \frac{U}{J} \]
\[ F = y_\eta z_\zeta \tilde{F} \]
\[ G = x_\xi z_\zeta \tilde{G} \]
\[ H = x_\xi y_\eta \tilde{H} \]
\[ F_v = y_\eta z_\zeta \tilde{F}_v \]
\[ G_v = x_\xi z_\zeta \tilde{G}_v \]
\[ H_v = x_\xi y_\eta \tilde{H}_v \]
\[ S = \tilde{S}/J \]

We use the method of lines in which a suitable discretization method is used to approximate the spatial derivatives and thereby converting the partial differential equations to a system of ordinary differential equations in time.

\[ \frac{dQ}{dt} = L_q(Q, P) \]

where \( Q \) is an array that represents all flow variables at the mesh nodes. Because the exchange of momentum and energy between carrier gas and particles depends on the instantaneous particles positions, velocities, and temperatures, the equations for the particles are also advanced.
in time simultaneously with the Navier-Stokes equations using the same time advancement scheme and time step. Particles are treated as discrete point masses and tracked using the Lagrangian approach. Hence their governing equations are ordinary differential equations in time

\[ \frac{dP}{dt} = L_p(Q, P) \] \hspace{1cm} (3.7)

where \( P \) is an array that stands for the positions, velocities, and temperatures of all solid particles in the field.

### 3.2 Fourth-Order Runge-Kutta Time Integration Scheme

Given initial conditions of all flow and particles variables, we advance the systems of equations Eqs(3.6)-(3.7) in time using the five-stage fourth-order Runge-Kutta scheme developed by Carpenter and Kennedy (49). This is a low-storage scheme where only two storage locations are required for each variable. Let \( Q^n \) and \( P^n \) be the solution at time step \( n \). The solution at time step \( n + 1 \) is obtained in five sub-steps. The algorithm is

\[
\begin{align*}
R_p &= 0 \\
R_q &= 0 \quad (3.8) \\
\text{For } m &= 1 \text{ to } 5 \\
R_p &\leftarrow L_p(Q, P) + a^m R_p \\
R_q &\leftarrow L_q(Q, P) + a^m R_q \\
P &\leftarrow P + b^m \Delta t R_p \\
Q &\leftarrow Q + b^m \Delta t R_q \\
\text{End For} \\
P^{n+1} &= P \\
Q^{n+1} &= Q \quad (3.11)
\end{align*}
\]
Table 3.1: Coefficients of low-storage Runge-Kutta Scheme

<table>
<thead>
<tr>
<th>$m$</th>
<th>$a^m$</th>
<th>$b^m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.1496590219993</td>
</tr>
<tr>
<td>2</td>
<td>-0.4178904745</td>
<td>0.3792103129999</td>
</tr>
<tr>
<td>3</td>
<td>-1.192151694643</td>
<td>0.8229550293869</td>
</tr>
<tr>
<td>4</td>
<td>-1.697784692471</td>
<td>0.6994504559488</td>
</tr>
<tr>
<td>5</td>
<td>-1.514183444257</td>
<td>0.1530572479681</td>
</tr>
</tbody>
</table>

The coefficients $a^m$ and $b^m$ are given in Table (3.1), and $\Delta t$ is the time step.

### 3.3 Weighted Essentially Non-Oscillatory Finite Difference Scheme

In this section, we present details of Weighted Essentially Non-Oscillatory Finite-Difference (WENO) scheme for approximating the spatial derivatives of the inviscid flux terms in the Navier-Stokes equations. This will be demonstrated for the term $\partial F/\partial \xi$, and similar treatments can be applied to the terms $\partial G/\partial \eta$, and $\partial H/\partial \zeta$. At node $(i,j,k)$, the derivative of the inviscid flux is written as

$$\left( \frac{\partial F}{\partial \xi} \right)_i = \frac{1}{\Delta \xi} \left( \hat{F}_{i+\frac{1}{2}} - \hat{F}_{i-\frac{1}{2}} \right) \quad (3.12)$$

where $\hat{F}_{i+\frac{1}{2}}$ is a numerical flux at the midpoint (interface) between nodes $i$ and $i+1$, that is constructed by a fifth-order WENO scheme according to the following steps. The indices $j$ and $k$ will not be shown.

1. The flux vector $F_i$ and the matrix of eigenvalues $\Lambda_i$ of the flux Jacobian matrix $\partial F/\partial U$ are computed at all nodes.

2. The right $\hat{R}_{i+1/2}$ and left $\hat{L}_{i+1/2} = \hat{R}_{i+1/2}^{-1}$ eigenvector matrices and the eigenvalues $\hat{\Lambda}_{i+1/2}$ of the Roe matrix are computed at the interface between cell $i$ and $i+1$. On
the left side of the interface \((i + 1/2)\) the primary variables are

\[
\begin{align*}
\rho^- &= \rho_i \\
u^- &= u_i \\
v^- &= v_i \\
w^- &= w_i \\
p^- &= p_i \\
E^- &= E_i \\
H^- &= E^- + \frac{p^-}{\rho^-}
\end{align*}
\] (3.13)

and on the right side they are

\[
\begin{align*}
\rho^+ &= \rho_{i+1} \\
u^+ &= u_{i+1} \\
v^+ &= v_{i+1} \\
w^+ &= w_{i+1} \\
p^+ &= p_{i+1} \\
E^+ &= E_{i+1} \\
H^+ &= E^+ + \frac{p^+}{\rho^+}
\end{align*}
\] (3.14)

The Roe matrix is the flux Jacobian matrix evaluated at the Roe-averaged state of the left and right primary variables that is given by

\[
\begin{align*}
\hat{\mathbf{u}} &= \frac{u^- \sqrt{\rho^-} + u^+ \sqrt{\rho^+}}{\sqrt{\rho^-} + \sqrt{\rho^+}} \\
\hat{\mathbf{v}} &= \frac{v^- \sqrt{\rho^-} + v^+ \sqrt{\rho^+}}{\sqrt{\rho^-} + \sqrt{\rho^+}} \\
\hat{\mathbf{w}} &= \frac{w^- \sqrt{\rho^-} + w^+ \sqrt{\rho^+}}{\sqrt{\rho^-} + \sqrt{\rho^+}} \\
\hat{\mathbf{H}} &= \frac{H^- \sqrt{\rho^-} + H^+ \sqrt{\rho^+}}{\sqrt{\rho^-} + \sqrt{\rho^+}} \\
\hat{\mathbf{a}}^2 &= (\gamma - 1) \left[ \hat{\mathbf{H}} - \frac{1}{2} (\hat{\mathbf{u}}^2 + \hat{\mathbf{v}}^2 + \hat{\mathbf{w}}^2) \right]
\end{align*}
\] (3.15)
The eigenvalues are

$$\hat{\Lambda}_{i+\frac{1}{2}} = \begin{bmatrix} \hat{u} - \hat{a} & 0 & 0 & 0 & 0 \\ 0 & \hat{u} & 0 & 0 & 0 \\ 0 & 0 & \hat{u} & 0 & 0 \\ 0 & 0 & 0 & \hat{u} & 0 \\ 0 & 0 & 0 & 0 & \hat{u} + \hat{a} \end{bmatrix}$$

(3.16)

and the right eigenvectors are

$$\hat{R}_{i+\frac{1}{2}} = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ \hat{u} - \hat{a} & \hat{v} & 0 & 0 & \hat{u} + \hat{a} \\ \hat{v} & 0 & 1 & 0 & \hat{v} \\ \hat{w} & 0 & 0 & 1 & \hat{w} \\ \hat{H} - \hat{a}\hat{u} & \hat{v}^2 - \frac{1}{2} \hat{V}^2 & \hat{v} & \hat{w} & \hat{H} + \hat{a}\hat{u} \end{bmatrix}$$

(3.17)

where $\hat{V}^2 = \hat{u}^2 + \hat{v}^2 + \hat{w}^2$

(3) Higher-order WENO flux is built from a low-order flux, and in this work we use the local Lax-Friedrichs (LLF) flux.

$$F_{i+\frac{1}{2}}^{+LF} = \frac{1}{2} \left[ F_i + \hat{\Lambda}_{i+\frac{1}{2}} Q_i(\xi_x)_i \right]$$

$$F_{i-\frac{1}{2}}^{-LF} = \frac{1}{2} \left[ F_i - \hat{\Lambda}_{i+\frac{1}{2}} Q_i(\xi_x)_i \right]$$

(3.18)

where $\hat{\Lambda}_{i+\frac{1}{2}}$ is a (positive) diagonal matrix to be defined later; it controls the dissipation of the WENO scheme. These flux vectors are projected onto the characteristic directions at the interface $i + 1/2$; each characteristic flux component is a linear combination of the components of the flux vector with the coefficient being the components of the left eigenvectors.

$$F_{i;i+\frac{1}{2}}^{+c} = \hat{L}_{i+1/2} F_{i}^{+LF}$$

$$F_{i;i+\frac{1}{2}}^{-c} = \hat{L}_{i+1/2} F_{i}^{-LF}$$

(3.19)
The double subscript \((i; i + \frac{1}{2})\) is introduced here to emphasize that Eq\((3.19)\) gives the characteristic flux at the cell center (or node \(i\)) projected onto the characteristic directions at the cell interface \(i + 1/2\). The characteristic flux at the cell interface \(i + 1/2\) is obtained by reconstruction (interpolation) of the flux at the neighboring cell centers.

In the fifth-order WENO scheme, three different interpolation stencils are possible and denoted by \(k = 0, 1, 2\). For \(F_{i+\frac{1}{2}}^{c+}\), the interpolated fluxes are

\[
F_{0,i+\frac{1}{2}}^{c+} = \frac{1}{6} \left( 2F_{i-2,i+\frac{1}{2}}^{c+} - 7F_{i-1,i+\frac{1}{2}}^{c+} + 11F_{i,i+\frac{1}{2}}^{c+} \right)
\]

\[
F_{1,i+\frac{1}{2}}^{c+} = \frac{1}{6} \left( -F_{i-1,i+\frac{1}{2}}^{c+} + 5F_{i,i+\frac{1}{2}}^{c+} + 2F_{i+1,i+\frac{1}{2}}^{c+} \right)
\]

\[
F_{2,i+\frac{1}{2}}^{c+} = \frac{1}{6} \left( 2F_{i+1,i+\frac{1}{2}}^{c+} + 5F_{i,i+\frac{1}{2}}^{c+} - F_{i-1,i+\frac{1}{2}}^{c+} \right)
\] (3.20)

For \(F_{i+\frac{1}{2}}^{c-}\), the interpolated fluxes are

\[
F_{0,i+\frac{1}{2}}^{c-} = \frac{1}{6} \left( 2F_{i+3,i+\frac{1}{2}}^{c-} - 7F_{i+2,i+\frac{1}{2}}^{c-} + 11F_{i+1,i+\frac{1}{2}}^{c-} \right)
\]

\[
F_{1,i+\frac{1}{2}}^{c-} = \frac{1}{6} \left( -F_{i+2,i+\frac{1}{2}}^{c-} + 5F_{i+1,i+\frac{1}{2}}^{c-} + 2F_{i,i+\frac{1}{2}}^{c-} \right)
\]

\[
F_{2,i+\frac{1}{2}}^{c-} = \frac{1}{6} \left( 2F_{i+1,i+\frac{1}{2}}^{c-} + 5F_{i,i+\frac{1}{2}}^{c-} - F_{i-1,i+\frac{1}{2}}^{c-} \right)
\] (3.21)

In Eqs\((3.20)-(3.21)\)

\[
F_{i+k,i+\frac{1}{2}}^{c+} = \frac{1}{2} \hat{L}_{i+1/2} \left[ F_{i+k} + \tilde{\Lambda}_{i+\frac{1}{2}} Q_{i+k}(\xi_x)_{i+k} \right]
\]

\[
F_{i+k,i+\frac{1}{2}}^{c-} = \frac{1}{2} \hat{L}_{i+1/2} \left[ F_{i+k} - \tilde{\Lambda}_{i+\frac{1}{2}} Q_{i+k}(\xi_x)_{i+k} \right]
\] (3.22)

where

\[
\tilde{\Lambda}_{i+\frac{1}{2}} = \chi \left( \max \left[ |\Lambda_{i+\frac{1}{2}}|, |\Lambda_{i-1}|, |\Lambda_{i-2}|, |\Lambda_{i}|, |\Lambda_{i+1}|, |\Lambda_{i+2}|, \epsilon_d \right] \right)
\] (3.23)

where \(\chi\) is an empirical parameter with values between 1.1 and 1.3. In all results presented in this dissertation, \(\epsilon_d = 0\) except for the cases of helium jet impingement, we used \(\epsilon_d = 0.05\). For the helium jet impingement at Mach number 2.8, simulations became unstable in the sonic regions as the flow re-expands from compressed gas zone.

A weighted flux is formed from the three interpolated fluxes

\[
F_{i+\frac{1}{2}}^{cw+} = \omega_1^+ F_{0,i+\frac{1}{2}}^{c+} + \omega_2^+ F_{1,i+\frac{1}{2}}^{c+} + \omega_3^+ F_{2,i+\frac{1}{2}}^{c+}
\]

\[
F_{i+\frac{1}{2}}^{cw-} = \omega_1^- F_{0,i+\frac{1}{2}}^{c-} + \omega_2^- F_{1,i+\frac{1}{2}}^{c-} + \omega_3^- F_{2,i+\frac{1}{2}}^{c-}
\] (3.24)
The procedure for computing the weighting parameters is as follows:

\[
\begin{align*}
\beta_1^+ &= \frac{13}{12} (F_{i+\frac{1}{2}}^+ - 2F_{i+\frac{1}{2}}^- + F_{i-\frac{1}{2}}^- )^2 + \frac{1}{4} (F_{i+\frac{1}{2}}^- F_{i+\frac{1}{2}}^- - 4F_{i+\frac{1}{2}}^-) \\
\beta_2^+ &= \frac{13}{12} (F_{i+\frac{1}{2}}^- - 2F_{i+\frac{1}{2}}^- + F_{i+\frac{1}{2}}^- )^2 + \frac{1}{4} (F_{i+\frac{1}{2}}^- F_{i+\frac{1}{2}}^- - 4F_{i+\frac{1}{2}}^-) \\
\beta_3^+ &= \frac{13}{12} (F_{i+\frac{1}{2}}^- - 2F_{i+\frac{1}{2}}^- + F_{i+\frac{1}{2}}^- )^2 + \frac{1}{4} (F_{i+\frac{1}{2}}^- F_{i+\frac{1}{2}}^- - 4F_{i+\frac{1}{2}}^-) \\
\beta_1^- &= \frac{13}{12} (F_{i-\frac{1}{2}}^- - 2F_{i-\frac{1}{2}}^- + F_{i-\frac{1}{2}}^- )^2 + \frac{1}{4} (F_{i-\frac{1}{2}}^- F_{i-\frac{1}{2}}^- - 4F_{i-\frac{1}{2}}^-) \\
\beta_2^- &= \frac{13}{12} (F_{i-\frac{1}{2}}^- - 2F_{i-\frac{1}{2}}^- + F_{i-\frac{1}{2}}^- )^2 + \frac{1}{4} (F_{i-\frac{1}{2}}^- F_{i-\frac{1}{2}}^- - 4F_{i-\frac{1}{2}}^-) \\
\beta_3^- &= \frac{13}{12} (F_{i-\frac{1}{2}}^- - 2F_{i-\frac{1}{2}}^- + F_{i-\frac{1}{2}}^- )^2 + \frac{1}{4} (F_{i-\frac{1}{2}}^- F_{i-\frac{1}{2}}^- - 4F_{i-\frac{1}{2}}^-)
\end{align*}
\]

where \( \epsilon = 10^{-8} \), \( \alpha_1 = 1/10 \), \( \alpha_2 = 3/5 \) and \( \alpha_3 = 3/10 \)

(4) Finally, the numerical flux at cell interface \( i + \frac{1}{2} \) is given by

\[
\hat{F}_{i+\frac{1}{2}} = \hat{R}_{i+\frac{1}{2}} \left[ F_{i+\frac{1}{2}}^+ cw + F_{i+\frac{1}{2}}^- cw \right]
\]

The WENO scheme is used only in a small box around the bow shock. A schematic diagram indicating a box around the bow shock wave where WENO scheme is used is shown in figure 3.1. The fifth-order WENO scheme is applied to points inside the box and six-order compact scheme is applied for points outside the box.
Figure 3.1: A box around the bow shock wave in the \(yz\)-plane. The fifth-order WENO scheme is applied to points inside the box and six-order compact scheme is applied for points outside the box.

### 3.4 Compact Sixth-Order Finite-Difference Scheme

To reduce the numerical dissipation due to space discretization in smooth regions, a sixth-order compact finite-difference scheme (39) is used for spatial derivatives of the inviscid fluxes with respect to the three Cartesian \((\xi, \eta, \zeta)\) coordinates for which the mesh is uniform. The derivatives \(F'_i = (\partial F/\partial \xi)_i\) at all nodes \(i = 1\) to \(i = n\) are determined by solving a tridiagonal linear system

\[
\alpha F'_{i-1} + F'_i + \alpha F'_{i+1} = \frac{1}{h} [a(F_{i+1} - F_{i-1}) + b(F_{i+2} - F_{i-2})] \tag{3.27}
\]

where \(\alpha = 1/3\), \(a = 7/9\), \(b = 1/36\), and \(h = \Delta \xi\) is the mesh size. This scheme is applied for \(i = 3, \ldots, n-2\). Fifth-order explicit schemes developed by Carpenter et al. (52) can be used at the boundary points \(i = 1\) and \(i = n\),

\(i = 1:\)

\[
F'_1 = \frac{1}{h}(c_0 F_i + c_1 F_{i+1} + c_2 F_{i+2} + c_3 F_{i+3} + c_4 F_{i+4} + c_5 F_{i+5} + c_6 F_{i+6} + c_7 F_{i+7}) \tag{3.28}
\]
\[ i = n: \]
\[ F'_i = -\frac{1}{h}(c_0 F_i + c_1 F_{i-1} + c_2 F_{i-2} + c_3 F_{i-3} + c_4 F_{i-4} + c_5 F_{i-5} + c_6 F_{i-6} + c_7 F_{i-7}) \quad (3.29) \]
and also a fifth-order explicit scheme can be used at the first point off the boundary \( i = 2 \) and \( i = n - 1 \),

\[ i = 1: \]
\[ F'_{i+1} = \frac{1}{h}(e_0 F_i + e_1 F_{i+1} + e_2 F_{i+2} + e_3 F_{i+3} + e_4 F_{i+4} + e_5 F_{i+5} + e_6 F_{i+6} + e_7 F_{i+7}) \quad (3.30) \]

\[ i = n: \]
\[ F'_{i-1} = -\frac{1}{h}(e_0 F_i + e_1 F_{i-1} + e_2 F_{i-2} + e_3 F_{i-3} + e_4 F_{i-4} + e_5 F_{i-5} + e_6 F_{i-6} + e_7 F_{i-7}) \quad (3.31) \]
The coefficients are given by Carpenter et al. (52) and also included in Appendix B for completeness.

In the version of the code used in this dissertation, there are variations of the schemes used at the boundary points. In the \( \xi \) and \( \eta \) directions (for cold spray applications, the \( \xi - \eta \) plane is normal to the jet axis) we used fourth-order Pade scheme at the first point off the boundary \( i = 2 \) and \( i = n - 1 \),
\[ \alpha F'_{i-1} + F'_i + \alpha F'_{i+1} = \frac{1}{h}[a(F_{i+1} - F_{i-1})] \quad (3.32) \]
where \( \alpha = 1/4, \) and \( a = 3/4 \). We used a first-order scheme at the boundary points \( i = 1 \) and \( i = n \),

\[ i = n, \]

\[ i = 1: \]
\[ F'_{i-1} = \frac{1}{h}(F_{i+1} - F_i) \quad (3.33) \]

\[ i = n: \]
\[ F'_{i-1} = \frac{1}{h}(F_i - F_{i-1}) \quad (3.34) \]

In the \( \zeta \) direction (for cold spray applications, the jet main velocity is in the negative \( \zeta \)-direction) we used the fifth-order explicit schemes at the top boundary (this the plane where the jet enters the computational domain) for the points \( i = n - 1 \) and \( i = n \). At the bottom
boundary (this is the wall representing the substrate surface) for the first point off the wall
\( i = 2 \) we used a second-order central difference scheme,

\[ F'_i = \frac{1}{2h}(F_{i+1} - F_{i-1}) \]  

(3.35)

For the point on the wall \( i = 1 \), we used a first-order scheme for the flux components in the
continuity, z-momentum and energy equations, \( i = 1 \):

\[ F'_i = \frac{1}{h}(F_{i+1} - F_{i}) \]  

(3.36)

but we set the \( \zeta \)-derivative of the flux to zero for the \( x \)- and \( y \)-momentum equations.

### 3.5 Compact Tenth-Order Filter

The compact tenth-order filter is a low-pass filter developed by Gaitonde and Visbal (51) for
application with the compact sixth-order central difference scheme. It is needed to remove
spurious high wavenumbers that can be produced by non-dissipative schemes when applied
to nonlinear problems. The filter is applied once per time step after the five stages of the
Runge-Kutta time scheme. It is applied sequentially in the \( x \), \( y \), and \( z \) directions. The flow
variables being filtered are the array \( Q \). Let \( Q_i \) denote the unfiltered quantity at node \( i \). A
tri-diagonal system is solved for the filtered quantity \( \tilde{Q}_i \), which is given by

\[ \alpha_f \tilde{Q}_{i-1} + \tilde{Q}_i + \alpha_f \tilde{Q}_{i+1} = \sum_{m=0}^{M'} \frac{1}{2} a_m (Q_{i+m} + Q_{i-m}) \]  

(3.37)

where \( M' = 5 \), and \( \alpha_f < 0.5 \). For the jet impingement problem, we used values of \( \alpha_f \) in the
range 0.49 to 0.495.

\[
\begin{align*}
    a_0 &= (193 + 126\alpha_f)/256, \\
    a_1 &= (105 + 302\alpha_f)/256, \\
    a_2 &= (-15 + 30\alpha_f)/64, \\
    a_3 &= (45 - 90\alpha_f)/512, \\
    a_4 &= (-5 + 10\alpha_f)/256, \\
    a_5 &= (1 - 2\alpha_f)/512
\end{align*}
\]
The stencil of the tenth-order filter is 11 points; the central point and five points on each side. As the central point approaches a boundary, we used filters of decreasing even order.

The coefficients for the eight-order filter \((M' = 4)\) are

\[
\begin{align*}
    a_0 &= \frac{(93 + 70\alpha_f)}{128}, \\
    a_1 &= \frac{(7 + 18\alpha_f)}{16}, \\
    a_2 &= \frac{(-7 + 14\alpha_f)}{32}, \\
    a_3 &= \frac{(1 - 2\alpha_f)}{16}, \\
    a_4 &= \frac{(-1 + 2\alpha_f)}{128}
\end{align*}
\]

The coefficients for the sixth-order filter \((M' = 3)\) are

\[
\begin{align*}
    a_0 &= \frac{0.5(11 + 10\alpha_f)}{16}, \\
    a_1 &= \frac{0.5(15 + 34\alpha_f)}{32}, \\
    a_2 &= \frac{0.5(-3 + 6\alpha_f)}{16}, \\
    a_3 &= \frac{0.5(1 - 2\alpha_f)}{32}
\end{align*}
\]

The coefficients for the fourth-order filter \((M' = 2)\) are

\[
\begin{align*}
    a_0 &= \frac{0.5(5 + 6\alpha_f)}{8}, \\
    a_1 &= \frac{0.5(1 + 2\alpha_f)}{2}, \\
    a_2 &= \frac{0.5(-1 + 2\alpha_f)}{8}
\end{align*}
\]

The coefficients for the second-order filter \((M' = 1)\) are

\[
\begin{align*}
    a_0 &= \frac{0.5(1 + 2\alpha_f)}{2}, \\
    a_1 &= \frac{0.5(1 + 2\alpha_f)}{2}
\end{align*}
\]

The points on the boundary are not filtered.

### 3.6 WENO Dissipation and Viscous Terms

After each complete five-stage Runge-Kutta time step, a WENO dissipation step \((40; 53)\) is executed for points in the domain outside the WENO box. The dissipative flux is obtained by subtracting the six-order explicit central-difference flux from the fifth-order WENO flux.
3.7 Viscous Terms

Fourth-order explicit central-difference schemes are used for the viscous and heat conduction terms.

3.8 Implementation of Two-way Coupling

The source term $-S^* = (0, -f_1^*, -f_2^*, -f_3^*, -q^*)$ represents force per unit volume ($-f_i^*)$ exerted by the particles on the gas and rate of heat transfer per unit volume $-q^*$ transferred from the particles to the gas. At the beginning of every stage of the five-stage Runge-Kutta time integration scheme, we compute the force $F_i^*$ acting on every particle [see Equation 2.33] and the rate of heat transfer to the particle $Q^*$ [equation 2.34] using local flow properties that are available at the that stage. To determine the flow properties at the particle location, we used trilinear interpolation. The force and the rate of heat transfer are divided by the volume of the cell containing the particle, hence we obtain $-f_i^* = -F_i^*/\Delta V$ and $-q^* = -Q^*/\Delta V$, where $\Delta V$ is the cell volume. The concentrated force and heat transfer (per unit volume) are allocated to the 8 nodes of the cell containing the particle. Each of the 8 nodes receives a fraction ($\beta$ of the total force and rate of heat transfer given by (54)

$$\beta = (1 - r_1)(1 - r_2)(1 - r_3)$$

(3.38)

where

$$r_1 = |x_p - x_g|/\Delta x$$
$$r_2 = |y_p - y_g|/\Delta y$$
$$r_3 = |z_p - z_g|/\Delta z$$

(3.39)

where $(x_p, y_p, z_p)$ are the particle current coordinates, $(x_g, y_g, z_g)$ are coordinates of any of the eight corners of the cell containing the particle, and $\Delta x$, $\Delta y$, and $\Delta z$ are dimensions of the cell. This process is done for each of the particles in the flow field.
Chapter 4

Supersonic Jet Impingement:
Results and Discussion

Despite extensive studies of jet gas-dynamics for cold spray technology, some issues have not been accurately addressed. One of the most important tasks in the cold spray process is to achieve high particle velocity and temperature at impact efficiently. This is not possible without complete understanding of all the important features of the gas flow process. Development of the boundary layer on the nozzle walls, the structure and instabilities of the supersonic jet, interaction of a supersonic jet with the substrate, locations and structures of the shock outside the nozzle, the compressed gas layer in front of the substrate, effects of stand-off distance and heat transfer between the jet and the particle/substrate, should be properly studied to achieve the optimal velocity and temperature of particles at impact on the substrate.

Generally, two types of nozzles are used in cold spray; circular and rectangular. A rectangular nozzle has an advantage over the circular nozzle. A rectangular nozzle can provide a wider spray beam normal to traverse direction. The thickness of the compressed gas layer is small in rectangular jets, which can also decrease the effects of particle deceleration in the compressed gas zone (7).

The purpose of the current chapter is to explore the flow characteristics associated with the impingement of rectangular supersonic jets. Helium and air are used as a deriving gas. All
the studies are performed for two cases of the standoff distance, which is the distance between nozzle exit and substrate; $Z_o = 10\text{mm}$ and $Z_o = 20\text{mm}$. In this chapter, the instantaneous and mean flow field characteristics are discussed. Grid sensitivity study is obtained for both cases. Comparison with experimental data is also presented.

### 4.1 Computational Domain and Initial Conditions

The model consists of a rectangular jet issuing from a plane which is at a distance of $Z_o = 10\text{mm}$ or $Z_o = 20\text{mm}$ above the substrate. The dimensions of the nozzle exit are $H = 10\text{mm}$ and $h = 3\text{mm}$ along $x$ and $y$, respectively. The jet mean velocity $W_0$, mean density $\rho_0$ and mean temperature $T_0$ at the center of the nozzle exit are used as reference values. The Mach number and Reynolds number of the jet are $M = 2.5$ and $Re = 0.552 \times 10^5$ for air (reference length is $1\text{mm}$) and $M = 2.8$ and $Re = 0.235 \times 10^5$ for helium. This model is closely related to the experimental setup of Papyrin et al. (7). The computational domain selected for this problem is shown in figure 4.1. The domain is a three-dimensional box with dimensions $-20\text{mm} \leq x \leq 20\text{mm}$, and $-20\text{mm} \leq y \leq 20\text{mm}$. The extent of domain along $x$ and $y$ was found to be adequate for capturing all important features of the flow.

The supersonic jet is issued from the middle of the domain and impinges at the center of the bottom wall ($z = 0$). In order to resolve the jet shear layers, wall boundary layer and to capture the shock clearly, a fine grid is necessary in these regions. Since the jet is issued over the rectangle $-5\text{mm} \leq x \leq 5\text{mm}$ and $-1.5\text{mm} \leq y \leq 1.5\text{mm}$, a fine grid is generated over the larger rectangle $-7.5\text{mm} \leq x \leq 7.5\text{mm}$ and $-3\text{mm} \leq y \leq 3\text{mm}$ and shown in figures 4.2, 4.3 and 4.4. The grid is clustered near the wall with a minimum $\Delta z$ spacing less than $0.015\text{mm}$. After preliminary simulations, it is found that the shock occurs nearly at a distance of $z = 1.25\text{mm}$ from the wall. The grid is also clustered in this region in order to capture the shock. Grid statistics are given in table 1 for $Z_o = 20\text{mm}$. The same grid parameters are used for $Z_o = 10\text{mm}$ except that $N_z = 161$.

Jet is released from the center of the top plane. The bottom plane represents a solid wall. The other four sides of the domain are the pressure outlets with static pressure equal to the atmospheric pressure. The direction of the velocity vector is obtained from the neighboring
Table 4.1: Grid Statistics

<table>
<thead>
<tr>
<th>Total no of points</th>
<th>Minimum Spacing (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_x )</td>
<td>201</td>
</tr>
<tr>
<td>( N_y )</td>
<td>201</td>
</tr>
<tr>
<td>( N_z )</td>
<td>201</td>
</tr>
</tbody>
</table>

cells. The normalized vertical velocity profile of the jet issuing from the inflow boundary plane is shown in figure 4.5. The continuous line is a curve fit to the experimental mean velocity data across the short side of the rectangular nozzle exit (7). Using the same approach the velocity profile along the long side of the nozzle exit is obtained and is shown in figure 4.6. The total velocity is multiplication of the both profiles i.e.

\[
W(x, y, Z_0) = W_0 f(x^+) g(y^+) \quad (4.1)
\]

and

\[
g(y^+) = \frac{1}{k} lny^+ + 5.5 \quad (4.2)
\]

**Boundary Conditions**

The bottom plane \((z = 0)\) is a solid wall where we apply no slip and adiabatic boundary conditions. At the top boundary \((z = Z_0)\) entrainment is allowed from the domain outside the nozzle exit. Speed of sound \((a_b)\) and velocity component normal to the boundary \((w_b)\) are obtained by extrapolating Riemann invariants of the locally one-dimensional flow normal to boundary.

\[
w_b = \frac{1}{2} (J_b^+ + J_b^-) \quad (4.3)
\]

\[
a_b = \frac{\gamma - 1}{4} (J_b^+ - J_b^-) \quad (4.4)
\]

where \(J_b^+\) and \(J_b^-\) are Riemann invariants at a boundary point. Their values are determined as follows. Let subscript \(b - 1\) denote the first grid below the top boundary.
\[ J_b^+ = J_{b-1}^+ \]
\[ = w_{b-1} + \frac{2a_{b-1}}{\gamma - 1} \] (4.5)

\[ J_b^- = J_{\infty}^- \]
\[ = w_{\infty} - \frac{2a_{\infty}}{\gamma - 1} \] (4.6)

with \( w_{\infty} = 0 \)

Knowing the speed of sound \( a_b \) we determine the temperature, \( T_b = \frac{a_b^2}{\gamma R} \). Then we use isentropic relations to determine density

\[ \frac{\rho_b}{\rho_{\infty}} = \left( \frac{T_b}{T_{\infty}} \right)^{\frac{1}{\gamma - 1}} \] (4.7)

The pressure is determine from the equation of state. Velocity components tangential to the boundary are \( (u_b = u_{b-1} \) and \( v_b = v_{b-1} \) for outflow \( (w_{b-1} > 0) \), otherwise they are zero. On the other four sides of the domain we prescribe the pressure to be atmospheric pressure for outflow and extrapolate all other flow variables from inside the domain. For inflow, we extrapolate Riemann invariants as prescribed above for the top boundary.

Figure 4.1: Computational domain.
Figure 4.2: y-z plane grid.

Figure 4.3: x-z plane grid.
Figure 4.4: 3D grid.

Figure 4.5: Jet velocity profile across the short side of rectangular nozzle exit.
4.2 Instantaneous Flow Field

4.2.1 Supersonic Jet Impingement

The jet is released from the top. At the inlet to the computational domain, a steady velocity vector \((u, v, w) = (0, 0, w(x, y, Z_0))\) is specified. The inflow velocity profiles are shown in figures 4.5 and 4.6. After impingement, a strong bow shock is formed in-front of the substrate. After impingement, the flow is deflected sideways. Pressure waves are reflected from the flat surface in the outward direction. Part of the wave also travels in within the jet. However, inside the jet waves propagate at an oblique angle to the downward supersonic velocity. The acoustic pressure waves also perturb the shear layer and induce disturbances in the shear layer (55). These disturbances are vortices that propagate downstream and grow in strength. If provided with more distance these disturbances and vortex structures grow and force the jet to oscillate as a result the jet is no more stable. For isobaric condition, the jet oscillates sinusoidally. The oscillation has strong implication on the bow shock, compressed zone and stagnation point.
Figures 4.7 to 4.9 show snapshots of an iso-surface of vorticity magnitude of 1.5 (normalized by $L_r$ and $W_r$) for $Z_0 = 20\text{mm}$ and figures 4.10 - 4.12 for $Z_0 = 10\text{mm}$. At the inlet, the vorticity vector has two components with the x-component (normal to the long side of the jet) being the dominant component. The streamwise vorticity ($\omega_z$) is identically zero. Due to shear layers at the jet boundary, instability waves develop. Large-scale vortical structures start to form at a distance about 8mm from the nozzle exit. These waves grow as the jet goes downward, as a result, the jet oscillates. The iso-surface is colored by the streamwise component of vorticity that is generated by vorticity titling mechanism. For $Z_0 = 10\text{mm}$ the standoff distance is not long enough for vortical structures to grow.

These large-scale vortical structures interact with the bow shock wave, and upon impinging on the substrate, further breakdown to smaller turbulent structures. For a distance $Z_0 = 20\text{mm}$ the flow is complex and the bow shock assumes a three-dimensional undulated surface, and hence shock strength and orientation vary continuously in the impingement zone. Multiple shocks are also observed. Figures 4.13(a)-4.13(c) show an iso-surface of density for $Z_0 = 10\text{mm}$ and figures 4.14(a)-4.14(c) show an iso-surface of density for $Z_0 = 10\text{mm}$ at different times. For $Z_0 = 10\text{mm}$ the shock surface is smooth and a clear bow shock is observed. The red rectangle is the projection of the jet inlet area (nozzle exit area). In all cases it is observed that the compressed gas is confined to the mirror image of the jet inlet area. For $Z_0 = 20\text{mm}$ the shock is not smooth and multiple/oblique shocks are observed. The shock surface is undulated by the interaction with large-scale turbulent structures developing on the jet shear layers.
Figure 4.7: Instantaneous iso-surface of vorticity magnitude = 1.5 colored by the vertical component of vorticity; air M=2.5, $Z_0 = 20 \text{mm}$, $t=1857$.

Figure 4.8: Instantaneous iso-surface of vorticity magnitude = 1.5 colored by the vertical component of vorticity; air M=2.5, $Z_0 = 20 \text{mm}$, $t=1913$. 
Figure 4.9: Instantaneous iso-surface of vorticity magnitude = 1.5 colored by the vertical component of vorticity; air $M=2.5$, $Z_0 = 20\, mm$, $t=1969$.

Figure 4.10: Instantaneous iso-surface of vorticity magnitude = 1.5 colored by the vertical component of vorticity; air $M=2.5$, $Z_0 = 10\, mm$, $t=1696$. 
Figure 4.11: Instantaneous iso-surface of vorticity magnitude = 1.5 colored by the vertical component of vorticity; air M=2.5, Z₀ = 10mm, t=1759.

Figure 4.12: Instantaneous iso-surface of vorticity magnitude = 1.5 colored by the vertical component of vorticity; air M=2.5, Z₀ = 10mm, t=1875.
Figure 4.13: Iso-surface of density = 1.5 in the compressed region; air $M = 2.5$, $Z_0 = 10\, mm$

Figure 4.14: Iso-surface of density = 1.5 in the compressed region; air $M = 2.5$, $Z_0 = 20\, mm$
4.2.2 Jet Oscillations

Due to shear layer instabilities and reflection of pressure waves from the flat surface the rectangular jet becomes unstable and flaps. The oscillations are more evident in the direction normal to the smaller side of the rectangular jet, although the vortical structures imply the existence of oblique waves on the jet shear layers. The oscillations magnitude, however, depends upon the standoff distance. As discussed earlier; for small standoff distance, the vortex structures do not have enough distance to mature, and the jet remains non-oscillatory. Figures 4.15 to 4.17 show the Mach number contours on the central plane for air at exit Mach number of 2.5. The jet flapping is evident. The jet oscillation has also been observed experimentally as reported by Papyrin et al. and Kosarve et al. (7; 14). To determine the frequency of oscillations in the present simulations, the time series of velocity, pressure and density were recorded by probes placed at fifteen locations in the jet shear layers and impingement region. A fast Fourier transform routine is then used to analyze the frequency contents of the time series. The energy spectrum for the velocity component parallel to the wall at $x = 0$, $y = 3$ mm, and $z = 1.5$mm is shown in Figure 4.18. There is a peak corresponding the jet oscillation frequency at non-dimensional frequency of 0.223, which is equivalent to 30KHz.

![Figure 4.15: Mach number contours at central plane for air, $X = 0$, $t=2413$ and $Z_0=20$mm.](image-url)
Figure 4.16: Mach number contours at central plane for air, $X = 0$, $t=2425$ and $Z_0=20\text{mm}$.

Figure 4.17: Mach number contours at central plane for air, $X = 0$, $t=2457$ and $Z_0=20\text{mm}$. 
Figures 4.18 to 4.21 show the Mach number contours on the central plane for helium at exit Mach number 2.8. For the same nozzle exit-to-throat area ratio, the difference in Mach number is due to the higher specific heat ratio of helium compared to that of air.

Figures 4.22 to 4.24 show the Mach number contours for \( Z_0 = 10\, \text{mm} \). For this smaller standoff distance the core of the jet is almost stable; however, the flow after impingement does not flow along the wall, rather it deflects from the wall and goes at an angle and strong circulation region forms on both sides. This phenomenon will be discussed in the next section.
Figure 4.19: Mach number contours at central plane for helium, $M = 2.8$, $X = 0$, $t=2420$ and $Z_0=20\text{mm}$.

Figure 4.20: Mach number contours at central plane for helium, $M = 2.8$, $X = 0$, $t=2431$ and $Z_0=20\text{mm}$. 
Figure 4.21: Mach number contours at central plane for helium, $M = 2.8$, $X = 0$, $t=2441$ and $Z_0=20\text{mm}$.

Figure 4.22: Mach number at central plane for air, $M = 2.5$, $X = 0$, $t=1696$ and $Z_0=10\text{mm}$. 
Figure 4.23: Mach number at central plane for air, $M = 2.5$, $X = 0$, $t=1759$ and $Z_0=10\text{mm}$.

Figure 4.24: Mach number at central plane for air, $M = 2.5$, $X = 0$, $t=1875$ and $Z_0=10\text{mm}$.
4.2.3 Vorticity Field

At the nozzle exit, the specified velocity vector \((u, v, w) = (0, 0, w(x, y, Z_0))\) is steady with zero z-vorticity \(\omega_z\). The vorticity vector has only two components with the x-component (normal to the long side of the jet) being the dominant component. Due to shear layer interactions and waves reflection from the flat surface, instability waves develop. Figures 4.25 to 4.27 show snapshots of an iso-surface of y-vorticity \(\omega_y\) of 1 and -1 (normalized by \(L_r\) and \(W_r\)) and figures 4.28 to 4.30 show snapshots of an iso-surface of x-vorticity \(\omega_x\) of 1 and -1 (normalized by \(L_r\) and \(U_r\)) for \(Z_0 = 20mm\). These figures show that the vortex layers in the \(x, y\) directions are undisturbed for some initial distance. The vortex structures breakup afterwards. Due to small stand-off distance for the case of \(Z_0 = 10mm\) these vortex structures would reach the flat substrate surface before further breakup. As the rectangular jet exists the nozzle, the component of vorticity \(\omega_y\) exists mainly on the short side of the rectangle as shown by the thin vortex layers in figures 4.25 to 4.27. Whereas the component \(\omega_x\) exists on the long side of the rectangle as shown in figures 4.28 to 4.30. As a result of shear layer instability, three-dimensional disturbances develop on the rectangular boundary of the jet, producing \(\omega_y\) on the long side as shown in figures 4.25 to 4.27 and \(\omega_x\) on the short side on jet as shown in figures 4.28 to 4.30. Figures 4.31 to 4.33 show snapshots of an iso-surface of z-vorticity \(\omega_z\) for \(Z_0 = 20mm\). There is no z-vorticity \(\omega_z\) at the inlet. As the oblique instability waves develop on the long and short sides of the rectangular jet, \(\omega_z\) appears on these sides as depicted in figures 4.31 to 4.33. The oblique waves is a characteristic of the mixing layers at high convective mach numbers (56). All these large-scale vortical structures interact with the bow shock wave, and upon impinging on the substrate, further breakdown to smaller turbulent structures.
Figure 4.25: Iso-surface of y-vorticity ($\omega_y$) 1 and -1 air M=2.5, $Z_0 = 20\text{mm}$ and $t=2413$.

Figure 4.26: Iso-surface of y-vorticity ($\omega_y$) 1 and -1 air M=2.5, $Z_0 = 20\text{mm}$ and $t=2425$. 
Figure 4.27: Iso-surface of $y$-vorticity ($\omega_y$) 1 and -1 air $M=2.5$, $Z_0 = 20\, \text{mm}$ and $t=2457$.

Figure 4.28: Iso-surface of $x$-vorticity ($\omega_x$) 1 and -1 air $M=2.5$, $Z_0 = 20\, \text{mm}$ and $t=2413$. 
Figure 4.29: Iso-surface of x-vorticity ($\omega_x$) 1 and -1 air $M=2.5$, $Z_0 = 20\text{mm}$ and $t=2425$.

Figure 4.30: Iso-surface of x-vorticity ($\omega_x$) 1 and -1 air $M=2.5$, $Z_0 = 20\text{mm}$ and $t=2457$. 
Figure 4.31: Iso-surface of z-vorticity ($\omega_z$) 0.5 and -0.5 on one side of shear layer of the jet $y = 0 - 5mm$, air $M=2.5$, $Z_0 = 20mm$ and $t=2413$.

Figure 4.32: Iso-surface of z-vorticity ($\omega_z$) 0.5 and -0.5 on one side of shear layer of the jet $y = 0 - 5mm$, air $M=2.5$, $Z_0 = 20mm$ and $t=2425$. 
Figure 4.33: Iso-surface of $z$-vorticity ($\omega_z$) 0.5 and -0.5 on one side of shear layer of the jet $y = 0 - 5 \text{mm}$, air $M=2.5$, $Z_0 = 20 \text{mm}$ and $t=2457$.

4.2.4 Linear Stability Analysis

Linear stability analysis of two-dimensional supersonic jet is performed to further understand the flow dynamics observed experimentally and numerically. We performed two-dimensional linear stability analysis to validate the oscillation frequency determined from the three-dimensional CFD calculations. The analysis is based on the linear disturbance equations. Spatial stability theory of propagating two-dimensional or oblique waves is considered. An eigenvalue problem is obtained and solved numerically. The details of the equation are given in (56). The basic state is a parallel (unconfined) two-dimensional jet whose velocity profile is a curve fit to the mean velocity in $z$–direction found in our CFD simulations for $Z_o = 20\text{mm}$. The velocity profile is given by

$$W(y) = B_o + A_o \frac{\tanh(b + y) - \tanh(y - b)}{2\tanh b}$$

(4.8)
where the curve-fitting parameters $B_o = 0.013$, $A_o = 0.987$, $b = 1.5$, and $\theta = 4$. The CFD mean velocity profile and curve fit are shown in figure (4.34). Similarly the mean temperature profile obtained from CFD is also approximated by a double-Gaussian profile

$$T(y) = C_o + D_o \left[ e^{-\delta(y+c)^2} + e^{-\delta(y-c)^2} \right]$$

(4.9)

where the curve-fitting parameters $C_o = 1.01$, $D_o = 0.49$, $c = 1.4$, and $\delta = 6$. The CFD mean temperature profile and curve fit are shown in figure (4.37). The high temperature regions at the edges of the 2D jet are imposed by the temperature profile at the nozzle exit. Here, we assumed that nozzle walls are insulated, and hence the wall temperature is adiabatic temperature, which is higher than the temperature in the core. The disturbances are assumed to be propagating waves in the $z$–direction. The velocity disturbance in $y$–direction is of the form

$$v(x, y, z, t) = \hat{v}(y) e^{i(\alpha x + \beta z - \omega t)} + c.c.,$$

(4.10)

where $\omega$ is the non-dimensional frequency, $\alpha$ and $\beta$ are wave-numbers. Similar wave forms are assumed for all other flow variables. We conducted spatial stability analysis for which $\omega$ and $\alpha$ are assumed to be real where as $\beta = \beta_r + i\beta_i$ is a complex eigenvalue. The differential eigenvalue problem is solved using a fourth-order finite difference method (57).

For two-dimensional waves ($\alpha = 0$), the growth rate ($-\beta_i$), wavelength $\lambda = 2\pi/\beta_r$, and phase speed $C_{ph} = \omega/\beta_r$ are shown in figure (4.36) against frequency $f = 2\pi\omega(W_r/L_r)$. The most amplified wave happens at frequency $f = 28.4kHz$, and the corresponding wavelength is 13.8mm. The eigenfunction of the $v$-velocity component is depicted in figure 4.35, and its symmetry about the jet center line indicates a sinuous mode. The frequency predicted by linear stability is remarkably close to the jet flapping frequency of 30kHz predicted by CFD. Papyrin et al. (table 3.4 of reference (7)) reported wavelength in the range of 4.5mm to 11.6mm. They used the gas velocity (460m/s–500m/s) as the wave speed and estimated the frequency to be in the range of 50 – 100kHz. However, the wave speed for the sinuous mode is less than the gas velocity. According to linear stability analysis the wave speed is about half of the gas velocity. Therefore, experimental frequency is in the range of 25 – 50KHz. Thus linear stability analysis and experimental data provide basic validation to the current CFD simulations.
Figure 4.34: Mean Velocity profile at central plane for air, $M = 2.5$, $X = 0$, $Z_0=20mm$. and $Z = 12.3mm$

Figure 4.35: Mean temperature profile at central plane for air, $M = 2.5$, $X = 0$, $Z_0=20mm$ and $Z = 12.3mm$. 
Figure 4.36: Growth rate, wavelength, and phase speed of 2D sinuous mode against frequency.

Figure 4.37: Eigen function \((v_r, V(i))\) of v-velocity disturbance for most amplified 2D sinuous mode.
4.2.5 Bow shock and compressed gas layer

The supersonic jet initially undergoes through a series of expansion and compression along its axis as a result of the growth of the varicose mode of the jet instability. After that transient state jet oscillates in the direction normal to the long side. The oscillations resemble the sinuous mode of jet instability. As a result of these oscillations, the compressed gas layer between the bow shock and substrate also oscillates laterally. It is commonly believed that in cold spray that there is a strong and stationary bow-shock in-front of the substrate. However, stable bow shock occurs only if the standoff distance is small. Steady RANS simulations do not capture these oscillations. For large standoff distance the shock orientation and location change due to jet oscillations. Figures 4.38(a) to 4.38(f) show instantaneous density contours at different times for $Z_0 = 20mm$. These results show that the compressed air layer oscillates parallel to the substrate surface to the extent that the entire region is shifted away from the center. The occurrence of a secondary shock/oblique shock is also clearly seen in figures.

For small distance $Z_0 = 10mm$, the large-scale structures of shear layer instability do not have enough distance to develop before impingement. Experimental results by Papyrin et al. (7) suggest that the length of the undisturbed region is up to 2-6 times the thickness of the jet (6mm-18mm). Figures 4.13(a) to 4.13(c) show an iso-surface density of level 1.5. The figure implies that the bow shock surface is smooth and the shock is almost normal everywhere in the impingement region. Although the shock remains nearly normal; however, the shock/compressed air region also oscillates in the vertical direction. The oscillation of the shock/compressed air region is up to 0.25mm. Figures 4.39(a) to 4.39(f) show instantaneous density contours at different times for $Z_0 = 10mm$. For small distance the stagnation point essentially remains at the same location and no significant oscillations along the wall are observed.
Figure 4.38: Density contours at central plane, air $M=2.5$, $X = 0$ and $Z_0=20$mm.
Figure 4.39: Density contours at central plane, air M=2.5, X = 0 and Z₀=10mm.
4.3 Mean Flow Field

The mean flow is obtained by averaging the unsteady flow field over a long period of time. The mean flow can be used for comparison to the experimental data, and other Reynolds averaged calculations. Figure 4.40 shows mean density contours in the central $yz$ plane i.e. $X = 0mm$. After the flow is compressed by the shock it continues to compress to stagnation conditions at the substrate. The maximum density on the substrate is 3.72 as compared to the theoretical value of 3.77 obtained by a normal shock at $M = 2.5$ followed by isentropic compression to stagnation conditions. The shock region extends from $y/h = -1$ to $y/h = 1$, where $h = 3mm$ is the narrow side of the rectangular jet. The mean distance of the shock from the substrate is approximately $h/3$. Figure 4.40 shows the mean density contours for $Z_0 = 20mm$. These mean contours show continuous compression and do not show any shock. As explained earlier for higher standoff distance the flow is complex and shock is less organized and varies significantly in orientation and position. Hence averaging over time smears the shock discontinuities and mean contours appear to be continuous; they are significantly different from the instantaneous contours in the same plane shown in figure 4.38. The instantaneous values of maximum densities were found to be higher for $Z_0 = 20mm$ compared to $Z_0 = 10mm$.

Figures 4.42 and 4.43 show the mean velocity magnitude contours for $Z_0 = 10mm$ and $Z_0 = 20mm$, respectively. The streamlines indicate the entrainment from the top boundary. Some characteristics of the mean flow field are different for the two cases of standoff distances. For $Z_0 = 10mm$, after impingement, flow expands and then re-expands. Mean flow calculations show that the jet does not completely adhere to the wall surface, instead it deflects at a small angle. This creates a separation region on the wall. For $Z_0 = 20mm$ the flow expands only once after impingement. This is because the jet diffuses for a longer distance.
Figure 4.40: Mean density contours air $M=2.5$, $X = 0$ and $Z_0 = 10mm$.

Figure 4.41: Mean density contours air $M=2.5$, $X = 0$ and $Z_0 = 20mm$. 
Figure 4.42: Mean velocity magnitude contours air $M=2.5$, $X = 0$ and $Z_0 = 10\text{mm}$.

Figure 4.43: Mean velocity magnitude contours air $M=2.5$, $X = 0$ and $Z_0 = 20\text{mm}$.
4.4 Grid Independence

We performed a grid independent study using three different grids resolution (course, medium and fine) for two cases of standoff distance $Z_0 = 10mm$ and $Z_0 = 20mm$. The details of the grids are given in table 4.2. The total number of nodes in coarse, medium and fine mesh are approximately 2 million, 4 million and 8 million, respectively. In three grids, grid refinement is used near the wall and in the jet region i.e. from $-7.5 mm \leq x \leq 7.5 mm$ and $-3 mm \leq y \leq 3 mm$. Figures 4.44 shows comparison of mean y-velocity near the wall, at a distance of $0.1 mm$ from the wall for the three grids for $Z_0 = 10mm$. The results agree very well especially in the jet region. Figures 4.46 shows comparison of mean pressure distribution on wall, for the three grids for $Z_0 = 10mm$. These figures show that the results obtained from different grids are very close to each other. Similar results were obtained for $Z_0 = 20mm$. Figures 4.46 and 4.47 show the y-velocity near the wall and pressure distribution on the wall for $Z_0 = 20mm$. These results show that velocity comparison near the wall is good. The pressure peak however, was slightly different. This could be possibly due to averaging time over which averaging is obtained. All these results suggest that the medium (4 million nodes) and fine grid (8 million nodes) are very close to each other. The results presented in this chapter are computed from the medium or fine grids.

<table>
<thead>
<tr>
<th>Grid</th>
<th>$Z_o = 10mm$</th>
<th>$Z_o = 20mm$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Course Grid</td>
<td>$121 \times 121 \times 91$</td>
<td>$121 \times 121 \times 111$</td>
</tr>
<tr>
<td>Medium Grid</td>
<td>$161 \times 161 \times 161$</td>
<td>$161 \times 161 \times 161$</td>
</tr>
<tr>
<td>Fine Grid</td>
<td>$201 \times 201 \times 161$</td>
<td>$201 \times 201 \times 201$</td>
</tr>
</tbody>
</table>
Figure 4.44: Mean $y$-velocity near the wall for air $M=2.5$, $Z_0=10\text{mm}$.

Figure 4.45: Mean pressure distribution on the wall for air $M=2.5$, $Z_0=10\text{mm}$.
Figure 4.46: Mean y-velocity near the wall for air M=2.5, \( Z_0=20 \text{mm} \).

Figure 4.47: Mean pressure distribution on the wall for air M=2.5, \( Z_0=20 \text{mm} \).
4.5 Comparison with Experimental Data

Mean pressure distribution on the wall is compared to the experimental data by Papyrin et al.(7) in figure 4.48, where $P_s$ is the pressure on the substrate, $P_{sm}$ is the maximum pressure on the substrate at $Y = 0$, $P_a$ is the ambient pressure. $Y_{0.5}$ is the half width of the pressure profile. The experimental data are available for $Z_0 = 9mm$, but the numerical simulations are for $Z_0 = 10mm$. The profile is well predicted by the current simulations. Akhtar and Ragab (58) obtained qualitative comparison for the wall pressure using a fifth order WENO scheme. The maximum mean Mach number distribution (based on velocity component parallel to the y-axis) is compared to the experimental data measured by Kosarev et al (14) as shown in figure 4.49. Excellent agreement is obtained in the first expansion region of the wall jet. Both experiments and simulations show the wall jet remains locally supersonic at least for $y/h = 10$. It is interesting that the deflected wall jet reaches a maximum Mach number higher than the Mach number of impinging jet ($M = 2.5$). The present numerical scheme provides a better comparison with experiments than that of WENO scheme by Akhtar and Ragab (58).

Figure 4.48: Normalized pressure profiles on the wall for air $M=2.5$, $X = 0mm$, $Z_0 = 10mm$. 
Figure 4.49: Distributions of $M_m$ along y-axis for air $M=2.5$, $Z_0 = 10mm$. 
Chapter 5

One-Dimensional Model For Cold Spray

In cold spray, compressed gas expands to supersonic speed through a convergent-divergent nozzle. The gas is released from a large chamber where certain stagnation pressure and temperature are maintained. Particles are injected in the convergent or divergent part of the nozzle depending on the pressure in the powder feeder.

In this chapter, a one-dimensional model for predicting particle and gas velocity and temperature inside and outside of the nozzle is presented. Many authors used one-dimensional models (59–62) employing different drag and heat transfer coefficients. Helfritch et al. (59) used a drag coefficient given by Carlson et al. (48) In our one-dimensional model, we combined the model with deposition criteria and is applied on powder with size distribution to obtain the deposition efficiency. Good agreement with available experimental data is obtained. The model can be used to obtain an accurate particle velocity and temperature at the exit of the nozzle, particle velocity and temperature at impact and information about particle deposition based on deposition criteria. The model provides an overview of the cold spray process. The model can be used to select suitable stagnation conditions for gas and optimum particle injection point/location and type of nozzle geometry, etc.

The gas is assumed to be released from a chamber where stagnation constant pressure and temperature are maintained. The gas flow calculation inside the nozzle is based on isentropic
flow analysis. Particles trajectories are calculated by integrating the equations of motion for the particles using a fourth-order Runge-Kutta method. Gas flow and particle motion are briefly described here.

## 5.1 Gas Flow Model Equations

The nozzle geometry is prescribed, hence the area at any stream wise station is known, \( A(x) \). The corresponding Mach number of the gas is calculated iteratively from the relation between area ratio and Mach number.

\[
\frac{A(x)}{A^*} = \left( \frac{1}{M} \right) \left[ \left( \frac{2}{\gamma + 1} \right) \left( 1 + \frac{\gamma - 1}{2} M^2 \right) \right]^\frac{\gamma + 1}{2(\gamma - 1)} \tag{5.1}
\]

where \( A^* \) is the cross section area at the nozzle throat, \( M \) is the Mach number at nozzle cross section \( A(x) \) and \( \gamma \) is the ratio of the heat capacity at constant pressure to heat capacity at constant volume. Typically, \( \gamma \) values is set 7/5 for diatomic gasses and 5/3 for mono atomic gasses. Once the Mach number is calculated at a given cross-sectional area of the nozzle, the remaining corresponding gas quantities can be calculated using the following isentropic relationships,

\[
\frac{T_0}{T} = 1 + \left( \frac{\gamma - 1}{2} \right) M^2 \tag{5.2}
\]

\[
\frac{\rho_0}{\rho} = \left[ 1 + \left( \frac{\gamma - 1}{2} \right) M^2 \right]^{\frac{1}{\gamma - 1}} \tag{5.3}
\]

\[
v = M \sqrt{\gamma RT} \tag{5.4}
\]

where \( T_0 \) and \( \rho_0 \) are the stagnation temperature and density. The dynamic viscosity and thermal conductivity are calculated from Sutherlands law given in chapter 2, Eq 2.14 and
Eq 2.15. Since the substrate distance from the nozzle exit is small compared to the nozzle length, in this one-dimensional model, the gas flow and thermodynamic properties are assumed constant from the nozzle exit until the bow shock near the substrate surface. The gas flow properties immediately after the shock are calculated using normal shock relations.

\[
M_2^2 = \frac{\frac{2}{\gamma-1} - M_1^2}{1 + \left[\frac{2\gamma}{\gamma-1}\right] M_1^2}
\]

(5.5)

Downstream of the shock the velocity is assumed to vary linearly to zero value at the wall. The temperature is calculated from the energy equation.

5.2 Particle Equations of Motion and Thermal Energy Equation

Once the gas velocity and temperature are determined, particle equations of motion can be integrated in the one-dimensional flow where all flow properties are known functions of \(x\). Particle motion and heat transfer equations are given chapter 2. For better understanding they are repeated here. Particle equations of motion are given by

\[
m_p \frac{du_p}{dt} = F_{\text{drag}}
\]

(5.6)

\[
\frac{dx_p}{dt} = u_p
\]

(5.7)

The drag is given by.

\[
F_{\text{drag}} = \frac{\pi}{8} d_p^2 \rho C_D |u - u_p|
\]

(5.8)

Where \(C_D\) is the drag coefficient (47). Details of the drag model are given in Appendix A. Thermal energy equation for the particle is

\[
\frac{d}{dt} (m_p c_{pp} T_p) = h (T_g - T_p) A_p
\]

(5.9)

where \(A_p = \pi d_p^2\) is the surface area of the spherical particle and \(m_p = \rho_p \frac{\pi d_p^3}{6}\) is the mass of
the particle. Simplifying the above equation, we obtain

\[
\frac{dT_p}{dt} = \frac{6h(T_g - T_p)}{\rho_p d_p c_{pp}}
\]  

(5.10)

where

\[
h = \frac{\kappa_g N u}{d_p}
\]  

(5.11)

is the coefficient of convection, \( \kappa_g \) is the gas conductivity and \( N u \) is the Nusselt number given by Carlson and Hoglund (48)

\[
N u = \frac{N u_c}{1 + 3.42 \left( \frac{M_p}{Re_{pp} Pr} \right) N u_c}
\]  

(5.12)

where

\[
N u_c = 2.0 + Re^{0.5} Pr^{0.32}
\]  

(5.13)

hence the final form of temperature equation is

\[
\frac{dT_p}{dt} = \frac{6\kappa_g N u}{\rho_p d_p^2 c_{pp}} (T_g - T_p)
\]  

(5.14)

where \( Pr \) is the Prandtl number. We assumed initial velocity and temperature values and integrated these equations using 4th order Runge-Kutta time marching scheme (49).

5.3 Results and Discussion

In this section, results obtained using the one-dimensional model are discussed. Both circular and rectangular nozzles are used in cold spray. A rectangular nozzle has an advantage over the circular nozzle as it gives both narrow and wider beam of particles in different directions. For one-dimensional model, a convergent-divergent rectangular nozzle is selected. Figure 5.1 shows a schematic diagram of a cold spray process. The length of the divergent section is 100 mm. The thickness of the nozzle is kept constant at 3 mm. The nozzle exit section height is 10 mm and throat height is 3 mm. The substrate distance from the nozzle exit is 20 mm.
5.3.1 Effects of particle diameter on particle velocity and temperature

Based on isentropic one-dimensional model, results are obtained for aluminum particles for diameters 1, 5, 10, 20 and 30 microns. Figure 5.2 shows velocity and temperature for carrier gas (air) and aluminum particle having a diameter 5 microns. The gas stagnation pressure and temperature are 1.72MPa and 750K, respectively. The particle initial temperature is 273K and initial velocity is equal to the gas velocity at the injection section (100 m/s). The figure shows that the particle is quickly heated by the gas until its temperature equals the gas temperature. This heating happens before the nozzle throat. As the gas continues to expand its temperature drops down and subsequently the particle cools down. However, the particle temperature remains higher than the local gas temperature until the nozzle exit. Particle velocity increases throughout the nozzle due to drag force.

The gas velocity between nozzle exit and the bow sock is assumed to be constant because the standoff distance is usually small, and the velocity is very high. Due to drag force particle velocity increases slightly until particles pass the shock and enter the compressed gas zone. Based on our numerical simulations and experimental work reported in (58; 63) the shock standoff distance is set at 1.5mm from the substrate. Downstream of the shock the gas velocity decreases and ultimately reaches to zero at the substrate surface. The gas temperature increases and reaches to the stagnation temperature at the wall. The particle temperature increases slightly in the compressed air zone, but the particle velocity decreases dramatically in that region.

Particle velocity and temperature are affected by its diameter. Figure 5.3 shows a comparison of particle velocity for different diameters of 1, 5 and 10 microns. It shows that
small particles tend to follow the fluid and reach velocity close to the gas velocity. The small particle, however, looses most of its kinetic energy in the compressed air region. Large particles though achieve relatively less velocity, but they maintain their velocity when they pass through the compressed air region. Large particles are less affected by the compressed gas region.

Similar observations are noted for particle temperature. Figure 5.4 shows particle temperature variations for different particle diameters. It is also interesting to note that the temperature of a small particle increases quickly in the subsonic region, but cools down in the supersonic region with the gas and heats up again in the compressed air region. However, large particles heat up slowly in the subsonic region and cool down in the supersonic region with slow cooling rate compared to small particles. As a result, at the nozzle exit, their temperature is higher than the gas temperature and of small particles temperature. Large particles temperature is not affected by the compressed gas region. This is because the thickness of the compressed gas region is small and large particle heat up slowly. As a re-
result, their temperature is relatively constant after the nozzle exit. At impact, small particles have high temperature but low kinetic energy or velocity. Small particles tend to follow the fluid. Increase in stagnation temperature will affect the small particles (diameter less than 1 micron) deposition.

Large particles have low temperature at impact, but they have high kinetic energy. For deposition, both temperature and velocity play important roles. Figure 5.5 shows the effect of particle diameter on its velocity and temperature at impact. Since the small particles lose their velocity in the compressed air region, their impact velocity is low. Particle impact velocity increases with the particle diameter, until 6–7 microns. Further increase in the particle diameter results in decrease in the particle impact velocity. It’s important to mention that particle with a very large diameter will have low velocity at the exit of the nozzle, but are less affected by the compressed air region. Their low-impact velocity is mainly due to low acceleration in the nozzle.

![Figure 5.3: Effects of particle diameter on its velocity, aluminum particles, working gas air, note the change in scale](image)

All results shown so far are for high-pressure cold spray where particles are injected into
Figure 5.4: Effects of particle diameter on its temperature, aluminum particles, working gas air

the convergent part of the nozzle. Particles can be added in the divergent part of the nozzle, that process is called low-pressure cold pray as explained in detail in chapter 1. Analyses were performed on LPCS, and particles are injected at \( Z = 50 \text{mm} \), this is 10mm downstream of the nozzle throat. Figure 5.6 shows particle velocities inside the nozzle when they are injected at \( Z = 50 \text{mm} \); where the gas flow is supersonic. It is surprising to see that all the particles reach the same velocities as if they were injected at the convergent section (inlet) of the nozzle as shown in figure 5.6. Particles approach these velocities in a distance of 25\text{mm} approximately. This distance varies with particle diameter and density. This indicates an optimum injection position for particles for LPCS. Results for particle temperature are different from particle velocities. Figure 5.7 shows particle temperature for different diameter when they are injected at \( Z = 50 \text{mm} \). The result show a reduction in particle temperature at the nozzle exit, especially for large particles. This is because heating of particles by the gas is ineffective in the supersonic (divergent)region. This is why LPCS has low deposition efficiency for cold particles. Higher deposition efficiency can be obtained if the particles are heated before injection into the divergent section.
Figure 5.5: Effects of particle diameter on particle velocity and temperature at impact, aluminum particles, working gas air.

Figure 5.6: Particle velocity for different diameters injected in the divergent section at Z=50mm
Figure 5.7: Particle temperature for different particle diameter injected at Z=50mm

5.3.2 Comparison with experiments

Comparisons were made with the experimental data by Gilmore et al.(64). The experimental nozzle has the exit area of 2mm by 10mm with a stand-off distance of 25mm. In all results presented below a spherical particle, gas-atomized copper powder (ACuPowder International, LLC No. 500A, Union, NJ) with a volumetric mean diameter of 19µm for one powder and a mean diameter of 22µm for another powder is used. Deposition efficiency is obtained by applying deposition criteria presented in chapter 6 on powder distribution such as shown in figure 6.10. Figure 5.8 shows a comparison between experimental data and results obtained by one-dimensional simulation. It shows that one-dimensional model can predict the inflight particle velocity accurately, both for helium or air as a carrier gas. Figure 5.9 shows a comparison of deposition efficiency with the experimental data vs impact velocity. The impact velocity was achieved by using different stagnation pressure and temperature of helium as a driving gas. The exact values of the corresponding stagnation temperature and pressure used
in the experiments are unknown.

![Graph](attachment:image.png)

Figure 5.8: Mean particle velocity vs temperature x=0, y=0, z=10mm (from nozzle exit), P=2.1 MPa, 22 \( \mu m \) copper powder

### 5.3.3 Limitations of One-Dimensional Model

Although the one-dimensional model predicts very accurately the in-flight and impact particle velocity, however, it has certain limitations. One-dimensional model only gives the velocity for the central particle plane at \( x = 0, y = 0 \) where uniform gas velocity and temperature may be assumed. Hence it cannot predict the distribution of particles at nozzle exit and the effects of shear layers. The model assumes small standoff distance and constant velocity between the shock and nozzle that is equal to the velocity at the exit of the nozzle. It can not estimate velocity reduction due to turbulence and shear layer growth. If the standoff distance is large, the model over-predicts the velocity. Figure 5.5 shows a comparison of numerical and experimental (64) mean particle velocity. Experimental work indicates that particle velocity remains nearly uniform for distances up to 80mm, and afterwards starts decreasing. However,
Figure 5.9: Variation of deposition efficiency with mean impact velocity for $Z_0 = 25\text{mm}$, for 19$\mu\text{m}$ copper powder, helium driving gas, and varying stagnation pressure and temperature.

for helium it keeps increasing for some distance and then remains constant. Such behavior cannot be predicted by one-dimensional model, as a result it will over-predict the particle velocity and efficiency. We recall that isobaric jet is assumed for one-dimensional model. For non-isobaric jet, there will be multiple shocks outside of the nozzle.

5.3.4 Conclusions

In this chapter, a one-dimensional model for predicting gas and particle velocity and temperature inside and outside of the nozzle is presented. The model is combined with deposition criteria and is applied on powder with size distribution to obtain the deposition efficiency. Good agreement with available experimental data is obtained. The model provides an overview of the cold spray process. However, the model is not applicable if the stand distance is large or if the jet is non-isobaric.
Figure 5.10: Mean particle velocity vs z-axis $P=2.1\text{MPa}, T=473\text{K}$
Chapter 6

Three-Dimensional Particle Tracking and Deposition

Supersonic jet impingement has applications towards cold spray. In cold spray, supersonic jet is released from a convergent-divergent nozzle. Particles are added either at the inlet of the nozzle or in the divergent section of the nozzle. The geometry of particle-laden jet impingement flow field is identical as supersonic jet impingement discussed in details in chapter 4. In this chapter results of particles-laden flow are discussed. Particles are tracked in the instantaneous flow field. Analyses were made to study particle interactions with bow shock, compressed gas layer and turbulent flow field. Particles initial conditions at the nozzle exit are determined using the one-dimensional model discussed in chapter 5. In this chapter first, the results of particles in the instantaneous flow field are presented. Quantitative comparison between the deposition efficiencies in high-pressure cold spray and low-pressure cold spray is presented. Deposition efficiency is obtained for aluminum and copper.

Simulation for jet impingement without particles is conducted for a long time before solid particles are injected. Aluminum and copper particles are injected into the computational domain at the nozzle exit. Separate simulations are run for each particle size in the same initial flow field. In each case 40,000 particles are injected at the same time but with different initial particle velocity and temperature.

As shown by Papyrin et al.(7) and Tabbara et al.(65), particles are concentrated at
the center of the nozzle exit. In the present simulations all particles are injected over a rectangular region smaller than the nozzle exit area. For the nozzle with exit cross-section $-5mm \leq x \leq 5mm$ and $-1.5mm \leq y \leq 1.5mm$, the particles are injected over a smaller rectangular section, $-4mm \leq x \leq 4mm$ and $-1.2mm \leq y \leq 1.2mm$.

Figure 16 shows the 40,000 particles as they reach the impingement zone. The particle diameter is 1 micron, and all particles are injected at the same elevation i.e. $Z_0 = 20mm$. The blue particles impact the substrate surface after passing through the bow shock. The red particles drift with the large-scale turbulent structures and do not succeed in reaching the substrate. These particles do not deposit on the wall.

Large particles of ($d > 3$ microns), however, impact the wall. For small standoff distance i.e $Z_0 = 10mm$, all the particles ranging from 1 to 40 microns impact the substrate; despite the presence of a strong bow shock compared to $Z_0 = 20mm$. For large standoff distance flow field is associated with jet oscillations. and dominant turbulence structure which influence the small particles and hence their deposition efficiency. In these cases, simple one-dimensional empirical models (66) fail to predict the correct particles trajectories and deposition efficiency.

![Figure 6.1: Blue particles impact substrate surface, red particles disperse sideways with large-scale turbulent structures $d = 1\mu m, Z_0 = 20mm$.](image)
6.1 Particles Deceleration in the Compressed gas Region

In cold spray particles are accelerated and heated inside the convergent divergent nozzle. Particles distribution at the nozzle exit is also important. Particles distribution is controlled by the precise injection method, such that particles are concentrated at the center to void strong boundary-layer effects due to nozzle. Precise injection is also necessary for targeted cavity filling. One dimensional models explained in chapter 5 can predict the velocity of the particles at the nozzle exit. The models give accurate particles velocity at the nozzle exit as validated by comparison with the experiments.

In the jet region before the shock particles are accelerated, decelerated and deviated from the center of the jet depending on standoff distance and carrier gas. For small standoff distance the velocity remain fairly constant. For large standoff distance in the case of air particles velocity decrease as the jet diffuses. For helium the particle velocity continue to increase after the nozzle for a good range of standoff distance, because of the gas expansion after the shock as shown in figure 5.8 (64). In the compressed gas region the particles decelerate due to low velocity and high density of the gas after the shock. The effects of these hydrodynamic parameters on particles deceleration will depend on particles diameter. To investigate particle diameter effects variations of particle vertical velocity (normal to the substrate surface) with elevation above the substrate surface for different diameters are given in figures 6.2 and 6.3 for $Z_0 = 10\text{mm}$ and $Z_0 = 20\text{mm}$, respectively. All particles are injected at the same location (center of the jet $x = 0, y = 0, z = Z_0$). Figures 6.2 and 6.3 show that particles velocity remains fairly constant before the shock, however, in the compressed gas region the particles velocity decreases especially for small particles. Small particles are severely decelerated as evident from the velocity of the 1 micron particle. For $Z_0 = 10\text{mm}$ the smallest particle i.e. $d_p = 1$ micron loses about 50% of its vertical momentum in the compressed gas region. Large particles ($d > 25\text{microns}$) are not affected by the compressed air region. Similar results are obtained for large standoff distance $Z_0 = 20\text{mm}$. 
Figure 6.2: Variation of particles vertical velocity with elevation above the wall. \((X = 0, Y = 0\text{and}Z_0 = 10mm)\). Note particle deceleration in the compressed air region.

Figure 6.3: Variation of particles vertical velocity with elevation above the wall. \((X = 0, Y = 0\text{and}Z_0 = 20mm)\). Note particle deceleration in the compressed air region.
6.2 Probability Density Function of Particle Velocity

In the previous section results for single particle, which is at the center of the jet, are discussed. To investigate all particles impact velocity, we computed the probability density function (pdf) of the velocity component normal to the substrate surface at impact.

Figures 6.4 and 6.5 show comparison of particle normal velocity ($w$) pdf at the nozzle exit (doted lines), pdf before the shock and pdf at impact (solid lines) for $Z_0 = 10mm$ and $Z_0 = 20mm$, respectively. The three pdf indicate that the particles velocity does not change significantly till the shock. However, after the shock particles are affected by the compressed gas region. The velocity pdf of small particles ($d_p = 1$ micron) is shifted from the high velocity region ($w_p/w_m = 0.98$) to a low velocity region ($w_p/w_m = 0.5$). The velocity pdf of large particles ($d_p > 25$ microns) experiences minor changes relative to its velocity pdf at the nozzle exit.

Velocity pdf for $Z_0 = 20mm$ are shown in figure 6.5. For $Z_0 = 20mm$ mechanisms of velocity modulation involve multiple shocks, compressed gas zone, and interaction with large-scale turbulence structures. The pdf of small particles ($d_p = 1$ micron) is shifted from the high velocity region ($w_p/w_m = 0.98$) to a lower velocity region ($w_p/w_m = 0.6$), but the pdf is also spread over a wider range of velocities. Some particles retain their high initial velocity because they may have passed through a shock weaker-than-normal shock or may not have encountered a shock at all due the lateral jet oscillations in the impingement zone. However, a fraction of the particles at the jet boundary loses their entire vertical momentum and never impacted the substrate surface, see figure 6.1. The pdf of large particles ($d_p > 25$ microns) experiences minor changes relative to its distribution at the nozzle exit. Figure 6.6 shows the comparison of velocity pdf before the shock for $Z_0 = 10mm$ and $Z_0 = 20mm$. It shows the particles velocity is almost same for both cases. This is because the stand of distance is small, although the flow field is different before the shock. Figure 6.7 shows the comparison of velocity pdf at impact for $Z_0 = 10mm$ and $Z_0 = 20mm$. Although, velocity pdf before the shock is identical for $Z_0 = 10mm$ and $Z_0 = 20mm$ 6.6, however at impact the velocity pdf is different. This difference is less for large particle ($d > 20$ microns).
Figure 6.4: Probability density function of vertical velocity of particles for air \( M = 2.5 \) and \( Z_0 = 10 \text{mm} \).

Figure 6.5: Probability density function of vertical velocity of particles for air \( M = 2.5 \) and \( Z_0 = 20 \text{mm} \).
Figure 6.6: Probability density function of vertical velocity of particles before the shock for air M=2.5, Z_0 = 10\,mm and Z_0 = 20\,mm.

Figure 6.7: Probability density function of vertical velocity of particles at impact for air M=2.5, Z_0 = 10\,mm and Z_0 = 20\,mm.
6.3 Deposition Criterion

In cold spray adhesion of particle and successful bonding with substrate occurs due to localized adiabatic shear instability by the pressure wave generated from the point of impact between particle and substrate (4; 18–22). This phenomenon occurs only if the particle impact velocity is above a critical velocity. Critical velocity depends on parameters such as particles melting temperature, yield stress and density. An empirical relation accounting for all of these effects is given by Assadi et al. (19).

\[ v_{\text{critical}} = 667 - 14\rho_p + 0.08(T_m - T_r) + (\sigma_y)10^{-7} - 0.4(T_i - T_r) \]  \hspace{1cm} (6.1)

where \( T_m \), \( T_i \), \( \rho_p \) and \( \sigma_y \) are particle melting temperature, temperature at impact (in Kelvin), density and yield stress (in Pa), respectively. \( T_r \) is the reference temperature equal to 273K. Equation 6.1 clearly indicates the effects of the particle temperature and material properties on critical velocity. Materials with higher melting point and higher yield stress will require higher critical velocity. Particle diameter influences particle velocity and temperature at impact, but does not appear explicitly in the expression of critical velocity. The particle diameter, however, is important while calculating the upper bound of the cold spray deposition as it determines the erosion velocity. Based on many experimental and numerical analyses the erosion velocity limit can be found by (3; 19).

\[ v_{\text{erosion}} = 900d_p^{-0.19} \]  \hspace{1cm} (6.2)

In this study critical velocity of copper and aluminum is determined using equation 6.1. Table 6.1 gives properties of aluminum and pure copper used in calculations.

6.4 Deposition Efficiency

Particle normal component of impact velocity, particle temperature, and physical properties of particle i.e. density and yield stress determine successful deposition of particles in cold spray. For a given powder particle size distribution function \( f(dp) \), the deposition efficiency \( \eta \) can be found quantitatively as follows (28):
Table 6.1: Material properties

<table>
<thead>
<tr>
<th></th>
<th>Aluminum</th>
<th>Copper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Temperature</td>
<td>934(K)</td>
<td>1356(K)</td>
</tr>
<tr>
<td>Density</td>
<td>2700 (Kg/m³)</td>
<td>8940 (Kg/m³)</td>
</tr>
<tr>
<td>Yield Stress</td>
<td>10MPa</td>
<td>70MPa</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td>900 (J/KgK)</td>
<td>386 (J/KgK)</td>
</tr>
<tr>
<td>(d_{min}, d_{max}, d_{mean})</td>
<td>1,40,18 (micron)</td>
<td>1,40,18 (micron)</td>
</tr>
</tbody>
</table>

\[
\eta = \int_{0}^{\infty} g(dp) f(dp) dp
\]  \hspace{1cm} (6.3)

where \(g\) is a size-dependent function that determines successful deposition, which is obtained in terms of the characteristic particle velocities as follows (28):

\[
g = \begin{cases} 
1 & v_{critical} < v_i < v_{erosion}, \\
0 & \text{otherwise},
\end{cases}
\]  \hspace{1cm} (6.4)

The stagnation pressure and temperature are 1.72 MPa and 750 K, hence the jet is isobaric. Nozzle dimensions are shown in figure 5.1. The particles size distribution is shown in figure 6.10, and the mean diameter is 18 (\(\mu m\)). Aluminum and copper particles are injected into the nozzle at two locations \(Z = 0 mm\) and \(Z = 50 mm\) (see figure 5.1). All the particles are injected in the identical flow-field, and tracked through the field until they impact the substrate or drift side-ways. We count the particles that successfully satisfy the deposition criterion by equation 6.1 to 6.4.

Figure 6.8 show the particles deposition efficiency vs particle diameter for aluminum particles. The particle are injected at inlet of nozzle. Figure 6.8 show that the deposition efficiency is high for particle in the rage \(5 \mu m \leq d \leq 20 \mu m\). Since particle mean diameter is 18 (\(\mu m\)), the over all powder efficiency is high. The deposition efficiency for both stand off distances are same. This could be mainly for two reasons. First, the stagnation conditions are high and overcome the adverse flow fields effects. Second, the difference in the standoff could be small.
For the same stagnation conditions low deposition efficiency is obtained if the particles are injected at $Z = 50\,\text{mm}$, as shown in the figure 6.9. However, the particles deposition efficiency can be increased by heating the particles slightly, before injection. Figure 6.9 shows that particle deposition efficiency increases by increasing the temperature of the particles, enabling the large particle deposition. Figures 6.11 and figure 6.12 show powder deposition efficiency for aluminum and copper. The results show that the particle efficiency can be increased by a moderate increase of the initial temperature of the particles. Copper efficiency is sightly lower than aluminum at a given initial temperature. Because of the higher density and low thermal conductivity of copper its critical velocity is higher than that for aluminum.

Figure 6.8: Particles Deposition efficiency vs particle diameter for aluminum, air $\text{M}=2.5$. 
Figure 6.9: Particles deposition efficiency vs particle diameter for aluminum, air $M=2.5$.

Figure 6.10: Particles size distribution vs diameter ($\mu m$).
Figure 6.11: Aluminum deposition efficiency vs particle initial temperature for Air M=2.5.

Figure 6.12: Copper deposition efficiency vs particle initial temperature for Air M=2.5.
6.5 Deposition Layer Portrait

Figures 6.13 to 6.18 show the locations of deposited particles on the substrate surface for selected particle diameter of 2, 3, and 25 microns. The large rectangle correspond to the nozzle exit cross section, whereas the small rectangle is where the 40,000 particles are injected. It is observed that for $Z_0 = 10\, mm$ the particles deposited in a continuous strip shape. The best uniform coating is obtained for particles in the range $5\, \mu m \leq d_p \leq 20\, \mu m$, where particles spread over entire small rectangle. Given a relative velocity between the nozzle and substrate a uniform layer of deposition can easily be achieved with rectangular nozzle. For $Z_0 = 20\, mm$ nonuniform and somewhat random coatings with gapes between them is observed for small particles. The coatings continuous for large particles as shown in figures 6.16 to 6.18.

Figure 6.13: Deposited layers; $d_p = 2$ microns for air $M=2.5$, $Z_0 = 10\, mm$.

Figure 6.14: Deposited layers; $d_p = 3$ microns for air $M=2.5$, $Z_0 = 10\, mm$. 
Figure 6.15: Deposited layers; $d_p = 25$ microns for air $M=2.5$, $Z_0 = 10\, mm$.

Figure 6.16: Deposited layers; $d_p = 2$ microns for air $M=2.5$, $Z_0 = 20\, mm$. 
Figure 6.17: Deposited layers; $d_p = 3$ microns for air $M=2.5$, $Z_0 = 20mm$.

Figure 6.18: Deposited layers; $d_p = 25$ microns for air $M=2.5$, $Z_0 = 20mm$. 
Chapter 7

Conclusions

Results for direct numerical simulations of a supersonic rectangular jets (air and helium) impinging on a flat substrate surface are obtained by solving unsteady Navier-Stokes equations. We have developed a code that uses a six-order compact scheme with tenth-order filter combined with WENO dissipation. Throughout the flow field except in a region around the bow shock where a fifth-order WENO scheme is used. A fourth-order low-storage Runge-Kutta scheme is used for time integration of gas dynamic equations simultaneously with solid particle equations of motion and energy equation. The nozzle exit area is a $3\, mm \times 10\, mm$ rectangle, and the jet Mach number is 2.5 for air and 2.8 for helium.

The flow structures, mean flow properties, particle deposition and particles impact velocity on a flat substrate surface are presented for two cases ($Z_0 = 10\, mm$ and $20\, mm$) for the distance between the nozzle exit and the substrate. Numerical results for the wall pressure and maximum Mach number in the wall jet are in good agreement with the available experimental data. Numerical results show that after impingement, the jet re-expands to a supersonic wall jet to a high Mach number close to jet Mach number at the exit of the nozzle. The pressure on the wall in the expansion region is locally lower than ambient pressure. For $Z_0 = 10\, mm$, numerical results show that the shock surface is smooth, and the bow shock is nearly normal everywhere in the impingement region. For $Z_0 = 20\, mm$, however, the jet is unstable and flap in the direction normal to the long side of the jet. The flapping frequency is about 30kHz. Linear stability analysis performed on the mean jet profile and available
experimental data validates the oscillation frequency observed in the three-dimensional numerical results. The flapping causes the undulation of the normal shock to multiple oblique shocks. However the time-averaged profiles do not show any shock. The entire compressed gas region also oscillates parallel to the wall which has adverse effects on particles deposition efficiency.

One-dimensional model for cold spray based on isentropic flow equations can predict reliable results for particle velocity and temperature at impact. The one-dimensional model can also be combined with a deposition criteria and predict deposition efficiency for powders of given particle size distribution.

Results for tracking spherical aluminum and copper particles of diameters from 1 to 40 microns in the three-dimensional instantaneous jet flow show that small particles are readily influenced by the large-scale turbulent structures developing on jet shear layers and drift sideways. However, large particles are not influenced by the large-scale structures or bow shock. Deposition efficiency indicates an optimum range of particle diameters for deposition efficiency. The deposition efficiency of low-pressure cold spray (LPCS) is found to be lower compared to high-pressure cold spray (HPCS). This is mainly because of low particle temperature at the nozzle exit. Deposition efficiency in LPCS can be improved by heating the particles before injecting into the nozzle.
Appendix A

The following equations are given in references (47). The formula for $C_D$ consists of three equations depending on the relative Mach number; a formula for the subsonic flow regimes, a formula for the supersonic flow regime at particle Mach numbers greater than 1.75, and a linear interpolation for the intervening region between particle Mach number of 1 and 1.75.

The detail equations for $C_d$ are given as follows:

For subsonic flow ($M_p < 1$)

$$C_{D_{(sub)}} = 24 \left[ Re_p + S \left( 4.33 + \frac{3.65 - 1.53 \frac{T_p}{T}}{1 + 0.353 \frac{T_p}{T}} \right) \right]$$

$$\times \exp \left( -0.247 \frac{Re_p}{S} \right) \right]^{-1} + \exp \left( - \frac{0.5M_p}{\sqrt{Re_p}} \right)$$

$$\times \left[ 4.5 + 0.38(0.33Re_p + 0.48 \sqrt{Re_p}) + 0.1M_p^2 + 0.2M_p^8 \right]$$

$$+ 0.6S \left[ 1 - \exp \left( - \frac{M_p}{Re_p} \right) \right]$$

(1)

Where $S$ is the molecular speed ratio and is given by $S = M_p \sqrt{\gamma/2}$. $Re_p$ and $M_p$ are particle Reynolds number and particle Mach number, respectively, based on the relative velocity between particle and fluid flow.

For supersonic flow ($M_p \geq 1.75$):

$$C_{D_{(supp)}} =$$

$$0.9 + \frac{0.34}{M_p^2} + 1.86 \left( \frac{M_p}{Re_p} \right)^{1/2} \left[ 2 + 2 \frac{2}{S^2} + \frac{1.058}{S} \left( \frac{T_p}{T} \right)^{1/2} - \frac{1}{S^4} \right]$$

$$\times 1 + 1.86 \left( \frac{M_p}{Re_p} \right)^{1/2}$$

(2)

For supersonic flow ($1 \leq M_p < 1.75$):

$$C_D(M_p, Re_p) = C_{D_{(sub)}}(1, Re_p) +$$

$$\frac{4}{3} (M_p - 1) \left[ C_{D_{(supp)}}(1.75, Re_p) - C_{D_{(sub)}}(1, Re_p) \right]$$

(3)

A formula for the Nusselt number given by Carlson and Hoglund (48) is given by
\[ Nu = \frac{Nu_c}{1 + 3.42 \left( \frac{M_p}{Re Pr} \right) Nu_c} \]  \hspace{1cm} (4)

where

\[ Nu_c = 2.0 + 0.459 Re^{0.5} Pr^{0.32} \]  \hspace{1cm} (5)

**Appendix B**

Coefficients for fifth order explicit are (52):

- \( A_0 = 1809.257 \)
- \( B_0 = -65.1944 \)
- \( A_1 = -62.16 \)
- \( B_1 = -26.6742 \)
- \( C_0 = -(A_0 - 28B_0 + 13068)/5040 \)
- \( C_1 = (A_0 - 27B_0 + 5040)/720 \)
- \( C_2 = -(A_0 - 26B_0 + 2520)/240 \)
- \( C_3 = (A_0 - 25B_0 + 1680)/144 \)
- \( C_4 = -(A_0 - 24B_0 + 1260)/144 \)
- \( C_5 = (A_0 - 23B_0 + 1008)/240 \)
- \( C_6 = -(A_0 - 22B_0 + 840)/720 \)
- \( C_7 = (A_0 - 21B_0 + 720)/5040 \)
- \( E_0 = -(A_1 - 21B_1 + 720)/5040 \)
- \( E_1 = (A_1 - 20B_1 - 1044)/720 \)
- \( E_2 = -(A_1 - 19B_1 - 720)/240 \)
- \( E_3 = (A_1 - 18B_1 - 360)/144 \)
- \( E_4 = -(A_1 - 17B_1 - 240)/144 \)
- \( E_5 = (A_1 - 16B_1 - 180)/240 \)
- \( E_6 = -(A_1 - 15B_1 - 144)/720 \)
- \( E_7 = (A_1 - 14B_1 - 120)/5040 \)
Bibliography


