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A novel model for the determination of nanoparticle impact velocity in low pressure impactors

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A B S T R A C T

The crucial parameter in the analysis of impact events is the impact velocity v_i. In case of inertial impactors v_i was assumed to be 85% of the average gas jet velocity, following the work of Marple. Numerical analysis of the impact process in low pressure impactors shows that this assumption is inappropriate and leads to overestimation of v_i near the inset of particle deposition, while v_i is underestimated in the regime of high impact velocities. In this paper the whole process of nanoparticle acceleration and impact in low pressure impactors is investigated numerically. In order to assure correct numerical procedures, the employed methods are thoroughly validated by comparison with experimental results. Finally, a new analytical model for the calculation of v_i on the basis of similarity theory is proposed that is independent of the impactor geometry and particle properties and holds well for the whole incompressible region. The model allows to perform defined collision experiments in low pressure impactors regarding impact velocity, without need of demanding numerical effort that is often beyond the scope of experimental studies. The model replaces the old rule of thumb and allows a quantitative re-evaluation of existing experimental data, e.g. on nanoparticle agglomerate fragmentation.

1. Introduction

Since its first description by Seipenbusch et al. (2002) impact fragmentation in low pressure impactors (LPI) has become a common tool in investigations of the nature and strength of bonds in nanoparticle agglomerates. This technique has been employed to study interparticular forces in airborne agglomerates of metal, ceramic and soot particles (Froeschke et al., 2003; Rothenbacher et al., 2008; Seipenbusch et al., 2007; Seipenbusch et al., 2010) to determine the degree of fragmentation as a function of the impact velocity.

However, this technique requires detailed knowledge of the particle impact velocity. This velocity can be calculated by simulation of the flow field in the LPI using common CFD methods and a subsequent calculation of the particle trajectories as explained later on in this paper. Although this is standard aerosol technology, these calculations require some computational effort and therefore are often beyond the scope of research projects. The velocity of impacting agglomerates, v_i, has so far been calculated following the work of Marple (1970), who developed and experimentally validated computational procedures for the solution of the Navier Stokes equations and the particles equation of motion in order to calculate the flow field and particle trajectories at near atmospheric pressure conditions, respectively. Marple found that for round nozzle impactors the impact

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velocity of deposited particles increases with the particle Stokes number from zero to a maximum of 85% of the average gas jet velocity and afterwards decreases again due to the lag of the particles during acceleration phase. As a first estimate this result was reduced to the assumption that particles impact on the plate with 85% of the average gas jet velocity, in order to show the feasibility of the method of agglomerate fragmentation. This estimate was retained in subsequent works for impact velocity determination, as it proved its value to retrieve qualitative information on the interaction mechanisms between nanoparticles, e.g. when combined with Weibull statistics (Seipenbusch et al., 2007). However, bond energies determined on the basis of this formula always were much greater than that predicted by theory, indicating some inadequacy of such a rough estimate for retrieving quantitative information.

Several numerical studies of inertial impactors have been performed regarding the influence of geometry and flow conditions on the collection efficiency starting from the fundamental work of Marple (1970). In case of nanoparticles under low pressure conditions less work has been done. Leduc et al. (2006) calculated the collection efficiencies of a low pressure impactor using the particle tracking option in Fluent and found good agreement for low velocities and Reynolds numbers. Arffman et al. (2011) used Fluent to calculate the flow field in the nozzle of an LPI in the compressible regime and separately calculated the particle trajectories using Lagrangian methods. They were able to predict the cut points of ELPI and QCM impactor stages with a deviation of 11% on average, compared to experimental results. As main sources of uncertainty they identified the inset of turbulence, when simulating cascade impactors under practical working conditions. However, the good agreement between experiment and theory shows clearly that the particle motion is described with reasonable accuracy by common numerical methods.

The aim of this study is to develop a general approximation for the impact velocity on the basis of similarity theory. To this end the impact velocity of nanoparticles is determined numerically. Process conditions were carefully chosen to assure that compressible effects and turbulence do not occur. The numerical model was validated by comparison of the collection efficiency curve for mono disperse particles vs. the chamber pressure. On the basis of the assumption that if the overall motion of particles is described precisely, also the underlying velocity components must be exact, the impact velocity of the particles can then be determined from the simulation data.

On the basis of the numerical results a general 1D model for the calculation of v_i is proposed, which is independent of particle properties, LPI geometry and flow conditions in the incompressible regime. The model also accounts for a possible lag of the particle motion in the acceleration zone compared to the gas velocity. Additionally, the radial distribution of impact velocities will be discussed. In order to emphasize the significance of the presented approach for the interpretation of already published impact fragmentation data, the new model is used to re-evaluate the data of the publication by Froeschke et al. (2003).

2. Theoretical background

2.1. Low pressure impactor model

A single stage low pressure impactor as first described by de la Mora et al. (1990) mainly consists of a critical orifice, which defines the aerosol mass flow into the impactor and a subsequent acceleration nozzle, directing the flow normal towards the impaction plate, where it is sharply redirected. When passing the critical orifice the aerosol will expand with hypersonic velocity. Based on CFD simulations the distance between critical orifice and acceleration nozzle was chosen large enough to give the aerosol the time necessary to relax to laminar flow conditions. Following the work of Marple (1970) for near atmospheric pressure impactors, the main geometry of an axially symmetric impactor is given by the diameter of the accelerating nozzle D, the nozzle throat length H and the plate to nozzle distance L, respectively, as shown in Fig. 1.

In order to enable the flow field for easy calculations, the gas is assumed to behave ideal, isothermal, laminar and incompressible. The axial velocity profile at the nozzle outlet is assumed to be parabolic. Then, the maximum axial gas velocity U_{max} will occur on the axis of symmetry being two times the mean gas velocity as derived from continuity equation. The jet is described by the jet Mach number, i.e. the ratio of U_{max} to the speed of sound, c_0, of the respective carrier gas, and the Reynolds number. Using the assumption made above, the jet Reynolds number can be rewritten independent of impaction pressure, p, as given in Eq. (1). As Ma depends on p (Eq. (2)) Mach and Reynolds number can be varied independently:

$$Re = \frac{U_{aver.} \cdot D \cdot \rho_{Gas}(p)}{\mu_{Gas}} = \frac{4 \cdot \dot{m}_{in}}{\pi \cdot D \cdot \mu_{Gas}} \tag{1}$$

$$Ma = \frac{8 \cdot \dot{m}_{in}}{\pi \cdot D^2 \cdot \rho_{Gas}(p) \cdot c_0} \tag{2}$$

where $\dot{m}_{in}$ denotes the aerosol mass flow rate defined by the critical orifice, μ_{Gas} is the dynamic viscosity and ρ_{Gas} the gas density. The deposition behaviour of particles in curvilinear streams due to their inertia is commonly described by means of the dimensionless Stokes number, representing the ratio of inertia force F_i to drag force F_d:

$$Stk = \frac{F_i}{F_d} = \frac{\tau \cdot U_m}{D/2} \tag{3}$$