Study on Numerical Investigation of Gas-Particle Supersonic Flow

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ABSTRACT

Particles lying in the sub-micron range have widespread applications in the pharmaceutical, ceramic and other related industries. Separation and classification of these particles is a very important step involved in the manufacturing of these products. Inertial separation, which involves forcing a rapid change in direction of flow of a particle laden gas flow, such that the solid particles separate from the gas streamlines due to their inertia, is the most commonly applied separation technique used for industrial applications. This rapid change in direction of the fluid can be forced by rapidly accelerating the mixture to high velocity and low pressure using a sonic nozzle, causing disequilibrium between the phases. This separation property of supersonic jets, called 'aerodynamic separation', has been widely used in molecular beam formation and mass spectrometry, techniques for analyzing properties of a substance. These processes isolate a narrow beam of molecules, ions, and heavy isotopes along the centerline axis, so that the beam can be introduced in a testing chamber for their analysis. Using Computational Fluid Dynamics (CFD), I have demonstrated how supersonic free jets can be applied for the large-scale isolation and separation of sub-micron solid particles. Optimum separation for particles of a particular diameter can be obtained, in the form of a very narrow distribution along the centerline axis. This separation regime is represented by the optimum value of the dimensionless parameter called as the Stokes number (St), which predicts the probability of particles to separate from the gas phase after encountering an obstacle in the flow. Straight nozzles or capillaries which provide maximum acceleration at its inlet have been found to be best suited for such applications. The acceleration experienced by the gasparticle mixture due to the sudden change in area of the nozzle, is the primary factor responsible for the separation of the path of both phases.

INTRODUCTION

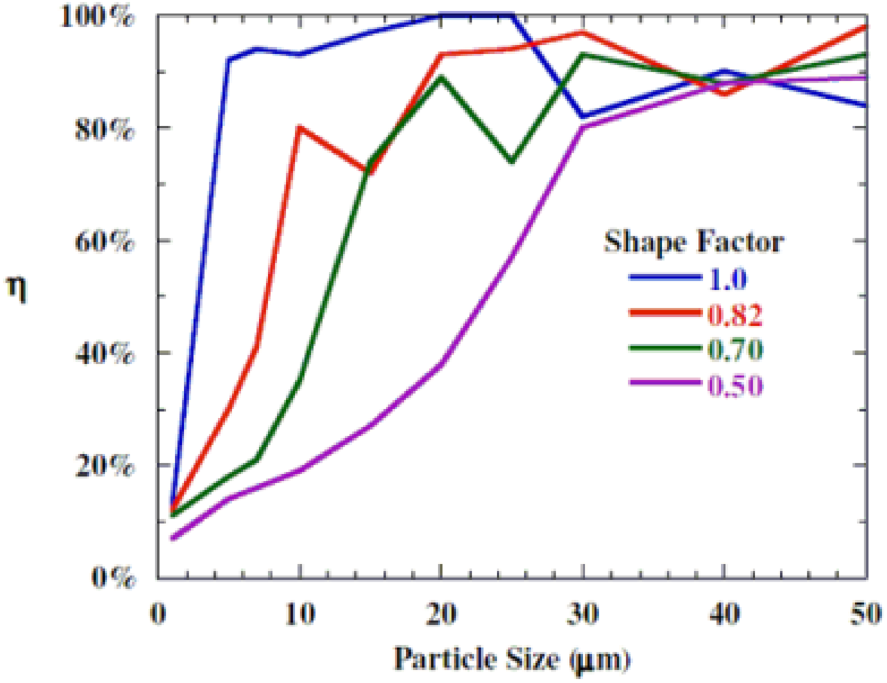
Particles lying in the sub-micron range have widespread applications in the pharmaceutical, ceramic and other related industries. They also have increasing application in processes such as'Gas dynamic cold spray process' [13,35], for the production of thin metallic films. Inertial separation is used to separate solid particles or droplets from a gas stream by enforcing a change in the velocity and direction of the gas. The particles, due to their inertia, find themselves unable to follow this change in direction and hence separate out of the gas flow. Cyclone separators have been one of the most popular categories of inertial separators on account of their simplicity in design and construction and high collection efficiency. In a typical cyclone separator, the gas-solid flow in injected into a cylindrical separator chamber in a direction tangential to its circumference. This results in a vortex flow about the axis. The particles, on account of their inertia, are hurled onto the walls of the chamber. On losing their momentum because of the impact with the walls, the particles fall to the bottom of the chamber where they are collected. In spite of the wide application of cyclone separation in dust removal processes, it is difficult to obtain satisfactory collection efficiency for sub-micron particles. Impact separators force the change in direction of the fluid by imposing an obstacle in its path. Common obstacles can come in many shapes. This obstacle causes causes a disequilibrium between the two phases, causing the particles to diverge from the gas after impacting the surface. Frain (2000) [17] designed a conical array of concentrically arranged circular rings which obtained collection efficiency in the range of 80-85% for a particle size of 10 µm. The separation of a particle is defined by the non-dimensional parameter called the Stokes number (St), which is the ratio of two-time scales, τp and τ. The τp, or the particle dynamics time scale is the time required by the particle suspended in a gas, to respond to the change in velocity of the gas, after experiencing an acceleration due to the obstacle. The τ, or the gas dynamics time scale is the time taken by the gas to travel around the obstacle. Micron and sub-micron sized particles have low inertia, and hence a smaller value of τp and St. This severely affects their separation at normal operating conditions. A review of particle dynamics in Chapter 3 shows that the value of τp and St can be increased by reducing the drag forces acting on the particles. This reduction can be achieved by operating the device at sub-atmospheric pressures. Witman (2005) [49] demonstrated this principle for particle sizes of 1 − 10µm at sub atmospheric pressures, using a louver separator with rectangular cross-section for the blades. A collection efficiency of 85% was obtained for 1µm particles at a pressure of 0.76 torr (101 Pa.), demonstrating its potential for its application in industry.

The application of under-expanded jets is prevalent in particle analyzer systems. Both systems use the properties of the jet to isolate and focus aerosol particles, molecules or heavy isotopes along the centerline of the nozzle. In these processes, the lighter specie or the carrier gas expands as it exits the nozzle. The heavier species, representing the particles to be analyzed, however due to their relatively higher value of τp, continue to travel in a straight trajectory. The nozzle geometry is known to have influence on the degree of concentration of the heavy molecules around the centerline. The size of the molecules and the ions separated in the particle analyzer systems is extremely small compared to the molecules. Here, the significance of the Stokes number (St) is important. The value of the St defines the effects of fluid dynamics and the geometry of the devices on the separation of the particle and gas phases. Therefore, an optimum value of St shall be used to match separation performance in different conditions.

LITERATURE REVIEW

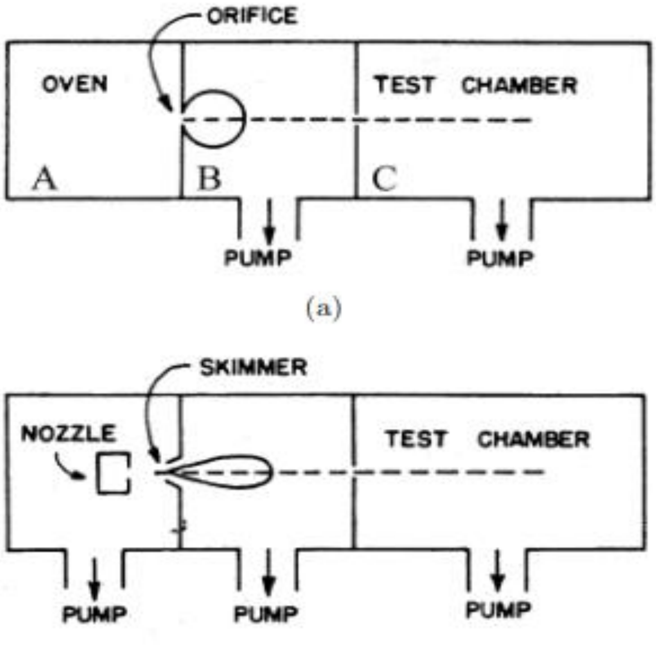
Inertial impact particle separation:

One of the earliest studies on a louver-array based inertial impact separator was conducted by Poulton and Cole (1981) [38]. The designers based the mechanism of the separation on the inertia of the solid particles suspended in the gas flow. The blade array was designed in a way that 90% of the incoming air was diverted through the blade spacing as 'clean air', while the remaining 10% with the particles continues in the original direction. The experimental results were backed up by numerical simulation of the particle trajectory using the Runge-Kutta-Merson method. The drag law acting on the particles was adopted as the one suggested by Serafini (1954) [41]. Poulton and Cole measured the performance of their device in terms of 'mass efficiency' of collection, i.e. simply by the ratio of the mass of the particles separated to the total inlet mass. Further, the variation of the collection efficiency was plotted against operating parameters such as the inlet air velocity and the design parameters such as blade thickness, pitch, and array angle. Since the designers were relying on the inertia of the particles for separation, they did not focus on the influence of the particle dynamics on collection efficiency. For example, no attention was given to study the effect operating pressure can have on the particle drag and how that can affect collection. Nevertheless, this study did successfully establish the effectiveness of louver-based separation for turbine engine applications, where the presence of solid particles suspended in the gas can cause heavy damage to the turbine blade surface.



Particle Focusing

The under-expanded jet is predominantly used by particle analyzer systems to separate and isolate molecules, ions of substances for analyzing their physical and chemical properties. Molecular beam method and mass spectrometry are the most prominent methods that make use of the under-expanded jet evolved due to rapid expansion of a carrier gas emerging from a sonic jet. The molecular beam method is used to isolate a stream of molecules of the carrier gas along the centerline of the nozzle, while mass spectrometry is used for the isolation of ions suspended in a lighter carrier gas. However, the principle of operation remains the same in both methods. In order to understand the application of the jet in separation of much heavier solid particles, it is necessary to conduct a brief review of both methods. Fenn [14] published an article in 2000, describing the history of the evolution of both the methods. Figure 2.2 shows the schematic representation of molecular beam methods. In the classical molecular beam method (Figure 2.2(a)), the gas effuses from source through a orifice into the collimating chamber. The beam of molecules, aligned close to the axis is generated in the collimating chamber and passed to the test chamber through a hole or a channel placed co-axially, called the 'skimmer'. However, the effusive method suffers limitations in the form of reduced beam intensity due to scattering of the molecules.the order of 100 − 400P a. The authors used a converging-diverging nozzle in order to obtain gas streamlines parallel to the centerline, thereby increasing the intensity of the beams. However, boundary layer effects, due to viscous flow interaction with the nozzle walls in the diverging section were observed to have a negative impact on the beam intensity. The influence of this effect was considered in the design of the nozzle geometry. Figure shows a typical molecular beam apparatus using the under-expanded jet.



METHODOLOGY

Eulerian phase:

The simulation of the under-expanded free jet flow in the separator chamber is performed using compressible flow solver rhoCentralFoam [18], which is a part of Open FOAM. High speed compressible flow is characterized by the presence of discontinuities such as shocks and contact discontinuities, the treatment of which is difficult to handle. Schemes such as the piecewise parabolic method (PPM) [9], essentially non-oscillatory (ENO) schemes [20], weighted ENO (WENO) [21] schemes have been popular in the numerical calculation of compressible flows. These schemes basically are approximate Riemann solvers that involve characteristic decomposition and Jacobian evaluation, which make them difficult to implement and are computationally expensive. RhoCentralFoam uses an alternate Riemann-free approach that is independent of characteristic decomposition and Jacobian evaluation. This approach, named the "central scheme" described by Nessyahu and Tadmor [32], has been derived from the Lax-Friedrichs scheme. The resulting numerical method has been proved to obtain accurate and inexpensive solutions for compressible flow problems [18].

Finite volume method:
In the Finite-Volume method [47] the computational domain is divided into polyhedral cells called Control Volumes (CV). Figure 3.1 shows a typical control volume. Neighboring CVs are connected to each other by a face f represented by the area vector Sf. The vector Sf points normally outwards from the cell designated as the “owner cell”. The cell that shares the face f with “owner cell” is named as “neighbor cell” for the sake of convenience. The cell centers of the owner and neighboring cells (named P and N respectively) are connected by the vector ¯d. The governing PDE’s are integrated over the CVs. Gauss’ theorem is implemented to convert these integrals into surface integrals over the face f.Discretization is the next step where the surface integrals are converted into a set of simple algebraic equations involving values of the flux of the primary variables ψf . The values on the face of the CV are interpolated from values at centers (ψP and ψN) of the cells connected by that face. The detailed procedure of discretization and interpolation has been explained in the following sections**.**

Boundary conditions:
Numerical simulations of compressible flow problems require a delicate treatment of the boundary conditions at the inlet and the outlet. As mentioned earlier the solution of high velocity compressible flow problems has a wave-like nature. Each of these waves has a local speed of propagation which can be obtained as an eigenvalue of the Jacobian matrix of the Navier-Stokes equations. Performing a characteristic analysis of the equations to yield the eigenvalues will help to understand their significance in specifying the boundary conditions. The detailed procedure for the same has been presented by Poinsett and Lele [37]. The eigenvalues for a 3-D compressible flow system obtained as a result of the procedure can be expressed as follows:

where λ1 is the eigen value obtained for the density equation. λ2, λ3, λ4 are the eigenvalues corresponding to the momentumequations. λ5 is the eigenvalue for the energy equation. The polarity of the values of λi denotes the direction of flow of the corresponding waves. The local speed of sound is denoted as ‘a’. If the wave enters the computational domain at a particular boundary, its “region of dependence” lies outside the domain, which means that it relies on information that is not present in the domain. Hence the values of the variable attached to that wave needs to be specified at that boundary. On the contrary, the waves that exit the computational domain have a “region of dependence” that lies entirely inside and thereby the value of the variables at the boundary must not be specified. The following boundary conditions are encountered during the simulation of an under-expanded supersonic jet**:**

Inlet: Supersonic conditions are present at the inlet. All the eigenvalues of the system at the inlet have values greater than 0. This means that they enter the domain. For such a system value for every variable viz. p, T, U needs to be specified at the inlet boundary.

Outlet: Subsonic conditions are prevalent at the outlet due to which the eigenvalue, $\lambda 1 = u - a < 0$. In order to deal with this incoming wave associated with the pressure boundary condition, non-reflective boundary conditions shall be used. The values of U and T, are allowed to float.

CONCLUSIONS

The particle trajectories calculated using CFD demonstrate that the straight nozzle geometry is more efficient towards focusing particles in an under-expanded free jet. The focusing is obtained for a very narrow range of particle diameters, which is of the order of 1 µm for the straight nozzle applied here. This performance can be characterized by an optimum Stokes number in the order of 0.6. Experimental results by Fernandez de la Mora et al [15] observed optimum focusing Stokes number in the similar range. The width of this particle beam is less than 0.1% of the nozzle diameter. Similar results were obtained by Fernandez de la Mora [15].

Dahneke and Chang [8] observed best focusing for particles with an optimum value of an inertia parameter ‘β’ which is closely related to the Stokes number. The focusing performance of the sharply converging nozzle is much less efficient than the one obtained for the straight nozzle. Even though the expansion of the gas from the reservoir pressure to the rarefied background pressure is largely independent of the nozzle geometry, the optimum separation of particles seems to be dependent to a great extent on the nozzle inlet conditions. By providing a high acceleration to the flow at its inlet due to the sudden change in cross-sectional area, the straight nozzle is better suited for this application than the converging nozzle. Moreover, straight nozzles are easier to design and fabricate. The particles that are tightly focused along the centerline can be separated from the rest of the flow by using apparatus like a skimmer or a probe placed coaxially. Most researchers note that the ideal position for such a skimmer would be at a distance upstream of the Mach disc [39, 40]. Moreover, additional focusing has been observed to have been brought about by the skimmers due to the inertial effects experienced at their inlets. We thereby conclude that aerodynamic separation of particles offers a very effective and simple way to separate and collect particles belonging to the sub-micron range.

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