Direct Numerical Simulation of Particle Behaviour in a Gas-Solid Three Dimensional Plane Jet

N. A. Qazi1, J. C. K. Tang1, E. R. Hawkes1, 2, G. H. Yeoh1, R. W. Grout3, H. Sitaraman4, M. Talei1, R. A. Taylor1, 2, M. Bolla1 and H. Wang1

1School of Mechanical and Manufacturing Engineering
2School of Photovoltaic and Renewable Energy Engineering
The University of New South Wales, NSW 2052, Australia
3Department of Mechanical Engineering
The University of Melbourne, Melbourne, Victoria 5005, Australia
4National Renewable Energy Laboratory
Computational Science Center, USA

Abstract
In this paper, direct numerical simulations (DNS) of a three-dimensional (3D), non-reacting, temporally evolving planar jet laden with mono-dispersed solid particles in the two-way coupling (TWC) regime are performed. Three different particles Stokes numbers (St = 0.1, 1, 10) have been considered. This has been achieved by varying the particle diameter while keeping the particle mass loading (φm = 1) and the jet Reynolds number \(Re_{jet} = 2000\) unchanged. The objective is to study the effect of the particle Stokes number TWC regime on the temporal development of the planar jet. Two-way coupled momentum and heat transfer has been studied by investigating mean relative velocity and temperature. Results indicate that the relative parameters are more pronounced on the edges of the jet and decrease in time in general. At the center of the jet however, the mean value first increases and then decreases again. Additionally, lighter particles spread farther than heavier particles from the center of the jet. Furthermore, the heavier particles delay the development of the jet due to TWC effects.

Introduction
Turbulent flows laden with solid particles are encountered in several engineering applications. In the area of energy technologies, examples include solar thermochemical systems, solid particle solar receivers, and coal/biomass combustion in power plants. In these applications, the TWC of heat transfer between particles and carrying fluid often plays an important role. In the last three decades, such flows have attracted much attention from both numerical and experimental perspectives [1].

Direct numerical simulation (DNS) can potentially provide a fundamental understanding of the interaction and dispersion of solid particles with the turbulent carrying fluid. However, most DNS studies of particle-laden flows have been conducted for isotropic turbulence. Here a multitude of physical processes have been investigated, including TWC of energy for decaying [8, 9] as well as for forced turbulence [8], with mono- and poly-dispersed particles [12, 2].

More recently, DNS with particles in jets started to appear [15, 5, 10] being more representative of typical industrial applications like coal/biomass combustion. For planar jets with particles, various DNS studies have been presented, focusing on different aspects of the physical problem. Examples include inter-particle collisions [15], turbulence modulation and particle dispersion [5], pulverized coal combustion [10], interaction of evaporating droplet with turbulent carrier flow [11]. However, to the authors best knowledge, to date no DNS work for energy TWC in a jet configuration laden with solid particles emphasising on temperature characteristics in the jet has been reported.

This is targeted in the current paper, where a three-dimensional, non-reacting, temporally evolving planar jet laden with monodispersed solid particles is performed with DNS including TWC of momentum and energy, with emphasis on energy exchange between the two phases. The primary objective is to study the effect of the particle Stokes number (St = 0.1, 1, 10) in the two-way coupling regime on the temporal jet development. This has been realized by varying the particle diameter while keeping the particle mass loading unchanged.

The remainder of the paper is organized as follows: first, the mathematical model with the particle and carrier phase governing equations are presented, followed by the numerical procedure and computational parameters. In the results and discussion section, simulation results for different Stokes number are analyzed with respect to the jet development. Finally, concluding remarks are drawn.

Mathematical Model
In the current simulations, the gas-phase fluid is considered to be Newtonian and compressible. The solid particles are assumed to be rigid and spherical, with constant density and uniform internal temperature. The particle equations utilised here and derived by [13] are based on the assumption that the particles are fine and heavy. The volume fraction, \(\phi_s\), is chosen such that the mixture is considered dilute. Under such conditions, particle collisions are infrequent and inter-particle interactions can be neglected [8]. The density of the particle is almost 2000 times to that of the gas phase, so that only Stokes drag is retained. The density of the particle is almost 2000 times to that of the gas phase, so that only Stokes drag is retained. The density of the particle is almost 2000 times to that of the gas phase, so that only Stokes drag is retained. The density of the particle is almost 2000 times to that of the gas phase, so that only Stokes drag is retained.

It should be mentioned here that for DNS of multiphase flows, the particle diameter should be less than the smallest scale, so as to resolve the turbulence characteristics, and at the same time, the wake due to spherical particles should not influence the turbulent scales. This assumption corresponds to several similar configurations adopted in the past [1].

In the following, subscript \((f)\) represents carrier fluid properties, interpolated at the particle location. Subscript \((p)\) represents the properties of the suspended particle, whereas the symbols without subscripts are considered as those for fluid variables.

Particle Governing Equations
Solid particles are treated in Lagrangian frame and drag force is calculated using the Stokes drag law. The particle equations can be expressed in normalised form as:

\[
\frac{dx_{pi}}{dt} = u_{p,i}, \tag{1}
\]

\[
\frac{du_{p,j}}{dt} = \frac{C_D}{\tau_p} (u_{f,j} - u_{p,i}). \tag{2}
\]
\[ \frac{dT_p}{dt} = \frac{Nu}{30Pr\tau_p} (T_i - T_p). \] (3)

In equations (1)-(3), \( Re_p = \frac{|u_f - u_p|d_p}{|u_f|} \) is the diameter of the particle, and \( v \) is gas kinematic viscosity. \( \tau_p \) is the particle relaxation time, calculated as, \( \tau_p = \frac{d^2 p_p}{18|\nabla u|} \). The drag coefficient \( CD \) is calculated via \( CD = 1 + 0.15R e_p^{0.88} \). \( T_p \) is the particle temperature where an infinite rate of heat conduction is assumed so that a uniform temperature within the particle is achieved at each instant in time. Furthermore, the Nusselt number, \( Nu = 2 + 0.6R e_p^{0.5}P r^{0.3} \), where \( Pr \) is the Prandtl number. The ratio of specific heat capacities of fluid and particle and kinematics viscosity of gas phase are represented by \( \alpha_1 \) and \( \nu \), respectively. Density of particle and gas phase are labeled as \( \rho_p, \rho_g \), respectively. The particle Stokes number, \( St \) is based upon \( \tau_p/\tau_k \) where \( \tau_k \) is the Kolmogorov time scale of turbulent flow, based upon \( \eta \). The Kolmogorov length scale, \( \eta \) is estimated from extensive analysis of similar temporal planar jet configuration in the past [3, 6, 7]. More specifically, \( \eta = H \times 0.5/150 \times (Re/10^5)^{-0.75} \), where \( H \) is slot width of the jet.

**Governing Equations of Carrier Phase**

The carrier fluid comprises of two species only. The fuel and oxidiser phases are chosen as Nitrogen (\( N_2 \)) and air, respectively. The transport equations of mass, momentum, total energy and scalar transport can be written as:

\[ \frac{\partial p}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \frac{\partial p u_i}{\partial x_i} + \rho_g + \Gamma_{m}. \] (4)

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = \frac{\partial \rho u_i}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho_g + \Gamma_{u}. \] (5)

\[ \frac{\partial E}{\partial t} + \frac{\partial (\rho u_i E)}{\partial x_j} = \frac{\partial \rho u_i}{\partial x_j} + \frac{\partial \tau_{ij} u_j}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + \Gamma_{e}. \] (6)

In equation (4), \( p \) is the fluid density, \( u_i \) is the fluid velocity in \( i \)-th direction. In addition to above, the mass fraction of \( N_2 \) is considered as a passive scalar with the assumption that Fickian approach is valid. In equation (6), \( E \) is total energy, \( \tau_{ij} \) is the stress tensor and \( q_j \) is the heat flux vector. These equations have been detailed comprehensively in previous works such as [7], [14] etc.

In these equations, \( \Gamma_{m}, \Gamma_{u}, \) and \( \Gamma_{e} \) represent the source terms contributed by the point particles. For the non-reacting case considered in this work, \( \Gamma_{m} = 0 \).

\[ \Gamma_{u} = - \frac{1}{\Delta V} \sum \alpha_p \frac{dm_p}{d\tau} |\nabla u_i| \] (7)

\[ \Gamma_{e} = - \frac{1}{\Delta V} \sum \alpha_p \frac{m_p}{\Delta t} |\nabla T_p| \] (8)

The coefficient, \( \alpha_p \), is a weighting factor determining how much of the particle source term is distributed to a particular grid node. There are many possible methods to distribute the particle source terms back to the Eulerian grid. These include weighted average and extrapolation techniques. However, care must be taken when applying such a technique, so that the solution is not prone to statistical noise and is discretely conserved. To account for particle source terms, the mollification kernel approach, as employed in [14, 2], was adopted. The main advantage of this technique is that it creates a smooth source term field on the Eulerian grid, consequently, removing the statistical noise which may lead to instabilities in the numerical solution.

---

![Figure 1: Particles colored by temperature in planar jet configuration.](image)

<table>
<thead>
<tr>
<th>Slot width, H (mm)</th>
<th>0.2592</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain size based on ( H )</td>
<td>16 × 24 × 10</td>
</tr>
<tr>
<td>Grid size</td>
<td>506 × 504 × 432</td>
</tr>
<tr>
<td>Jet Reynolds number, ( Re_{jet} )</td>
<td>2000</td>
</tr>
<tr>
<td>Jet temperature, ( T_{jet}(K) )</td>
<td>400</td>
</tr>
<tr>
<td>Surrounding Temperature, ( T_s(K) )</td>
<td>1000</td>
</tr>
<tr>
<td>Velocity difference, ( \Delta U ) (m/s)</td>
<td>186</td>
</tr>
<tr>
<td>Jet time, ( \tau_{jet} ) (( \mu s ))</td>
<td>1.39</td>
</tr>
<tr>
<td>Fluid viscosity, ( \mu ) (Pa.s)</td>
<td>1.67 × 10⁻⁵</td>
</tr>
<tr>
<td>Stokes number, ( St )</td>
<td>0.1; 1; 10</td>
</tr>
<tr>
<td>Particle diameter, ( d_p(\mu m) )</td>
<td>0.054; 0.171; 0.541</td>
</tr>
<tr>
<td>Computational Particles, ( m_c ) (( 10^8 ))</td>
<td>3.84; 8.08; 0.23</td>
</tr>
<tr>
<td>Real to Mc ratio, ( M_r / M_c )</td>
<td>59.57; 8.95; 1.0</td>
</tr>
<tr>
<td>Time step, ( \Delta t ) (ns)</td>
<td>3.9</td>
</tr>
</tbody>
</table>

**Table 1: Simulation parameters for particle-laden temporal jet with \( \phi_f = 0.005, \phi_m = 1.0, \rho_p/\rho_e = 2048 **

**Numerical Procedure and Computational Parameters**

The flow configuration is a temporally-evolving planar slot-jet consisting of a slab of fuel, surrounded by oxidiser. The problem is set up for a cold jet in a hot environment. The boundary condition for streamwise and spanwise direction is periodic, while in the lateral direction, the non-reflecting outflow boundary is selected. The simulation parameters are presented in Table 1. Figure 1 presents the schematics of the flow domain with the particles coloured by temperature when the jet has progressed to a later time.

The DNS was performed using the massively parallel, FORTRAN based computer code, 3D which explicitly integrates the compressible, reacting Navier-Stokes equations. The numerical solution is advanced in time by employing a fourth order, six-stage, low-storage Runge-Kutta method [4]. The particles are assumed to distribute randomly in the jet area with initial temperature and velocity regarded same as the local fluid. The local properties of the fluid are interpolated at the particle locations using fourth order Lagrangian interpolation scheme. For efficiency purposes, computational particle approach was adopted; where a single computational particle represents a collection of real particles with the same properties. Particle St is varied by changing the particle diameter and decreasing the number of particles to retain the same mass loading, whereas all other parameters are kept constant.
Results and Discussion

Figure 2 shows the fluid velocity, normalised by velocity difference, $\Delta U$, superimposed with particles (For St 0.1 case, the particles behave like tracers and significant statistics could not be observed, hence their results have not been included in the current work.) A slice of thickness $\Delta z = 5$ grid points is chosen in the middle of the span-wise direction to envisage the particle clustering more noticeably. A qualitative comparison can be made to study in detail, the effects of particle feedback on the jet development. Initially, particles in both cases are spread homogeneously in the domain. At $t = 10 \mu s$, fluctuations in the shear regime of the jet cause increase of vortical structures and the spreading of jet takes place. Figures 2a and 2d show that for St = 1 the jet has spread farther in the lateral direction as compared to St = 10. The clustering mechanisms are different in both cases as well. For lighter particles (St = 1), the particles follow the flow closely and are generally homogeneously distributed in the domain, with some clustering visible. However, in the case with St = 10, it is shown that they preferentially concentrate in the outer boundaries of large-scale vortex structures. This can be clearly observed in figures 2b and 2e. As the simulation progresses in time, the particles in both cases settle to the flow conditions, hence the jet spreads to almost same locations in the lateral direction in both cases. However, the clustering of particles in the case of St = 10 can be clearly observed (see figures 2c and 2f). Such a qualitative comparison between the width of the jet for the two cases, at same time stamps indicate the suppression of fluid fluctuations due to presence of laden particles. This is in compliance with similar works carried out in the past [15, 5].

Figure 3 presents the profiles for mean relative velocity, $\overline{u_{rel}}$ and mean relative temperature, $\overline{T_{rel}}$, for various simulation times, normalized by initial jet velocity difference, $\Delta U$, and jet temperature ($T_{jet}$), respectively. The value of $\overline{u_{rel}}$ is highest towards the edges of the jet and generally decay in time, except at early times in the center of the jet where it first increases then decreases again (see figure 3a). At $10 \mu s$, the particles in the center of the jet have already settled to the flow conditions, resulting in $\overline{u_{rel}} \approx 0$. However, on the edges, the jet starts to develop and various vortex structures with different time and space scales start to appear in the flow field. The particles respond to this disturbance according to their relaxation times which is larger for heavier particles, consequently increasing the relative velocity. At later time, $30 \mu s$, as the jet progresses and becomes turbulent, particle clustering is much more evident. However, at the same time, the particles on the edges of the jet start to respond to the fluid velocity and the relative velocity decreases. The increase in the mean relative velocity at the center of the jet can be explained by considering the fact that particles clustering causes mixing and particles are introduced in the center from the edges.

At $50 \mu s$, the turbulence starts to dissipate, and the particles settle to the flow conditions in all the regions of the jet. This eventually causes a decrease $\overline{u_{rel}}$ in the center as well. Furthermore, it can be seen that there is more spreading for lighter particles (St = 1) as compared to heavier particles (St = 10). At earlier times, particles with St = 1 spread to $-3 < y/H < 3$, whereas St = 10 have only spread to $-2 < y/H < 2$, approximately. The physical explanation of this lies in the fact that once again, the heavier particles respond much slowly to the fluctuating conditions in their surroundings with the jet development. On the other hand, the lighter particles respond readily and spread much rapidly along with the jet. Later in the simulation, the spreading of the jet causes the particles to spread accordingly, finally both St 1 and 10 particles spread to approximately same locations, while maintaining the difference in $\overline{u_{rel}}$.

Similar behavior is observed for $\overline{T_{rel}}$, as well, presented in figure 3b. Although along the edges of the jet, the decrease in mean relative temperature is not as significant as in velocity for both St values. The mean relative temperature decreases in general, with the values much larger in the case of heavier particle. The root mean square (RMS) of relative parameters behaves generally in the same manner as the mean values and therefore not included here.

Conclusions

Turbulent flows laden with solid particles are an important class of flows which occur in many natural and engineering situations. Particle-laden turbulent jets are studied extensively for combustion and related applications. In this work, a DNS is per-
形成了三维粒子含混流的槽流, 在两种方式下, 模拟结果表明粒子的相对温度对各种 Stokes 数有显著影响。结果表明, 党存在粒子时, 模拟具有抑制效应, 该效果在粒子质量更重时更为显著。此外, 相对参数在初始模拟时刻在边界处较大, 随着时间的推移, 值先增加然后减少, 之后再次增加。其变化规律在中心区域更为明显。这表明更重的粒子扩散比更轻的粒子更远。