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# CFD simulations of the Andersen cascade impactor: Model development and effects of aerosol charge

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ABSTRACT

Cascade impactors are commonly used to assess the size characteristics of aerosols in toxicology and pharmaceutical applications. These aerosol instruments have been developed and refined over decades. However, a number of questions remain related to impactor performance, including the influence of electrostatic charge on measured size distributions. The objective of this study was to develop a validated CFD model of the Mark II Andersen cascade impactor (ACI) and apply this model to evaluate the effects of particle charge on deposition. The flow field was simulated using a commercial CFD code for incompressible laminar and transitional flows. Particle trajectories and deposition were evaluated using a well tested Lagrangian tracking approach that accounts for impaction, sedimentation, diffusion, and electrostatic attraction. Particle charge levels typical of dry powder inhaler (DPI) and metered dose inhaler (MDI) aerosols were considered for a particle size range of 0.3–12 μm. As a model validation, computational predictions of cutoff $d_{50}$ diameters for each of the eight ACI stages were found to be within 10% difference of existing experimental and manufacturer data. Results indicated that charges consistent with DPI and MDI aerosols increased deposition fraction in Stages 0–3 by up to 30% and increased deposition fraction in Stages 4–7 by up to an order of magnitude. For Stages 0–3, both DPI and MDI charges reduced the $d_{50}$ value by approximately 10% or less. In contrast, charged aerosols reduced the $d_{50}$ values in Stages 4 and 5 by 200% and 60%, respectively. All charged submicrometer aerosols considered deposited in Stages 6 and 7. Increasing the particle charge by an order of magnitude from DPI to MDI values had a relatively small effect on further decreasing the cutoff size of each stage. In conclusion, these results can be used to approximate the actual aerodynamic diameter of a charged pharmaceutical aerosol based on measurements in a standard ACI. Future applications of the developed ACI model include evaluating the influence of space charge on deposition and quantifying the effects of aerosol condensation and evaporation on size assessment.



## 1. Introduction

Cascade impactors are frequently employed to evaluate the aerodynamic mass-weighted size distributions of aerosols from a variety of sources. For example, cascade impactor testing is the standard practice for determining the aerosol size distribution from respiratory drug delivery devices, such as dry powder inhalers (DPIs), metered dose inhalers (MDIs), nebulizers, and new softmist technologies (USP, 2005). Similarly, cascade impactors are frequently used to assess the size distribution of environmental

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pollutants (e.g., combustion products) and bioaerosols (e.g., airborne viruses and bacteria) (Hinds, 1999; Kittelson, 1998). An accurate determination of the size distribution for these aerosols is essential to predict inhalability, the occurrence and site of deposition in the respiratory tract, uptake into the tissue and blood, and subsequent drug effectiveness or potential adverse health effects. High flow rate ($Q \geq$ approximately 30 L/min) cascade impactors that are frequently implemented in the fields of inhaled drug delivery and toxicology include the Mark II Andersen Cascade Impactor (ACI) and the Next Generation Impactor (NGI). The NGI was developed specifically for pharmaceutical aerosol testing applications with appropriate stage cut points over a wide range of flow rates and minimal overlaps in the collection efficiency curves (Marple et al., 2003). However, the ACI remains widely used for testing aerosol size characteristics in both pharmaceutical and toxicological applications (Dunbar & Mitchell, 2005; Garmise & Hickey, 2008; Holzner & Muller, 1995; Janssens, de Gongste, Hop, & Tiddens, 2003; Longest, Hindle, Das Choudhuri, & Byron, 2007; Marple, 2004; Nichols, Brown, & Smurthwaite, 1998; Nichols & Smurthwaite, 1998; Stein, 1999, 2008; Veranth et al., 2000).

Theoretical and numerical studies have been conducted to evaluate the effects of impactor design and flow conditions on the determination of aerosol size distributions. Several primary studies described the underlying principles governing impactor design (Andersen, 1966; Cohen & Montan, 1967; Lundgren, 1967). Subsequent studies focused on improving and characterizing the performance of impactors, as well as developing impactors for specific applications (Marple, 2004; Marple & Liu, 1974; Marple & Liu, 1975; Marple & Willeke, 1976a; Rader & Marple, 1984; Swanson, Muzzio, Annapragada, & Adjei, 1996; VanOort, Downey, & Roberts, 1996; Vaughan, 1989).

Numerous experimental studies have assessed the performance of the ACI. Mitchell, Costa, and Waters (1988) experimentally studied the deposition of 10 μm particles in a calibrated Mark II ACI impactor attached to a pre-separator. This study concluded that for particles in the size range of 10 μm and above, wall losses could account for up to 20% of the total deposited mass, and that the wall losses increased significantly with moisture content of the aerosol particles. Vaughan (1989) calibrated the ACI and determined that S-shaped size distribution curves for particle deposition on individual stages and wall losses between stages compared well with the manufacturer's data. This study concluded that removing preceding stages increased wall losses, but negligibly affected the assessed size distribution. The higher end of wall losses was reported to be in the range of 20–40% of the total mass of initial particles. Dunbar, Kataya, and Tiangbe (2005) experimentally analyzed the effects of particle bounce, entrainment, and overload on uncoated impactor plates using large porous placebo particles and concluded that there were significant differences between the mass median aerodynamic diameter and geometric standard deviation of the ACI and a multistage liquid impinger. Roberts and Romay (2005) studied the ACI and NGI and recommended regular measurements of nozzle diameters on each stage of the impactor. Stein and Olson (1997) studied 14 different ACIs to test the reproducibility of particle size distribution results obtained experimentally and compared the results to theoretically obtained data. The size distributions were significantly different for various Mark II ACI impactors because of differences in stage cutoff values associated with usage and particle accumulation.

No available CFD study has considered the performance of a high flow rate impactor, such as the widely used ACI. The only previous CFD study to evaluate impactor performance was conducted by Swanson et al. (1996) for a low flow rate device (240 mL/min) with one orifice per stage, which was referred to as the PC-2 impactor. This analysis included the effects of gravity, inertia and viscous friction. Sticking probability and restitution were defined for the model and S-shaped particle deposition curves were obtained. Particles within a critical size range were observed to be trapped in recirculation zones close to the impactor walls. This study illustrates the utility of CFD analysis to evaluate and potentially improve the performance of impactors and other aerosol characterization devices. However, high flow rate impactors like the ACI and NGI can have on the order of 500 nozzles in a single stage resulting in significantly more complex flow patterns compared with a single nozzle design, especially near the collection plates (Fang, Marple, & Rubow, 1991). It is expected that interactions among the jets and differences in flow velocities and system geometries prevent the results of Swanson et al. (1996) from being directly extrapolated to analyze higher flow rate systems with multiple nozzles.

Considering the performance of impactors like the ACI, a number of open questions remain. In the airflow field, unknowns include the degree of flow distribution among jets of a single stage, the amount of flow recirculation, and airflow characteristics responsible for wall losses. Size change of aerosols within the impactor due to hygroscopic growth or evaporation is also known to influence impactor performance (Stein, 2008). However, the extent of these effects have not been fully quantified. Furthermore, standard pharmaceutical aerosols from DPI and MDI devices as well as some environmental particles are known to carry a significant electrostatic charge (Buckley, Wright, & Henshaw, 2008; Byron, Peart, & Staniforth, 1997; Kwok & Chan, 2007; Kwok, Chan, & Glover, 2005; Peart, 2001; Peart & Byron, 1999; Peart, Staniforth, & Meakin, 1995). Aerosol charge is reported to have an effect on deposition in aerosol generation (Janssens et al., 2004; Mitchell, Coppolo, & Nagel, 2007) and sampling (de Juan et al., 1997) devices, the mouth-throat region (Ali, Reddy, & Mazumder, 2007), as well as in the lungs (Balachandran, Kulon, Koolpiruck, Dawson, & Burnel, 2003; Cohen, Xiong, Asgharian, & Ayres, 1995; Cohen, Xiong, Fang, & Li, 1998) based on image and space charge effects (Finlay, 2001). However, the extent of aerosol charge on deposition in the ACI has not been quantified. As a result, size sampling un-neutralized aerosols with an ACI may produce a size distribution that is affected by both the particle aerodynamic diameter and electrostatic effects in the impactor. These impactor performance issues are difficult to address and quantify using only experimental techniques. However, a CFD model of the ACI can readily determine the internal airflow characteristics, the effects of recirculation on wall losses, and the effects of aerosol charge on deposition.

The objective of this study is to develop a validated CFD model of the Mark II Andersen cascade impactor that can be used to assess performance and highlight internal transport characteristics. Validation of the CFD model is based on comparisons