Semi-resolved CFD-DEM modeling of gas-particle two-phase flow in the micro-abrasive air jet machining

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Abstract:

Abrasive air jet (AAJ) machining is attractive for micromachining hard and brittle materials, while it is usually a big challenge to numerically investigate the particle velocity and concentration distribution in the particle erosion process in the AAJ. In this work, a recently developed semi-resolved CFD-DEM approach which bridges the simulation gap between the resolved and unresolved CFD-DEM, is further improved to reconstruct the background information with a double cosine kernel function. The semi-resolved CFD-DEM is then employed to numerically investigate the gas-particle two-phase flow in the AAJ and numerical results show that this semi-resolved CFD-DEM is more accurate in modeling particulate flow in the fine AAJ nozzle than the conventional unresolved CFD-DEM. We further conduct mechanism investigations on the AAJ micromachining process including particle flow characteristics inside the cylindrical nozzle, velocity, and concentration distribution over the nozzle exit, which are essential jet characteristic features. We identified the particle flow patterns, analyzed the particle distribution, and its correlation with air pressure, abrasive mass flow rate, and turbulence effects. The present simulation results and analyses can be great helpful in understanding the erosion mechanism and optimizing the setting parameters to improve the cutting performance of AAJ.

Keywords: Micro-abrasive air jet; Semi-resolved CFD-DEM; Particle distribution; Process parameter; Turbulence effect

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1. Introduction

Abrasive air jet (AAJ) machining, also known as abrasive jet micromachining (AJM), has become an attractive approach for micromachining hard and brittle materials such as glass, ceramics, quartz, and silicon, which are frequently used for the micro-fluidic, micro-electromechanical systems (MEMS) and opto-electronic device fabrication [1–3]. AAJ machining utilizes pressurized air to accelerate abrasive particles through a fine nozzle to form a jet of high-speed particles. The abrasive air-jet impinges the workpiece surface for mechanically etching required part features such as micro-channels and micro-holes into the target material [4]. In the AAJ machining process, the comprehensive understanding of the erosion process enables the development of more accurate models for the erosion rate and surface integrity, etc., as a function of process and material variables [4]. Many researchers have dedicated to developing the erosion and surface evolution models for the AAJ process [5–8]. In modeling the erosion process, it was found that the particle velocity and spatial distribution are essential jet characteristic information to develop reliable material removal models in AAJ [1,4]. Furthermore, such information is requisite to understand kerf characteristics and formation process, and further optimize the jetting parameters to enhance the jet performance for AAJ [4].

There are extensive investigations on AAJ to understand the particle velocity and its characteristics for particular jetting status through theoretical [1,9], experimental [4,10], and numerical approaches [11–12]. Li et al. [1] developed an analytical velocity model, in which a one-dimensional numerical solution was utilized to estimate the centerline particle velocity, and then the radial distribution across the jet, using the Gauss error function to approximate the radial velocity profile. Such particle velocity models can well describe the measured velocity distribution from a set of PIV measurements. Fan et al. [4] used particle image velocimetry (PIV) to measure the particle velocities and the characteristics in micro-abrasive jets, showing that the axial velocity profile consists of three stages and the radial profiles are relatively flat at a jet cross-section near the nozzle exit. Burzynski et al. [10] used a direct particle capture technique to obtain the particle and velocity distribution in a micro-abrasive jet. The results indicated that the spatial distribution of particles in the abrasive jet usually follows a Weibull distribution. Since the theoretical method cannot well describe the effect of nozzle wall and turbulence on air velocity, and the experimental measurement of velocity and pressure distributions in the flow field are hardly implemented [10,12]. Numerical simulation is a good complementary way to get comprehensive information on the particle distribution. Melentiev et al. [9] employed both theoretical and numerical approaches to analyze particle velocity in AAJ fields at the lower end of the micro-scale. They predicted the particle velocity data satisfyingly in theory and analyzed the influence of the process parameters on the particle velocity characteristics. Lv et al. [12] utilized the CFD with discrete phase model to study the effects of characteristics of velocity and pressure distributions on impact erosions in abrasive water jet machining. Fan et al. [11] used computational fluid dynamics (CFD) software to investigate the velocity distributions and particle behaviors of free jet and impinging jet in and out of the nozzle under the different input and boundary conditions. The simulation results could be helpful to optimize the nozzle structure for improving the jet performance.

Despite the various reported investigations, there still exist deficiencies in the understanding of particle velocity and spatial distribution in the AAJ micromachining process. In the previous research on the evolution of machined holed on glass, it was found that the variation of abrasive particle distribution in the jet would be an important role in the resultant profiles of the holes [14]. The practical range of the standoff distance between the nozzle exit and the target surface used in the AAJ is usually small [1]. Thus, a further study of the particle distribution in and around the nozzle and its variation with the process parameters need to be conducted, which will be conducive to understanding the erosion mechanism and optimizing the setting parameters to improve the cutting performance of AAJ.

Among the variety of numerical models available in the literatures [15–19], the computational fluid dynamics-discrete element method (CFD–DEM) is a frequently used approach to describe fluid-particle two-phase flow in industrial applications and it combines CFD for the fluid phase with the discrete element method (DEM) for the solid particles. A major advantage of CFD–DEM is that it can predict accurate particle-scale information, such as the trajectories of and forces acting on individual particles [16,17]. Based on the ratio of fluid mesh size to particle diameter, CFD-DEM can be classified into two categories, i.e., resolved CFD-DEM and unresolved CFD-DEM [20]. In the resolved CFD-DEM, the fluid flow around and covering each particle is resolved into a finer mesh whose grid size is much smaller than the size of the particle [21]. The interaction force between the particle and the surrounding fluids is calculated directly by the integral of the fluid stress over the boundary surface of the particle [22]. To accurately capture the boundary of particles, the sizes of the fluid meshes are required to be at least 8-10 times smaller than the particle diameter [23]. Therefore, in the resolved modeling, a number of fluid meshes are needed that lead to much heavier computational cost, and thus limit the applications of resolved CFD–DEM in industrial systems with a large number of particles. In contrast, the empirical drag force models are used to characterize particle–fluid interaction in the unresolved CFD–DEM. As integration along the particle boundary is not necessary, the particle boundary does not need to be resolved, and larger mesh sizes are feasible to compute the fluid flow. Therefore the unresolved CFD–DEM method is much more efficient than the resolved CFD–DEM method, and is frequently used for modeling different problems in engineering and scientific research [21,24–26]. In order to ensure the accurate calculation in the drag force models, mesh size should be at least 3 times larger than the particle diameter [27].

In a previous study, Li et al. [13] used the conventional unresolved CFD-DEM to numerically study the high-velocity jet dynamic characteristics such as air and particle velocity distribution within the jet, especially for the flow downstream from a nozzle fine exit. Micro-AAJ usually employs a cylindrical nozzle with an internal diameter below 1 mm and abrasive particles with diameters ranging from 5 to 50 μm shown in Table 1. When modeling the particulate flow with a number of big particles in a fine nozzle in the AAJ, the resolved CFD–DEM modeling is usually not applicable due to the extremely heavy computational cost. When using the conventional unresolved CFD–DEM, the mesh size is usually comparable with the particle diameter, and the normal size ratio is no longer satisfied. Otherwise, if the size ratio is bigger than 3, the mesh along the cross-section of the fine nozzle can be very coarse (sometimes even with only several mesh cells), leading to large numerical errors in modeling the flow field. Corresponding to the requirement of the grid size and particle size induced by the usage of the local volume average technique [28], many studies have been conducted to improve the accuracy of the CFD-DEM method [21,29]. Takabatake [29] developed a dual grid approach combining the distance function and the immersed boundary method in the CFD-DEM simulation. In this approach, two types of grids are used to calculate the void fraction and the fluid flow, and this makes it possible to simulate a gas-solid flow including thin walls. Wang et al. [21] recently developed a new semi-resolved CFD-DEM approach, which bridges the particle-mesh size gap between the resolved CFD-DEM and unresolved CFD-DEM. For cases where the particle has comparable or larger size as compared to the FVM grid, the developed approach reconstructs the background fluid velocity by kernel approximation and then corrects the relative velocity and volume fraction to obtain a more accurate drag force. The developed semi-resolved CFD-DEM is validated through a number of examples and it has comparable efficiency with the conventional unresolved CFD-DEM and as accurate with the resolved CFD-DEM. Therefore, the semi-resolved CFD-DEM is more accurate than the conventional unresolved-CFD, and it is applicable to numerically investigate the gas-particle two-phase in a fine nozzle of micro-AAJ.

In this work, this semi-resolved CFD-DEM method [21] is further developed to investigate the gas-particle two-phase flow in the micro-abrasive air jet machining. Instead of using the Gaussian kernel function, a double cosine kernel function is used to reconstruct the background information to remove truncation error on the boundary. The developed semi-resolved CFD-DEM is first compared with the unresolved CFD-DEM to model the gas-particle two-phase flow in the AAJ process, while the obtained axial particle velocity distributions by semi-resolved CFD-DEM show better agreement with theoretical results than those by the unresolved CFD-DEM. We then investigate the essential jet characteristic features of the AAJ micromachining process including particle flow characteristics inside the nozzle, velocity, and concentration distribution over the nozzle exit. The influences of key process parameters including air pressure and abrasive mass flow rate, additionally turbulence effect, on the variation of abrasive particle distribution in the air jet in AAJ are analyzed and discussed. The results and analyses can be great helpful in understanding and optimizing the characterization of micro-channels and micro-holes machined using AAJ.

2. Governing equations for gas-particle two-phase flow

2.1 Governing equations of the particle phase

According to Newton's second law of motion, the equations governing the translational and rotational motions of a particle *i* are given by [30,31]:

$$m_i \frac{d\mathbf{u}_i}{dt} = m_i \mathbf{g} + \sum_{j=1}^{N} \mathbf{F}_{c,ij} + \mathbf{F}_{d,i} + \mathbf{F}_{b,i}, \tag{1}$$

$$\mathbf{I}_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{N} (\mathbf{T}_{t,ij} + \mathbf{T}_{r,ij}), \tag{2}$$

where m_i is the mass of the particle, $\mathbf{g}$ is the gravitational acceleration, $\mathbf{u}_i$ is the particle velocity, $\mathbf{F}_{c,ij}$ is the contact force, $\mathbf{F}_{d.i}$ is the drag force due to gas-particle interaction and is usually calculated from empirical expressions. $\mathbf{F}_{b,i}$ is the Archimedes buoyance force caused by the pressure gradient. $\mathbf{I}_i$ is the rotational inertia of the particle, $\boldsymbol{\omega}_i$ is the angular velocity of the particle, and $\mathbf{T}_{t,ij}$, $\mathbf{T}_{r,ij}$ are the moment of the tangential force generated by the contacting particles and the rolling friction toques.

It should be noted that the time-related drag force and virtual mass force are neglects in Eq. (1), which may cause some discrepancies between the numerical and the experimental results. To fix that, Guo's model is employed [32] and Eq. (1) becomes

$$\frac{\pi}{6} d^3 (\rho_p + \rho_g C_A) \frac{d\mathbf{u}_i}{dt} = \frac{\pi}{6} d^3 (\rho_p - \rho_g)\mathbf{g} + \sum_{j=1}^{N} \mathbf{F}_{c,ij} + \mathbf{F}_{d,i}, \tag{3}$$

where d is the particle diameter, ρ_p is the particle density and ρ_g is the gas density. C_A is a constant about time-related drag force and virtual mass force, and $C_A = 2$ in this simulation [32]. The Hertz-Mindlin (no-slip) model is employed to calculate the inter-particle collision force $\mathbf{F}_{c,ij}$ [33]. In the Hertz-Mindlin model, each force and moment on the particle can be treated as a spring or a damper [31]. The tangential micro-slip is neglected, and the tangential contact force is limited by Coulomb's law [17,34,35].

2.2 Governing equations of gas phase

The continuity and momentum equations are used to compute the motion of the gas phase [16,17], given by

$$\frac{\partial}{\partial t}(\varepsilon_g\rho_g) + \nabla\cdot(\varepsilon_g\rho_g\mathbf{U}_g) = 0, \tag{4}$$

$$\frac{\partial}{\partial t}(\varepsilon_g\rho_g\mathbf{U}_g) + \nabla\cdot(\varepsilon_g\rho_g\mathbf{U}_g\otimes\mathbf{U}_g) = -\nabla p + \nabla\cdot\boldsymbol{\tau} + \varepsilon_g\rho_g\mathbf{g} - \mathbf{F}_{p,i}, \tag{5}$$

where ε_g is the gas volume fraction, ρ_g is the density of the gas, $\mathbf{U}_g$ is the gas velocity, p is the pressure, and $\boldsymbol{\tau}$ is the viscous tensor.

$$\boldsymbol{\tau} = \varepsilon_g(\mu+\mu_t)[\nabla\mathbf{U}_g + (\nabla\mathbf{U}_g)^T - \tfrac{2}{3}(\nabla\mathbf{U}_g)\delta_k] \tag{6}$$

where μ is the gas dynamic viscosity, μ_t is the turbulent viscosity and δ_k is the identity tensor.

$$\mu_t = C_u\rho_g\frac{k^2}{\varepsilon} \tag{7}$$

where C_u is the empirically constant, k is the turbulent kinetic energy and ε is the turbulent dissipation rate.

The momentum exchange term $\boldsymbol{F}_{p,i}$ from the particles to the fluid [17], is computed from

$$\boldsymbol{F}_{p,i} = \frac{\sum_{i=1}^{n_p}\boldsymbol{F}_d}{\Delta V} \tag{8}$$

where $\boldsymbol{n}_p$ is the number of particles and ΔV is the number of the computational cell.

Turbulence effects cannot be neglected due to the high Reynolds number of the air in the AAJ. The k-ε turbulence model is widely used for turbulent flow in many industrial processes [13,30,36]. Here, the k-ε turbulence model is implemented for the turbulent flow simulation and the turbulent flow near the wall is computed with the wall function method. The governing equations of the k-ε turbulence model are

$$\frac{\partial}{\partial t}(\varepsilon_g\rho_g k) + \nabla(\varepsilon_g\rho_g k\mathbf{U}_g) = \nabla\left[\varepsilon_g\left(\mu+\frac{\mu_t}{\sigma_k}\right)\nabla k\right] + \varepsilon_g G_k - \varepsilon_g\rho_g\sigma_k + S_d^k, \tag{9}$$

$$\frac{\partial}{\partial t}(\varepsilon_g\rho_g\varepsilon) + \nabla(\varepsilon_g\rho_g\varepsilon\mathbf{U}_g) = \nabla\left[\varepsilon_g\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right] + \varepsilon_g\frac{\varepsilon}{k}(C_1G_k - C_2\rho_g\varepsilon) + S_d^\varepsilon, \tag{10}$$

where σ_k and σ_ε are the turbulent Prandtl numbers for k and ε, C_1 and C_2 are model constants [37], G_k represents the turbulence kinetic energy because of the velocity gradient, S_d^k and S_d^ε denote the defined turbulent kinetic energy [30].

2.3 Particle-fluid interaction

The drag force acting on individual particles is given by the drag force model of Di Felice [38], as

$$F_d = \frac{1}{8} C_d \rho_g \pi d_p^2 \left|\mathbf{U}_g - \mathbf{U}_p\right| (\mathbf{U}_g - \mathbf{U}_p) {\varepsilon_g}^{1-\chi} \tag{11}$$

where C_d is the drag force coefficient, $\mathbf{U}_p$ is the particle velocity and χ is the empirical constant. The definition of drag force coefficient in Eq. (11) is given as

$$C_d = \begin{cases} \frac{24}{Re_p} & Re_p \leq 1 \\ (0.63 + \frac{4.8}{\sqrt{Re_p}})^2 & Re_p > 1 \end{cases} \tag{12}$$

where $Re_p = \frac{\varepsilon_g \rho d_p |\mathbf{U}_g - \mathbf{U}_p|}{\mu}$ is the particle Reynolds number. The expression for the term χ is

$$\chi = 3.7 - 0.65\exp[-\frac{(1.5 - \lg Re_p)^2}{2}] \tag{13}$$

3. Semi-resolved CFD-DEM

3.1 Methodology of semi-resolved CFD-DEM modeling

In the conventional unresolved CFD–DEM, for situations where the cell size is smaller than 3 times of the particle diameter, the computed fluid velocity $\mathbf{U}_g$ and fluid volume fraction ε_g are not accurate, and the resultant C_d and drag force will certainly cause a large numerical error in an unresolved CFD–DEM coupling [21]. To overcome this shortcoming, a semi-resolved CFD-DEM model was recently proposed in Ref. [21]. The model used a kernel function to reconstruct the background information from all the cells whose centers locate within the smoothing distance, which leads to eliminating the grid-size dependency. This kernel-based approximation bridges the gap between CFD-DEM simulations based on unresolved and resolved meshes, and have a wide application to particulate flows with a fine mesh, especially gas-particle two-phase flow in the narrow AAJ nozzle. Based on Ref. [21], the basic implementation of semi-resolved CFD-DEM is described as follows.

As shown in Fig. 1, the fluid domain is expanded from the local cell containing a specific particle with a diameter of d, to neighboring cells which are covered by a circular or spherical region with a diameter of κd (where the scalar factor κ determines the range of surrounding flow domain and the number of neighboring cells). After the expansion of the fluid background domain from the local cell to neighboring cells, the kernel-based approximation is used to estimate the background fluid velocity from the fluid velocities in the neighboring cells. Kernel-based approximation has wide applications in estimating the field value of a function over randomly distributed points on which data is sampled, as in the smoothed particle hydrodynamics (SPH) [39,40].

Based on this normalized kernel approximation [41,42], the background fluid velocity ($\mathbf{U}_g$) of particle i from the neighboring cells can be estimated as

$$\mathbf{U}_g = \frac{\sum_{j=1}^{N} \mathbf{U}_g(\mathbf{r}_j) W(\mathbf{r}-\boldsymbol{r}_j) \Delta V_{c,j}}{\sum_{j=1}^{N} W(\mathbf{r}-\boldsymbol{r}_j) \Delta V_{c,j}} \tag{14}$$

where j is the index of a CFD cell within the smoothing distance κd, $\mathbf{U}_g(\mathbf{r}_j)$ *and* $\Delta V_{c,j}$ is the volume and the fluid velocity of the cell j. N is the total number of CFD cells within the smoothed region around particle i. $W(\mathbf{r}-\boldsymbol{r}_j)$ is the value of particle i's kernel function on cell j, and $\mathbf{r}-\boldsymbol{r}_j$ is the relative position vector of the particle and the cell.

Different from the previous semi-resolved CFD-DEM method [21], in this work, a double cosine kernel function [43] rather than the Gaussian kernel is used to reconstruct the background information. Similar to the Gaussian kernel, the double cosine kernel is sufficiently smooth. It is noted that the Gaussian kernel function does not rigorously have normalization property (integration of the kernel function to be unity) for a finite smoothing distance κd, unless κ approaches infinity [44]. The kernel function is truncated at κd, and this produces a numerical error in SPH kernel and particle approximations, while the error decreases when increasing κ with the more computational expense. In practical applications, κ is usually taken as 3 to balance accuracy and efficiency. Different from the Gaussian kernel function, the double cosine kernel function has rigorous normalization property and the function value is exactly zero on the boundary (κd). This theoretically removes the truncation error arisen from non-zero boundary value as in the Gaussian kernel function. The double cosine kernel function is given by

$$W(\mathbf{r}-\boldsymbol{r}_j)=\alpha\begin{cases}4\cos\left(\frac{\pi}{\kappa}\frac{|\mathbf{r}-\boldsymbol{r}_j|}{\kappa d}\right)+\cos\left(\frac{2\pi}{\kappa}\frac{|\mathbf{r}-\boldsymbol{r}_j|}{\kappa d}\right)+3, & 0\le|\mathbf{r}-\boldsymbol{r}_j|\le\kappa d\\ 0, & |\mathbf{r}-\boldsymbol{r}_j|>\kappa d\end{cases} \quad (15)$$

where the normalized coefficient $\alpha = \pi/[(4\pi^2\text{-}30)(\kappa d)^2]$ in three-dimensional space, κd is the smoothing distance and κ is taken as 3 for general kernel approximations [43,45]. It is noted that κ determines the expanded fluid domain, which is the cells overlapping a circular or spherical region with a diameter, κd.

The corrected relative velocity difference $\widetilde{\mathbf{U}}_r$ between the particle and the fluid within the expanded fluid domain is then written as

$$\widetilde{\mathbf{U}}_r = \mathbf{U}_g - \mathbf{U}_p = \frac{\sum_{j=1}^{N} \mathbf{U}_g(\mathbf{r}_j)(4\cos\left(\frac{\pi}{\kappa}\frac{|\mathbf{r}-r_j|}{\kappa d}\right)+\cos\left(\frac{2\pi}{\kappa}\frac{|\mathbf{r}-r_j|}{\kappa d}\right)+3)\,\Delta V_{c,j}}{\sum_{j=1}^{N}(4\cos\left(\frac{\pi}{\kappa}\frac{|\mathbf{r}-r_j|}{\kappa d}\right)+\cos\left(\frac{2\pi}{\kappa}\frac{|\mathbf{r}-r_j|}{\kappa d}\right)+3)\,\Delta V_{c,j}} - \mathbf{U}_p \quad (16)$$

Similarly, the corrected fluid volume fraction for drag force calculation (Eq. (11)) is recalculated as

$$\tilde{\varepsilon} = 1 - \frac{\sum_i^N \Delta V_{p,j}}{\sum_i^N \Delta V_{c,j}} \quad (17)$$

where $V_{p,i}$ is the volume of particle i within the total identified neighboring FVM cells, and $V_{c,j}$ is the volume of the total identified FVM cells within the smoothing distance. In the boundary region, the smoothing distance should be increased to make sure that the volume of the smoothing spherical region still equals to $4\pi(\kappa d)^3/3$, as it is approaches the wall [46]. Additionally, reconstructing the background information from many other cells whose centers locate within the kernel-based approximation region, it is expected that the estimation of fluid velocity and volume fraction are more reasonable, and thus the resultant unresolved CFD–DEM modeling results can be more accurate.

3.2 Implementation of semi-resolved CFD-DEM technique

In this work, modeling of the gas-particle two-phase flow in the AAJ is implemented by using the semi-resolved CFD-DEM model [19]. This model is integrated within open-source code, CFDEM [47,48], in which the open-source CFD code, OpenFOAM [49], is employed to model the continuous fluid phase, and discrete particle motion modeling is accomplished using the discrete element method (DEM) code, LIGGGHTS [50,51].

In the CFDEM framework, the gas phase is solved using a pressure implicit with the splitting of operators (PISO) method [52,53]. Besides, a second-order implicit backward time integration scheme and centered gradient and interpolation schemes are adopted to preserve the second-order accuracy for pressure and velocity [17]. The coupling routine between CFD and DEM can be detail described as follows [30,31].

- The DEM solver calculates the particle positions and velocities.
- The particle positions and velocities are passed to the CFD solver.
- The continuity equation Eq. (4) and momentum equation Eq. (5) of the gas phase are resolved by the CFD solver.
- For each particle, the range κd of surrounding fluid domain from the corresponding local cell is expanded and the neighboring cells in the CFD mesh are determined.
- The background fluid velocity from the fluid velocities in the neighboring cells is estimated by the kernel-based approximation (Eq.(14-15)).
- For the neighboring cells, the corrected void fraction based on Eq.(17) as well as a mean particle velocity is determined.
- Based on the corrected void fraction and corrected relative velocity (Eq.(16)), the fluid forces (Eq.(11)) acting on each particle are calculated.
- Particle–fluid momentum exchange terms are assembled from particle-based forces by ensemble averaging over all particles in the CFD neighboring cell.
- The fluid forces acting on each particle are calculated and sent to the DEM solver and used within the next time step.
- The routine is repeated.

4. Simulations and discussions

4.1 Computational setup

In this simulation, to simplify analysis and to reflect the practice in the AAJ [1], only cylindrical nozzles and a free jet area are considered. Computational geometry is similar to previous experiments conducted by Li et al. [14]. The computational domain is a cylindrical nozzle with an inside diameter of 0.28 mm and a length of 7 mm, and a free jet region in an axial range of 0.5 mm from nozzle exit downstream, as shown in Fig. 2(a). The computational domain is divided into structural grid cells shown in Fig. 2(b). Based on the mesh sensitivity analyses shown in Fig. 3, the grid size is taken as 25×25×40 μm^3 considering the computational accuracy and efficiency [15,17,21,30]. The computational field containing 57744 CFD cells is chosen in this work.

The abrasive particles are assumed to be spherical and have a uniform size. The abrasive particles with a diameter of 27 μm are released continuously at the nozzle inlet. The air pressures corresponding to operating pressures of 0.43, 0.60, and 0.69 MPa are imposed at the nozzle inlet. Subsequently, the abrasive particles are accelerated by the airflow within the nozzle at different operating pressures. The abrasive air-jet enters the free jet domain initially filled with air. The outer boundary of the free jet region is set as the pressure outlet of immersing air and side flow with atmospheric pressure. The nozzle wall is set as a no-slip condition and the Neumann's condition $\partial p/\partial z = 0$ is applied at the upper, and lower boundaries of the free jet region (see Fig. 2(b)). The time step for a stable DEM scheme is determined via the contact time in the normal direction as

$$\Delta t_{contact} = \sqrt{m^* \frac{\pi^2 + ln^2 e_n}{k_n}} \tag{18}$$

When calculating the particle positions in the DEM procedure, the time step should be chosen sufficiently small so that the detection of contact between particles persists over several time steps [13]. Therefore, the DEM time step is set to be 1×10^{-8}s, which is smaller than the calculated contact time via Eq. (18) in the normal direction of 5×10^{-7} s. It is noted that the value of the normal spring stiffness adopted here is much lower than the real value of abrasive particles. Since the normal spring stiffness determined from Young's Modulus for the abrasive particle yields a very high value, which results in the usage of an even smaller particle time step, it is thus found to be undesirable from a computational perspective [13]. For the gas phase part, Courant–Friedrich–Lewy (CFL) condition is employed to determine the CFD time step [17], which can be given as:

$$CFL = \Delta t_{CFD} \max\left(\frac{|\mathbf{U}_g|}{\Delta}\right) < 1 \tag{19}$$

where Δ is a characteristic length of the FVM cell. For example, when the gas phase $|\mathbf{U}_g|$ = 500 m/s and the mesh size Δ = 25 μm, the CFD time step is calculated to be 5×10^{-8} s according to the CFL condition. Here, a conservative value of $\Delta t_{CFD} = 1 \times 10^{-9}$ s is adopted to ensure stability when modeling the gas phase in a whole computational domain. Detailed physical and numerical parameters chosen in the simulation of the AAJ are listed in Table 2.

4.2 Validation of the semi-resolved CFD-DEM model

To verify the accuracy of the semi-resolved CFD-DEM model used in this paper, the data of particle velocities from the theoretical model [1] and the PIV experiments [4] were utilized for comparisons. According to Ref. [1], a basic introduction of the particle velocity model is described as follows. A mathematical solution is utilized to estimate the centerline particle velocities by discretizing the nozzle into small segments and assuming the constant acceleration within those segments. After the centerline particle velocity is determined, the particle velocities in the free jet flow are predicted by the jet radial and axial location [1,54], which can be estimated as

$$\mathbf{U}_{p(x,z)}=\mathbf{U}_{p(x=0,z)}\exp\left(-\ln 2\left(\frac{x}{\frac{d_n}{2}+100d_n\tan\frac{\theta_A}{2}}\right)\right) \tag{20}$$

where $\mathbf{U}_{p(x,z)}$ is the particle velocity at an axial distance z from nozzle exit and a radial position x from the jet centerline, as shown in Fig. 4, $\mathbf{U}_{p(x=0,z)}$ is the centerline particle velocity at an axial distance z from the nozzle exit, and θ_A is the expansion angle of a pure air jet flow. The expansion angle of 13.5° is used here [1].

In the validation examples of the semi-resolved CFD-DEM model, the cylindrical nozzles with the inner diameter of 0.28, 0.36, and 0.46 mm are chosen respectively in the CFD–DEM analysis, and the other parameters are the same as those used in the experiments [4]. Except for the computational parameters shown in Table 2, other numerical parameters are given in Table 3. We simulated the abrasive particle passing through the nozzle by using the unresolved and semi-resolved CFD-DEM, and compared the numerical particle velocity with theoretical results, as shown in Fig. 5. In this simulation, the nozzle diameter is 0.28 mm, the operating pressure is 0.60 MPa and other parameters are given in Table 3. The particle velocity distribution obtained from unresolved CFD-DEM differs a lot from the theoretical results, because of the computational error in estimating the background velocity and solid volume fraction in the drag force model [21]. In contrast, the semi-resolved CFD-DEM calculates the background velocity and solid volume fraction in an expanded fluid region, and its simulation results agree more with the theoretical analyses than those from unresolved CFD–DEM. The comparison of numerically obtained particle velocity distributions from the nozzle exit with experimental and theoretical data is shown in Fig. 6. The numerical results exhibited a consistent variation trend with the experimental and the theoretical results within the axial length of 2 mm downstream. The practical range of the standoff distance between the nozzle exit and the target surface used in AAJ is usually small (within 2mm) [1]. It indicates that the present semi-resolved CFD-DEM model can qualitatively analyze the flow characteristics of abrasive particles within the air jet in the AAJ micromachining. Given the fact of simplification in numerical simulation and numerous factors affecting experimental accuracy [36], the simulation error is within an acceptable range and the simulation results of the gas-particle two-phase flow in the AAJ are relatively accurate.

4.3 Flow and distribution characteristics of particle jet flow in the AAJ micromachining

The typical evolution of abrasive particle flow in the AAJ micromachining is shown in Fig. 7. In the simulation, the nozzle diameter is 0.28 mm, the operating pressure is 0.60 MPa, and the abrasive mass flow rate is 0.04 g/s. It is based on simulations with a physical time of 1.5 ms, and a series of instantaneous snapshots are generated every 0.1 μs. Different colors are used to distinguish the magnitudes of particle velocity while red color represents the maximum particle velocity, and blue color represents the minimum particle velocity. The gray areas in Fig. 7 represent the wall of the nozzle and the boundaries of the free jet region, respectively.

The evolution of abrasive particle flow in the air jet exhibits different patterns in the whole process of the AAJ micromachining. As shown in the uppermost picture of Fig. 7(a), the initial abrasive particles are randomly generated in the nozzle inlet region. Subsequently, the solid particles inside the nozzle are driven by the high-pressure air until they pass through the nozzle. During the evolution of gas-particle flow inside the nozzle, it is observed that there exist two distinct flow patterns along the jet flow including an initial acceleration region with lower velocity and denser particle concentration, and the full-developed region with higher velocity and sparser particle concentration. After leaving the nozzle exit and traveling downwards, the particles disperse into a wider area shown in Fig. 7(b). Moreover, the typical particle trajectory distributions in the AAJ are shown in Fig. 8. The balls with different colors correspond to the abrasive particles in the AAJ. Particle trajectory distribution is obtained by a series of particle spatial locations at different times. The numerical results indicate particle trajectory is not a straight line or the solid particles move toward the vertical jet direction while it flows along the jet direction. It is mainly attributed to the particle-particle and particle-wall collision, and the turbulence produced by the high-velocity gas in the AAJ [55].

The numerical results of the particle velocity and trajectory distributions in AAJ are statistically analyzed on the conditions of the abrasive mass flow rate of 0.04 g/s, 0.28 mm diameter nozzle, and 0.60 MPa operating pressure. Fig. 9 illustrates the particle velocity and drag force distributions along the jet flow direction from the point of nozzle inlet through an axial length of 0.5 mm downstream. In the initial acceleration region near the nozzle inlet, the drag force applied to the particle by the air flow increases rapidly due to the large gas-solid slip velocity, and this results in a fast acceleration of the particle. The drag force acting on the particle gradually decreases with the particle velocity increasing in the full-developed region, and hence leads to a decaying acceleration of the particle within the nozzle. It should be noted that the drag force decreases rapidly at the nozzle outlet. This is attributed to the entrainment effect by the surrounding air, which reduces the speed of the air jet as it travels downstream from the nozzle exit.

When the particles pass through a jet cross-section at the nozzle exit, the particle properties (particle position, velocity, and concentration) are extracted from the numerical results of 1.5 ms physical time. In Fig. 10(a), the position distribution of the particles is obtained by accumulating particle trajectories over the nozzle exit section. The cross-section of the nozzle exit is divided into individual regions by the radial distance. And the individual regions are exhibited between the red and the blue lines in Fig. 10(a). The radial particle velocity distribution at the nozzle exit exhibits a compressed bell-shape, as shown in Fig. 10(b). It can be observed that the polynomial fitting curve of particle velocity distribution has a local maximum value at the centerline of the jet, and the particle velocity decreases continuously from the jet centerline toward the jet rim. It may be caused by the uneven distribution of the air velocity in the jet cross-section. As shown in Fig. 11(b), the velocity of the air jet reaches a maximum close to the centerline of the nozzle and decreases gradually towards the border of the nozzle. Moreover, we obtain the particle concentration distribution by calculating the particle number density within the individual regions, as shown in Fig. 10(c). It is found that the radial particle concentration distribution is non-uniform in the jet cross-section at the nozzle exit in the AAJ micromachining. The numerical result indicates that the radial concentration profile of the particle is preferentially distributed towards the near-wall region. The central core of the particle jet exhibits a 'U-shaped' concentration profile, with the lowest concentration occurring at the nozzle center. It might be explained by the influence of the turbophoretic force that is induced by the inhomogeneous turbulent flow field in Fig. 11(c)-(f). The turbophoretic force $\mathbf{F}_{tur}$ on the particle is proportional to [56–58]

$$|\mathbf{F}_{tur}| \sim -G^* = -\frac{\partial (u'/U_{g,c})^2}{\partial r'} \tag{21}$$

where G^* is the pseudo-gradient, r' is the radial distance, and $u'/U_{g,c}$ is the normalized root-mean-square value of wall-normal particle velocity fluctuation at the nozzle exit.

As shown in Fig. 12, the pseudo-gradient G^* related to the turbophoretic force $\mathbf{F}_{tur}$ is small throughout the central region of the nozzle (0 mm ≤ r' < 0.10 mm). It is related to the relatively low magnitude of the turbulent kinetic energy and the turbulent dissipation rate in the central region of the flow field in Fig. 11(c)-(f). In the closer wall region (0.10 mm ≤ r' < 0.12 mm), G^* has a positive value and it is negative while very close to the nozzle wall (0.12 mm < r' < 0.14 mm). It should be noted that the negative value of G^* close to the wall is induced by the damping of turbulent fluctuations by the wall [57]. Thus, the turbophoretic force on the particles dominates in the near-wall region of the nozzle, causing the particles to migrate towards the nozzle wall [56,57]. This numerical observation of the particle concentration in the turbulent pipe flow is in agreement with the previous theoretical, experimental, and numerical results [56–59].

To study the evolution of the particle flow as it transports from the nozzle exit into the free jet region, the radial distributions of particle velocity and concentration at the nozzle exit and in the free jet region are comparatively plotted in Fig. 13. The results indicate that the particles will accelerate to a higher value of the velocity in the free jet region than they pass the nozzle exit, as shown in Fig. 13(a). Comparing to the velocity distribution at the nozzle exit, there is a larger variation of the particle velocity from the jet centerline toward the jet rim in the free jet region. To quantify the radial distribution of the particle concentration, the individual regions are further subdivided into three subregions: the region 1 ($0 \leq r' < 0.05$ mm), region 2 ($0.05 \leq r' < 0.10$ mm) and region 3 ($r' \geq 0.10$ mm). The particle number percentages of the nozzle exit and free jet region in each subregion are counted as shown in Fig. 13(b). It is demonstrated that the particle concentration in region 3 would decrease as the particle jet flow travels downstream from the nozzle exit. The reason may be attributed to that the turbophoretic force near the jet boundary weakens in the free jet region, and this is consistent with a lower value of $G^{*}_{\max}$ in Fig. 13(c).

4.4 Parameters effects on particle distributions in the AAJ micromachining

The air pressure and abrasive mass flow rate have a key role in the processing results in the AAJ micromachining [14]. To investigate their influences on the particle velocity and concentration distributions over the nozzle exit in the AAJ, different air pressures and abrasive mass flow rates are used in the numerical model. In the present simulation, the detailed analyses of parameter effects are conducted on the conditions of the operating pressures of 0.43, 0.60, and 0.69 MPa along with the abrasive mass flow rates of 0.02, 0.04, and 0.09 g/s. The radial particle velocity distributions under the operating pressure of 0.43, 0.60, and 0.69 MPa are illustrated in Fig. 14(a). The numerical results show that a rise in the operating pressure at the nozzle inlet increases the particle velocity in the AAJ. It is reasonable as higher operating pressures yield higher dragging forces acting on the particles shown in Fig. 15(a), which further results in a larger acceleration and a higher particle velocity. The radial particle velocity distributions under the abrasive mass flow rate of 0.02, 0.04, and 0.09 g/s are shown in Fig. 14(b). The particle velocity drops with the abrasive mass flow rate increases, which is attributed to a decline in the drag force acting on the particle shown in Fig. 15(b). It should be noted that, for comparative purposes, the drag force acting on the same number of particles is considered here. These observations agree with the reported phenomena in experiments [60]. In summary, the operating pressure has obvious effects on the particle velocity distribution in the AAJ micromachining. The greater the pressure of the air jet, the bigger will be the velocity imparted to the abrasive particle in the jet cross-section. Moreover, a rise in particle mass flow rates would decrease the particle velocity due to the decline of the drag force acting on particles.

The particle number percentages in each subregion on the different operating pressures and particle mass flow rates are shown in Fig. 16(a) and (c), respectively. It can be observed in Fig. 16(a) that the particle concentration in region 3 decreases with the increasing pressure, which is consistent with the variation of G^{*}_{max} in the near-wall region in Fig. 16(b). It shows that a decrease of the particle concentration in the nozzle central region (region 1 and 2) and an increase in the near-wall region (region 3) with the particle mass flow rate rises, as shown in Fig. 16(c). It is attributed to the enhanced influence of the turbophoretic force during the near-wall region, as shown in Fig. 16(d). It should be noted that the particle mass flow rate has a more obvious effect on the variation of radial particle distribution compared with the operating pressure. This may be substantiated with the flow field information of the air jet at the nozzle exit under different operating parameters in Fig .17. In a denser particle jet of high mass flow rate, more solid particles significantly weaken the air velocity and turbulent fluctuation, which could transform the turbophoretic force and causes particle distributions to change distinctly.

5. Conclusion

Abrasive air jet (AAJ) machining is attractive for micromachining hard and brittle materials, while the particle velocity and concentration distributions are essential jet characteristic features of the particle erosion process in the AAJ. In this work, a semi-resolved CFD-DEM approach is used to numerically investigate the gas-particle two-phase flow in the AAJ. The semi-resolved CFD-DEM model is validated first and then used to investigate the particle flow characteristics inside the nozzle, velocity and concentration distributions over the nozzle exit during the AAJ machining process. From the results and discussions, we can conclude:

1. The recently proposed semi-resolved CFD-DEM coupling approach is further developed to investigate the gas-particle two-phase flow in the AAJ micromachining while the background fluid velocity is reconstructed using a double cosine kernel function. The numerical results are in better agreement with theoretical and experimental observations than the conventional unresolved CFD-DEM, demonstrating that the effectiveness of the semi-resolved CFD-DEM model in simulating the fluid-particle two-phase flow in the AAJ.
2. There are two distinct particle flow patterns inside the nozzle along the jet flow including an initial acceleration region with lower velocity and denser particle concentration, and the fully-developed region with higher velocity and sparser particle concentration. The particles continue to accelerate and disperse into a wider area after they leave the nozzle exit.
3. The radial particle velocity distribution in the jet cross-section exhibits a compressed bell-shape, which has a local maximum at the centerline of the jet and decreases continuously from the jet centerline toward the jet rim. The radial profile of the particle concentration is non-uniform and preferentially distributed towards the outer edges of the abrasive jet flow, which is attributed to the influence of the inhomogeneous turbulence in the AAJ.
4. The greater the pressure of the air jet, the bigger will be the velocity imparted to the abrasive particle, and a rise in particle mass flow rate decreases particle

velocity due to the decline of the drag force. The particle concentration of the near-wall region decreases with the increasing pressure and increases with the particle mass flow rate rises. This is attributed to the variation of the turbophoretic force during the near-wall region.

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Nomenclature

C_1	turbulent model constants
C_2	turbulent model constants
C_A	constant about time-related drag force and the virtual mass force
C_d	drag force coefficient
C_u	empirically constant
d_n	nozzle inner diameter
d	particle diameter
e_n	coefficient of restitution
$\boldsymbol{F}_{ba}$	basset force
$\boldsymbol{F}_b$	buoyance force
$\boldsymbol{F}_d$	drag force
$\boldsymbol{F}_m$	Magnus force
$\boldsymbol{F}_s$	Saffman force
$\boldsymbol{F}_{vm}$	virtual mass force
$\boldsymbol{F}_{c,ij}$	contact force between two specific particles *i* and *j*
$\boldsymbol{F}_{\text{normal}}$	normal contact force between two specific particles *i* and *j*
$\boldsymbol{F}_{\text{tangential}}$	tangential contact force between two specific particles *i* and *j*
$\boldsymbol{F}_{\boldsymbol{tur}}$	turbophoretic force
$\boldsymbol{F}_{d.i}$	drag force on a specific particle *i*
$\boldsymbol{F}_{p,i}$	momentum exchange term on a specific particle *i*
$\mathbf{g}$	gravitational acceleration
G_k	turbulence kinetic energy from velocity gradient
G^*	pseudo-gradient
H	Standoff distance
$\boldsymbol{I}_i$	rotational inertia of particle
k	turbulent kinetic energy
k_n	normal stiffness coefficient
k_t	tangential stiffness coefficient
L	nozzle length
m_i	mass of particle
m^*	equivalent mass
m_p	abrasive mass flow rate
p	pressure
p_g	nozzle inlet air pressure
$\mathbf{r}$	position vector of the particle
$\boldsymbol{r_j}$	position vector of the cell *j*
r'	radial distance
Re	Reynolds' number
S_d^k	defined turbulent kinetic energy
S_d^ε	defined turbulent kinetic energy
$\boldsymbol{T}_{t,ij}$	torque by tangential forces
$\boldsymbol{T}_{r,ij}$	rolling friction torque
$\mathbf{u}_i$	particle velocity
u'	root-mean square value of wall-normal particle velocity fluctuation
$\mathbf{U}_g$	gas velocity
$\mathbf{U}_{\boldsymbol{g},\boldsymbol{c}}$	gas velocity of nozzle centerline at nozzle exit
$\mathbf{U}_p$	particle velocity
$\mathbf{U}_{p(x=0,z)}$	centerline particle velocity at an axial distance z from the nozzle exit
$\mathbf{U}_{p(x,z)}$	particle velocity at an axial distance *z* from nozzle exit and a radial distance *x* from the jet centerline
$\widetilde{\mathbf{U}}_r$	relative velocity difference between the particle and the fluid
Δt_c	coupling time step
Δt_{CFD}	CFD time step
Δt_{DEM}	DEM time step

$V_{p,i}$	the volume of particle i
$V_{c,j}$	volume of the FVM cells within the smoothing distance
W	free jet region length and width
Y	Young's modulus of material
Greek symbols	
α	normalized coefficient
γ	Poisson ratio
ε	turbulent dissipation rate
ε_g	gas volume fraction
$\tilde{\varepsilon}$	corrected fluid volume fraction
η_n	normal damping coefficient
η_t	tangential damping coefficient
θ_A	expansion angle of a pure air jet flow
κ	scalar factor for the smoothing distance
μ	gas dynamic viscosity
μ_c	coefficient of friction
μ_t	turbulent viscosity
ρ_g	density of the gas
ρ_p	density of the particle
σ_k	turbulent Prandtl number
σ_ε	turbulent Prandtl number
τ	viscous tensor
φ	dimensionless coefficient
χ	empirical constant
$\boldsymbol{\omega_i}$	angular velocity of particle
Subscripts	
i	index
j	index
g	*gas*
n	*normal*
p	*particle*
t	*tangential*

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