Numerical simulation of particle beam focusing in a supersonic nozzle with rectangular cross-section

A A Shershnev¹ and A N Kudryavtsev¹,²
¹Khristianovich Institute of Theoretical and Applied Mechanics, Russian Academy of Sciences, Siberian Branch, 630090 Novosibirsk, Russia
²Novosibirsk State University, 630090 Novosibirsk, Russia
E-mail: antony@itam.nsc.ru

Abstract. Particle-laden flow in 3D supersonic micronozzle with rectangular cross-section and side walls convergent/divergent in both lateral and transversal direction is studied numerically using a one-way coupled Eulerian/Lagrangian approach. The carrier gas flow is simulated numerically on the basis of the Navier-Stokes equations and then is used to calculate the particles trajectories. It is shown that a collimated beam of particles can be produced using the effect of aerodynamic focusing and the beam collimation is observed in two different ranges of particle sizes. Obtained results are consistent with previously obtained data for plane and axisymmetrical nozzles.

1. Introduction
Multiphase flows in micronozzles are of great interest for their possible industrial applications. One of the most promising applications is generation of high-speed collimated beams of microparticles which can be used in different technologies, such as Cold Gas Spraying [1, 2, 3] or relatively new material deposition method known as Collimated Aerosol Beam Direct-Write (CAB-DW) [4]. In the CAB-DW, an “aerosol gun” is employed for printing solid materials on a substrate for producing solar cells and electronic chips. It was demonstrated both numerically and experimentally [5, 6] that collimated beams can be successfully generated by subsonic (convergent) nozzles. Supersonic (convergent/divergent) nozzles could be used to create high-speed beams; however, in the supersonic part, flow streamlines are divergent, hence the possibility of aerodynamic focusing in such nozzles is questionable.

It was shown numerically [7] that for plane and axisymmetrical supersonic convergent-divergent nozzles aerodynamic focusing of particles into a collimated beam can be obtained. Moreover, it is observed for two different sizes of particles. As for 3D nozzle it was demonstrated, that when a nozzle has a constant width in the lateral direction the focusing is only feasible in the transversal direction. Apparently, the displacement of streamlines in the supersonic part of the nozzle caused by the growth of the boundary layer thickness on the lateral walls is not sufficient for beam collimation in this direction. Hopefully, introduction of subsonic nozzle part, convergent in both lateral and transversal direction will produce particle trajectories focused into a narrow beam rather than a plane sheet. Thus, the present paper is a continuation of the cited study performed to confirm that conclusions above hold for 3D nozzle with rectangular cross-section convergent/divergent in both lateral and transversal direction.
2. Problem statement and numerical techniques

Two-phase flow in a 3D nozzle with a throat width 200 $\mu$m is simulated numerically using the Eulerian-Lagrangian approach. The nozzle contour is based on the nozzles used in experiments of Rothe [8]. Unlike [8], where the author used axisymmetrical nozzles with round cross-section, in the present paper the nozzle with convergent/divergent side walls and rectangular cross-section is considered. Nozzle geometry and computational mesh are shown in figure 1a. The design Mach number of the nozzle is $M_d = 7.52$ and the Reynolds number based on the nozzle half-width and parameters in the nozzle throat is equal to $Re = 350$. The Navier-Stokes equations are used to compute the carrier monatomic gas (argon) flowfield, then Lagrangian approach is applied for calculating the particle trajectories. The stagnation temperature and the nozzle wall temperature are equal to 300 K, the stagnation pressure is 21,790 Pa. It is assumed that the gas exhausts into a chamber with an ambient pressure that is lower than the jet pressure at the nozzle exit so that the exhausting plume is underexpanded.

The particles are introduced into the flow in the nozzle pre-chamber. The flow around small micro- and nanoparticles can occur in the transitional or even the free molecular regime and strong velocity nonequilibrium between the carrier gas and particles can be observed. Therefore, the drag force acting on a particle is calculated with a formula which interpolates between continuum and free molecular expressions and takes into account particle inertia, gas compressibility, and rarefaction effects [9].

When solving the Navier-Stokes equations a shock capturing TVD scheme of 3rd order is used for calculating the convective terms. The 2nd order central differences are used to approximate the diffusive terms. Stagnation temperature, stagnation pressure and flow direction are specified on the inflow boundaries. All gasdynamic quantities are extrapolated from within the computational domain on the outflow boundary. Particle equations of motion are integrated with the 4th order Runge–Kutta scheme. Carrier phase flow parameters in particle locations are calculated using the bilinear interpolation.

3. Results and discussion

Numerical simulation of the carrier phase was performed on a mesh consisting of $295 \times 40 \times 40$ cells. The local Mach number flowfield obtained in this computation is shown in figure 1b. As can be seen, the effective cross-section of the nozzle is reduced considerably because of the rapid growth of the boundary layer in the supersonic part of the nozzle. As a result, computed Mach number of the flow at the nozzle exit is $M = 4.5$, i.e. only 60% of the design Mach number. The flow pattern is typical for low-Reynolds number nozzle flows considered in previous study.

Figure 1. Computational domain sketch and grid used in carrier gas simulation (a) and local Mach number flowfield (b).
Figure 2. Trajectories of particles of different radii.

(a) 5 μm (b) 2.7 μm
(c) 0.5 μm (d) 0.23 μm (e) 0.05 μm

Figure 3. Distribution of the longitudinal velocity of the carrier and dispersed phases (a and b) and the particle Mach number and particle Reynolds number (c and d) along the trajectory in the cases of collimation.
The gas and particle velocities (normalized to the critical velocity) along particle trajectories are shown in figures 3a and b for the particle sizes for which aerodynamic focusing occurs. In case of large particles, the difference in velocity values is significant. Nevertheless, the particle velocity continues to grow in the supersonic part of the nozzle. This acceleration is much more pronounced for smaller particles. Evolution of the particles Reynolds and Mach numbers along the trajectories is presented in figures 3c and 3d. It can also be seen, that both parameters change quite drastically as the particle travels through nozzle. This fact emphasizes the need for formulas for the drag force approximation applicable in a wide range of flow regimes, from the creep flow to supersonic flow and from continuum to free molecular flow.

4. Conclusion
The particle-laden flow in the 3D supersonic micronozzle with a rectangular cross-section and side walls convergent/divergent in both lateral and transversal directions was investigated numerically using the one-way coupled Eulerian/Lagrangian approach. The carrier gas flow was simulated numerically on the basis of the Navier-Stokes equations and then is used to calculate the particles trajectories. It was shown that a collimated beam of particles can be produced using the effect of aerodynamic focusing and the beam collimation is observed in two different ranges of particle sizes. Obtained results are consistent with previously obtained data for plane and axisymmetrical nozzles. Further investigations are required to study the plume interaction with a transversal plate (substrate) which is of great importance for practical applications such as material deposition processes.

Acknowledgments
The work is supported by the Russian Science Foundation (grant No. 18-11-00246). This support is gratefully acknowledged.

Computational resources were kindly provided by Siberian Supercomputer Center of the Institute of Computational Mathematics and Mathematical Geophysics SB RAS (sscc.ru), Computational Center of Novosibirsk State University (musc.nsu.ru) and Moscow State University Supercomputing Center (parallel.ru).

References
[1] Klinkov S V, Kosarev V F, Ryashin N S and Shikalov V S 2016 Experimental study of cold gas spraying through a mask. Part 1 Thermophys. Aeromech. 23 735-40
[2] Klinkov S V, Kosarev, V F and Ryashin N S 2017 Experimental study of cold gas spraying through a mask. Part 2 Thermophys. Aeromech. 24 213-24
[3] Klinkov S V, Kosarev V F and Shikalov V S 2019 Influence of nozzle velocity and powder feed rate on the coating mass and deposition efficiency in cold spraying Surface and Coatings Technology 367 231-43
[4] Han S et al 2008 Printed silicon as diode and FET materials – preliminary results J. Non-Crystalline Solids. 354 2623-6
[5] Akhatov I S, Hoey J M, Thompson D, Lufturakhmanov A, Mahmud Z, Swenson O F, Schulz D L and Osip’tsov A N 2009 Aerosol flow through a micro-capillary Proc. of the ASME 2nd Micro/Nanoscale Heat & Mass Transfer International Conference (Shanghai, China) Paper MNHMT2009-18421
[6] Bhattacharya S, Lufturakhmanov A, Hoey J M, Swenson O F, Mahmud Z and Akhatov I S 2013 Aerosol flow through a converging-diverging micro-nozzle Non-linear Eng. 2 103-12
[7] Kudryavtsev A, Shershnev A and Rybdylova O 2019 Numerical simulation of aerodynamic focusing of particles in supersonic micronozzles Int. J. Multiph. Flow 114 207-18
[8] Rothe D E 1971 Electron-beam studies of viscous flow in supersonic nozzles AIAA J. 9 804-11
[9] Molleson G V and Stasenko A L 2008 Acceleration of microparticles in a gasdynamic facility with high expansion of flow High Temperature 46 100-7