Stochastic modeling of classifying aerodynamic lenses for separation of airborne particles by material and size

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\textbf{ABSTRACT}
A novel method to separate airborne particles by size and material is presented. The particles are separated via a setup of aerodynamic lens orifices. Varying the size of the orifices, the focusing pressure and the mass flow rate through the lens, leads to focusing of particles of distinct aerodynamic properties on the central axis. The separation process is transferred into a stochastic model, which uses a transfer function to describe the passage probability of particles. The distribution of feed particles and the changes of the distribution itself is described via probability densities. The modeling process is applicable to various kinds of separation methods and allows to optimize construction and operation parameters. To this end the model utilizes flexibly defined separation performance measures which are illustrated in a case study which considers the separation of Cu particles from SiO\textsubscript{2} particles. The spherical particles in the considered virtual mixtures are described by their log-normally distributed diameters and their normally distributed mass densities. Furthermore, the cases are selected in such a manner that the mean aerodynamic diameters of both Cu and SiO\textsubscript{2} particles are equal. The results of this study indicate that the aerodynamic ambiguity can be resolved when the operation and construction parameters are optimized via stochastic modeling. Even the inaccuracy of the separation process — the width of the transfer function — can be advantageous.

\textbf{KEYWORDS}
aerodynamic sampling; material separation; aerosol; stochastic modeling; aerodynamic lens; classifying aerodynamic particle sizer

1. Introduction

From the very beginning, when mankind melted ore and forged it into crude shapes, up to the sophisticated semiconductor engineering of today, the purity of the source materials has and always will be critical for the quality of the product made from these materials. Thus, the separation of mixed materials is a problem common to different industry sectors and applied sciences. The mixture of materials is often broken down into smaller parts, which are subsequently separated into value and waste material. When exposed to influences like buoyancy or inertia, the different physical and chemi-
cal properties of these parts lead to different behavior, which consequently is exploited in the design of separation processes. Even though the purity of the separated target material can be high, the waste material, often present in form of microscopic particles, can still contain non-negligible amounts of target material. A cost-efficient, scalable solution to separate mixtures of such particles is presented and theoretically analyzed in this work.

1.1. Background

Dispersed within a gaseous phase, particles are usually classified by their size. But when we want to separate them by material, their different densities provide the leverage we need. Before we introduce our approach in detail, we take a look at different methods for aerodynamic separation of particles, while delivering some needed background.

1.1.1. Ambiguity in aerodynamic separation

As an example we consider an impactor – a device commonly used for separation of airborne particles: An aerosol flowing through a pipe is exposed to a rapid change in the flowing conditions, when a plate is introduced at an orthogonal angle into the flow. The gas molecules follow the new flowing conditions and thus predetermine the streamlines on which the particles circumvent the obstacle. Whether a particle is able to follow the streamlines or whether it will impact on the surface of the plate is usually described via the dimensionless Stokes number Stk given by

\[ \text{Stk} = \frac{\tau_p u}{\ell} \]  

(1)

where \( \ell \) is the length of the obstacle, \( u \) is the gas velocity and \( \tau_p \) the particle relaxation time, describing the time a body needs to adapt to changing flow conditions. The particle relaxation time \( \tau_p \) depends on the particle density \( \rho_p \) and the volume equivalent diameter \( d_p \), and is given by

\[ \tau_p = \frac{\rho_p d_p^2 C_c(d_p)}{18 \eta}, \]  

(2)

where \( \eta \) is the viscosity of the gas and \( C_c \) the Cunningham correction. (Friedlander (2000); Willeke (2011)). Smaller, lighter particles possess a Stokes number Stk \( \ll 1 \) and thus follow the streamlines perfectly. Bigger and denser particles with higher Stokes numbers will collide with the surface of the impactor. This behavior can be modeled by a transfer function which describes the probability of a particle passing the CAL, depending on the particle’s Stokes number. The transfer function of an impactor is described using an integral curve. The impactor is comparable to a sieve, keeping particles over a certain size in, while letting all particles under this size pass through. This crossover point is called Stk_{50}, for which particles with this Stokes number possess a 50 % chance to pass the impactor. The slope of the transfer function describes how precisely the impactor is working. Ideally the transfer function would just be a step function, but in reality separation is never this kind of perfect. There is an additional ambiguity involved which is not often discussed: Equation (2) is not bijective, so that
there will be cases where particles with distinguishable size and density possess equal particle relaxation time, equal Stokes number and thus equal aerodynamic properties. This ambiguity can be described by the aerodynamic diameter $d_a$ which is given by

$$d_a = d_p \sqrt{\frac{\rho_p}{\rho_0}},$$

(3)

where $d_p$ is the volume equivalent diameter of a particle with mass density $\rho_p$ and $\rho_0$ is the unit density (Willeke (2011)). The aerodynamic diameter describes the diameter of a sphere of unity density, which behaves aerodynamically equally to the particle in question.

Even though non-spherical particles are not within the scope of this work, equivalent diameters are a useful tool, for describing particles, because they contain information about the behavior of the particle in a prescribed situation. For example, the hydrodynamic diameter is based on the movement of a particle in a solution, and thus takes hydration into account. The measured diameter of one and the same particle can vary, depending on the type of measurement. Even when high-resolution imaging techniques like scanning electron microscopy (SEM) are used, the measured diameter varies depending on the perspective, because particles are only in the rarest of cases perfect spheres, which they are often assumed to be. For the purpose of the present paper, the particle diameter $d_p$ refers to the volume equivalent diameter if not stated differently.

1.1.2. Classifying aerodynamic lenses

Classical impactors provide an easy to understand model for aerodynamic separation, but have the disadvantage of losing the impacted fraction from the gas stream. There are multiple approaches to counter this drawback, like virtual impactors and similar devices (Marple and Chien (1980)). In this work we rely on the separating capabilities of classifying aerodynamic lenses (CAL). Aerodynamic lenses are often applied to focus aerosols into a thin, particular beam (Liu et al. (1995)). An aerosol is injected into the center of a radial symmetrical pipe and often encased in sheath air. The aerodynamic lens contains an orifice leading to a temporary flow contraction, thus focusing the stream of the aerosol. In contrast, a classifying aerodynamic lens behaves more like a prism than a lens: The aerosol is injected at a well-defined radial area offside the centerline of the pipe, which results in a separation of the particles after they passed through the lens, due to their distinct relaxation time $\tau_p$. This behavior is enabled by the same principle as for the classical impactor. Before passing through the lens, the aerosol must follow the narrowing stream lines. Once passed through, the stream lines shift again, to accommodate for the space that is now available. Like in the impactor inertia plays a vital role here, because depending on its inertia, a particle will either stay on its original streamline, which is the direction that was determined while passing through the lens, or it will either partially or fully adapt to the new streamline. The consequence is that particles, possessing a specific relaxation time $\tau_L$, characterized by the flowing conditions and the design of the lens, will be focused right on the centerline of the CAL. Lighter and smaller particles will follow the new streamline, while larger, denser particles will not adapt to the new streamline and move towards the walls of the pipe. The part of the aerosol, that is focused on the centerline however is collected via an orifice, which we will call the sampler. This separation process (depicted in Figure 1) results in a transfer function different from the transfer function of the impactor.
Figure 1. Working principle of a classifying aerodynamic lens (CAL) according to Babick et al. (2018): The aerosol is injected into a stream of sheath gas at a defined radial position. After passing the lens, only particles with Stokes numbers close to Stk \( \approx 1 \) are collected via the sampler (dash-dotted green or blue line).

The new function shows classifying behavior, thus the name “classifying aerodynamic lens”.

Using this classifying characteristic it is possible to separate a “mono-aerodynamic” aerosol. Another device having similar capabilities is the “Differential Mobility Analyzer” (DMA). The DMA separates particles based on their mobility, when passing through an electrical field, thus creating a “mono-mobil” aerosol. The DMA has become somewhat of a gold-standard in aerosol science, but it has one drawback: For the DMA to work properly the particles have to be charged. Particles bigger than 100 nm often carry multiple charges, introducing another ambiguity of particles.

Different CALs target different particle relaxation times. The relaxation time \( \tau_L \) of a particle which is optimally focused by a CAL is given by

\[
\tau_L(d_L, \dot{Q}_v, p) = \frac{\text{Stk}_o \cdot \pi d_L^3 \cdot p}{\dot{Q}_v},
\]

(4)

where \( \tau_L \) depends on the diameter of the lens \( d_L \), the volume flow \( \dot{Q}_v \) through it, and the pressure \( p \). Equation (4) allows to calculate the relaxation time of the focused particles, when an appropriate value for the optimal Stokes number \( \text{Stk}_o \) is known (Wang et al. (2005)). For micro and sub micron particles the optimal Stokes number is close to unity. For nanoparticles, however, lower values of \( \text{Stk}_o \) have been reported (Wang et al. (2005)).
1.2. Previous research

One of the first theoretical works regarding aerodynamic focusing has been done by de La Mora and Riesco-Chueca (1988). They emphasize the most salient features of aerodynamic focusing and conclude that it might be the basis for new aerosol measurement techniques. In 1993, La Mora together with Rao et al. (1993) continued investigating the focusing of particles in viscous jets, showing that focusing is possible even when the flow conditions are not laminar. Two years later, Liu et al. (1995) published a two part paper, which to date still accomplishes to be the most cited paper in the topic of aerodynamic lenses. Liu et al. (1995) use a dimensionless contraction factor to characterize the focusing quality of aerodynamic lenses and describe in detail the factors that contribute to the broadening of particle beams. Mallina et al. (1999) describe the rapid single-particle mass spectrometry technique, for analyzing the chemical content of ultrafine aerosols, including a particle inlet, which is able to transmit particles of different sizes, by varying the nozzle pressure – a principle that is similar to the approach utilized in the present work. A thorough numerical investigation of particle trajectories in aerodynamic lenses is performed by Zhang et al. (2002). They found that the contraction of a focused particle is highest at a Stokes number smaller, but close to one. At higher Stokes numbers, significant impact losses occurred. Lee et al. (2003) investigated the performance of aerodynamic lenses numerically and experimentally, concluding that at Reynolds numbers between 300 and 700 a strongly focused beam is obtainable. Wang et al. (2005) proposed a procedure for designing aerodynamic focusing lenses for small particles, based on numerical simulations. In their algorithm, design decisions are dictated by the minimum reachable pressure. The pressure limit is introduced by the available equipment. Having a general guideline to follow is a prerequisite for this work. One year later Wang & McMurry released a tool for designing aerodynamic lenses, which uses an optimal Stokes number for focusing nanoparticles that was calculated beforehand via CFD simulations (Wang and McMurry (2006)). Whether this Stokes number is also best for micro particles is still subject of ongoing investigations. One of the most recent works on aerodynamic focusing stems from Ruiz et al. (2014), who investigated the effect of low material density on the focusing of small particles. In the run-up to this work, other authors like Lee et al. (2008) mainly considered focusing very small nanoparticles < 50 nm. In 2018, a new device to measure the aerodynamic diameter of nanoparticles was characterized as part of a project on multiparameter characterization of aerosols (MPAC) (Babick et al. (2018)). The Differential Aerodynamic Particle Sizer (DAPS) is based on the previously described principle of classifying aerodynamic lenses. While scanning through a range of different working pressures, the DAPS is able to focus different particle sizes, thus selecting a specific nearly monodisperse particle fraction for further investigation.

2. Theory

2.1. Design challenges

There are several challenges to overcome when setting up a separation experiment with classifying aerodynamic lenses. The most important parameters are focusing pressure $p$, mass flow $\dot{Q}_m$ and the diameter of the CAL orifice $d_L$, which influence the relaxation time $\tau_L$ of the particles focused by the lens given in Equation (4). Even when the importance of additional details, such as the geometric shape of nozzles and sampler
and the radial position of the aerosol inlet, are neglected, the interdependence of pressure, mass flow and orifice diameter creates a complex optimization problem. To focus particles with given size and density the characteristic relaxation time of the particle $\tau_p$ must be equal to the relaxation time $\tau_L$ of particles focused by the lens. Combining Equations (2) and (4) the following formula is obtained:

$$d_L = \left( \frac{2\rho_p d_p^2 C(p, d_p) \dot{Q}_m}{9\pi \rho_g \eta \text{Stk}_o} \right)^\frac{1}{3},$$

(5)

where $\rho_g$ is the gas density and all dimensions are given in SI Units. Note that for every particle of volume equivalent diameter $d_p$ and density $\rho_p$, there are infinitely many possible combinations of pressure $p$, mass flow $\dot{Q}_m$ and the lens diameter $d_L$ that focus the particle and thus allow to separate it from particles with deviating diameter or density.

We investigate constraints on the lens parameters $p, \dot{Q}_m, d_L$, in order to describe the space of valid parameter configurations. As stated by Wang et al. (2005) focusing of small particles is not possible, when certain limits for Reynolds $Re$, Mach $Ma$ and Knudsen $Kn$ numbers are exceeded, where the limits are denoted by $Re_c, Ma_c$ and $Kn_c$, respectively. Additionally, the available pumping capacity is a further limiting factor. The equations for computing $Re, Ma, Kn$ and their respective critical values given by Wang et al. (2005) are provided below. The Reynolds number $Re$ is calculated via the mass flow rate of the gas $\dot{Q}_m$ by

$$Re = \frac{\rho_g(p) \cdot \bar{u} \cdot d_L}{\mu_g} = \frac{4 \cdot \dot{Q}_m}{\pi \mu_g d_L} < 200 = Re_c,$$

(6)

where $\mu_g$ is the gas viscosity. The Mach number $Ma$, given by

$$Ma = \frac{u}{c_g} < 1 = Ma_c,$$

(7)

compares gas velocity $u$ with the velocity of sound $c_g$ in the gas. The Knudsen number $Kn$, which indicates whether a fluid flows as a continuum is given by

$$Kn = \frac{2 \cdot \lambda_g(p)}{d_L} < 0.1 = Kn_c,$$

(8)

where $\lambda_g$ is the mean free path of the gas.

The pumping capacity mentioned above limits the volume flow rate that can be pumped out of the system at a given pressure. In this work we use measurements from a rotary vane pump (RUVAC 1001 Leybold) as exemplary data. This limits the pressure range to values between $10^1$ and $10^5$ Pa. The pressure dependent volume pump rate $S_0$ handled by the rotary vane pump is depicted in Figure 2a. The actual mass flow $S_m$, which the pump is able to handle, is calculated from the fit and is given by

Figure 2a indicates a minimum pressure of 5 Pa, but pressure drop may be an issue, even if connections are kept as short as possible.
Figure 2. a) Fitted pumping speed curve for the RUVAC 1001, original data was extracted graphically from Leybolds product catalog (Leybold GmbH (2018)) b) Parameter space (grey volume) delimited by Reynolds limit Re₉ = 200, Mach limit Ma₉ = 1, Knudsen limit Kn₉ = 0.1, and pumping speed limit.

\[ S_m = S_0 \cdot \rho_g \cdot (p/p_0) \cdot (T_0/T), \]  

where \( p_0 = 101325 \) Pa is the standard pressure and \( T_0 = 263.15 \) K is the standard temperature. Note that both the volume pump rate \( S_0 \) and the density of the gas \( \rho_g \) depend on pressure.

When we apply the constraints that result from the calculation of the critical values for \( \text{Re}_c, \text{Ma}_c, \text{Kn}_c \) and the pumping capacity, we are left with all feasible combinations of pressure, flow rate and lens diameter. Using Equation (4) we can calculate the values of \( \tau_p \) belonging to the constrained parameter space, as shown in Figure 2b. For every particle with density \( \rho_p \) and diameter \( d_p \), there exists a surface, see Equation (5), in the 3D parameter space of pressure \( p \), lens diameter \( d_L \) and mass flow \( \dot{Q}_m \) such that the particle is optimally focused. Due to the constraints for the lens parameters given by Equations (6)-(8) the surface can be empty, but in our application there are usually a multitude of combinations of \( p, d_L \) and \( \dot{Q}_m \) which satisfy the constraints and for which the particle is optimally focused.

For a given particle system with various density \( \rho_p \) and diameter \( d_p \) configurations the question of the optimal parameter combination is reduced to the question: “Which point on the plane leads to the best performance?” Thus, we have to define measures for the separation performance that enable us to analyze the outcome of the experiments in theory for a given application. Since the goal of the CAL is to separate particles composed of value materials from non-value materials, e.g., particles with a large density like Cu from low density materials like SiO₂, the performance measures have to reflect this. In the present paper we will mainly consider the product yield \( Y_p \), the enrichment \( E \) and the yield of value material \( Y_v \). The definition of these measures is given within Chapter 3.3.

Once a set of lens geometry and operating parameters is chosen, the manufacturing and testing of the prototype is costly in time and money. And there still is the risk that the set up does not work in the intended way, which involves more calculations, redesigning and manufacturing again. To minimize the risk, it is usually good practice to simulate the separation process that would be manufactured, using numerical
fluid dynamics and particle trajectory analysis. However, CFD simulations of CALs are difficult, because they make use of critical orifices. These possess high aspect ratios and creating appropriate meshes is an elaborate process. This means that there is a need for a fast, reliable prediction method. The present paper utilizes stochastic models for predicting the most promising setup. For that purpose, based on Equation (4), we propose a stochastic description of CALs, which provides a realistic probability for passing through a lens to the particles based on their relaxation time. The passing probability is highest for particles for which $\tau_p \approx \tau_L$ holds. Furthermore, we describe incoming particle mixtures stochastically with the help of two-dimensional probability distributions for the random vector of particle size and mass density. By combining such probability distributions with the stochastic description of CALs we are able to determine the distribution of size and mass density for outgoing particles. Moreover, this approach makes it possible to derive formulas for the performance measures $Y_P$, $E$ and $Y_v$, such that fast numerical computation of performance measures for arbitrary lens parameters and particle mixtures, represented by two-dimensional probability distributions, is possible. Thus, the performance measures can be maximized efficiently for any known particle mixture by finding optimal operating parameters for the CAL. Last but not least, we conduct a case study for exemplary Cu-SiO$_2$ particle mixtures, for which we compute performance measures and investigate several optimization strategies.

3. Methods

In the following sections we first translate the problem at hand into the concise language of mathematics, so that it subsequently can be considered in a stochastic setting. In a first step we describe a CAL as a stochastic model which provides a probabilistic rule on the basis of a known transfer characteristic. In a second step we describe particle mixtures by stochastic models, i.e., a particle mixture is described by the joint distribution of particle size and mass density. By combining the stochastic description of particle mixtures with the stochastic model of the CAL we obtain an analytical description of the size-mass density distribution of particles that pass through the CAL. Furthermore, this approach allows us to calculate measures which will quantify the separation performance.

3.1. Classifying aerodynamic lens as a stochastic model

The relaxation time $\tau$ of a particle with size $d_p$ and mass density $\rho_p$ is given by

$$\tau(d_p, \rho_p) = \frac{\rho_p d_p^2 C_r(p, d_p)}{18 \eta},$$

see Equation (2), where $p$ is the pressure at which the CAL operates. The particle is focused by the CAL with relaxation time $\tau_L$ if

$$\tilde{\tau}(d_p, \rho_p) = \frac{\tau(d_p, \rho_p)}{\tau_L} = 1.$$  

We call $\tilde{\tau}(d_p, \rho_p)$ the normalized relaxation time of the particle. The set of configurations $\{(d_p, \rho_p) \in \mathbb{R}_+^2 : \tilde{\tau}(d_p, \rho_p) = 1\}$ which fulfill Equation (11) form a curve. These
so-called iso-τ lines are visualized in Figure 3a for three different pressures $p$, while the remaining lens parameters $Q_m$ and $d_L$, which influence the lens relaxation time $\tau_L$, are kept constant in the visualized three scenarios. An “optimal” lens would solely separate particles for which the tuples $(d_p, \rho_p)$ belong to the CAL’s iso-τ line, i.e., which fulfill Equation (11). However, particles with $\tilde{\tau}(d_p, \rho_p)$ values close to 1 can be separated with some probability. To model this, we define a trapezoidal transfer function $\Omega$: $(0, \infty) \rightarrow [0, 1]$ by

$$\Omega(\tilde{\tau}) = \frac{1}{2\beta(1-\delta)} (|\tilde{\tau} - (1+\beta)| + |\tilde{\tau} - (1-\beta)| - |\tilde{\tau} - (1+\beta\delta)| - |\tilde{\tau} - (1-\beta\delta)|), \quad (12)$$

where $\beta, \delta$ are model parameters. The transfer function $\Omega$ is taken from the work of Stolzenburg and McMurry (2008), where it is used to describe the behavior of differential mobility analyzers. Figure 3b shows such a transfer function $\Omega$ with parameters $\beta = 0.4$ and $\delta = -0.25$. The value $\Omega(\tilde{\tau})$ describes the probability that a particle with normalized relaxation time $\tilde{\tau}$ passes through the CAL. Furthermore, the transfer function $\Omega$ is symmetrical around $\tilde{\tau} = 1$, while the parameter $\beta$ controls the width of the trapezoid transfer function. For wider transfer functions particles with $\tilde{\tau}$ values different from 1 can pass through the lens more easily. The parameter $\delta$ influences the height of the trapezoid, which influences how likely particles with normalized relaxation times $\tilde{\tau} = 1$ pass through the lens.

By combining Equations (11) and (12) we obtain the transfer probability function $T_L$: $(0, \infty)^2 \rightarrow [0, 1]$ of a lens with relaxation time $\tau_L$ and transfer function $\Omega$ by

$$T_L(d_p, \rho_p) = \Omega(\tilde{\tau}(d_p, \rho_p)) = \Omega\left(\frac{\tau(d_p, \rho_p)}{\tau_L}\right). \quad (13)$$

The value of $T_L(d_p, \rho_p)$ is the probability that a particle with size $d_p$ and mass density $\rho_p$ passes through the lens, see Figure 3c. It can be considered as a two-dimensional transfer function which describes the separation behavior of a CAL with respect to particle size and mass density.
3.2. Stochastic modeling of the separation process

In the previous section we gave a stochastic description of DALs in the form of transfer probability functions $T_L$. On the other hand, particle mixtures themselves can be described by two-dimensional probability distributions, i.e., the relevant particle descriptors size $d_p$ and mass density $\rho_p$ of a particle mixture can be described by means of their joint distribution. More precisely, let $(D, R)$ be a random vector consisting of size $D$ and mass density $R$ of a random particle. In many applications the distribution of the random vector $(D, R)$ can be described by its two-dimensional probability density $f : \mathbb{R}^2 \to [0, \infty)$ whose values have the unit m$^2$/kg, i.e., we assume that $(D, R)$ is absolutely continuous. This allows us to derive various properties of particle mixtures, like for example the relative frequency of particles in the mixture with size $d_p \in [a, b]$ by computing

$$
\mathbb{P}(D \in [a, b]) = \mathbb{P}((D, R) \in [a, b] \times \mathbb{R}) = \int_0^b \int_a^b f(d, \rho) \, dd \, d\rho.
$$

(14)

The two-dimensional probability density $f$ of mixtures of two types of dispersed particles, denoted by $A$ and $B$, with two-dimensional probability densities $f_A$ and $f_B$, respectively, can then be modeled by

$$
f(d, \rho) = \lambda f_A(d, \rho) + (1 - \lambda) f_B(d, \rho),
$$

(15)

where the parameter $\lambda \in [0, 1]$ describes the mixing ratio of particles of type $A$ and $B$. Figure 4a depicts such a probability density of a particle mixture of Cu and SiO$_2$ where the task of a CAL will be to separate the desired Cu particles from SiO$_2$. Note that Figure 4a shows a bimodal probability density, where the mode centered at the mass density of 8900 kg/m$^3$ originates from the Cu particles. The red line depicts an iso-$\tau$ line of a CAL. Since the iso-$\tau$ line avoids the mode of the probability density induced by SiO$_2$ particles, it can be expected, that the separation task will be performed rather well. We already mentioned that a CAL does not only separate particles whose size-mass density configurations $(d_p, \rho_p)$ are located on the iso-$\tau$ line, but also particles whose size-mass density configurations are in the vicinity of this line. The transfer probability function $T_L$ of a CAL takes this effect into account.

Using the transfer probability function $T_L$, we can compute the probability $c_L$ that a particle, selected at random among all particles, with random size-mass density vector $(D, R)$ passes through a CAL. For this purpose, we introduce an additional random variable $U$ which is uniformly distributed on the unit interval $[0, 1]$ and stochastically independent of $(D, R)$. Then, the event that the random particle passes the CAL can be equivalently described by the event that the inequality

$$
T_L(D, R) \geq U
$$

(16)

holds. Note that for deterministic $D$ and $R$ the probability $c_L$ of the event $T_L(D, R) \geq U$ is the value of the transfer probability $T_L(D, R)$ itself. On the other hand, for a

\footnote{An absolutely continuous real-valued random variable $X$ has a probability density $f_X : \mathbb{R} \to [0, \infty)$ such that the probability of the event that the values of $X$ belong to some interval $[a, b] \subset \mathbb{R}$ is given by $\mathbb{P}(X \in [a, b]) = \int_a^b f_X(x) \, dx$. Analogously, an absolutely continuous random vector $X = (X_1, X_2)$ has a probability density $f_X : \mathbb{R}^2 \to [0, \infty)$ such that $\mathbb{P}(X_1 \in [a_1, b_1], X_2 \in [a_2, b_2]) = \int_{a_1}^{b_1} \int_{a_2}^{b_2} f_X(x_1, x_2) \, dx_2 \, dx_1$ holds (Jacod and Protter (2003); Karr (1993)). Note that the probability density $f_X$ is normalized, i.e., $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_X(x_1, x_2) \, dx_2 \, dx_1 = 1$ holds.}


random size-mass density vector \((D, R)\) with joint density function \(f\), this probability is given by

\[
c_L = \mathbb{P}(T_L(D, R) \geq U) = \int_0^\infty \int_0^\infty f(d, \rho) T_L(d, \rho) \, d\rho \, dd,
\]

where \(\mathbb{1}\) denotes the indicator function which is defined by

\[
\mathbb{1}_{T_L(d, \rho) \geq u} = \begin{cases} 
1, & \text{if } T_L(d, \rho) \geq u, \\
0, & \text{if } T_L(d, \rho) < u.
\end{cases}
\]

Moreover, it is possible to determine the two-dimensional probability density \(\tilde{f}\) of the vector \((\tilde{D}, \tilde{R})\), which describes the random size \(\tilde{D}\) and density \(\tilde{R}\) of those particles which pass through the lens. The distribution of this random vector is equal to the conditional distribution of \((D, R)\) under the condition that the random particle described by the vector \((D, R)\) passes through the CAL. By computing the probability that the value of \((D, R)\) belongs to a rectangle \(C_1 \times C_2 \subset \mathbb{R}^2\), where \(C_1, C_2 \subset \mathbb{R}^2\) are some intervals, it is possible to determine the probability density \(\tilde{f}\) of \((\tilde{D}, \tilde{R})\). Namely, it holds that

\[
\mathbb{P}(\tilde{D} \in C_1, \tilde{R} \in C_2) = \mathbb{P}(D \in C_1, R \in C_2 \mid T_L(D, R) \geq U) = \frac{1}{c_L} \int_{C_1} \int_{C_2} f(d, \rho) T_L(d, \rho) \, dd \, d\rho.
\]

Thus, the probability density \(\tilde{f}\) of the random size-mass density vector \((\tilde{D}, \tilde{R})\) of those particles which pass through the lens is given by

\[
\tilde{f}(d, \rho) = \frac{1}{c_L} f(d, \rho) T_L(d, \rho).
\]

The conditional probability density \(\tilde{f}\) is visualized in Figure 4b for the input probability density \(f\) shown in Figure 4a.
3.3. Evaluating the separation performance

We now introduce some further quantities in order to evaluate the quality of separation. Figure 5 shows how these quantities are denoted: The mass fractions of the feed are labeled with the subscript \( F \). Value material is labeled with \( v \), while non-value material is labeled with \( \text{nv} \). Thus, the mass \( m_F \) of the feed material consists of the mass \( m_{v,F} \) of the value material in the feed and the mass \( m_{\text{nv},F} \) of the non-value material. The feed is separated in product and waste fractions denoted by \( P \) and \( W \), respectively.

\[
\begin{align*}
\text{feed } F & \quad \text{separation} & \quad \text{product } P \quad \text{waste } W \\
m_F &= m_{v,F} + m_{\text{nv},F} & m_P &= m_{v,P} + m_{\text{nv},P} \\
m_W &= m_{v,W} + m_{\text{nv},W}
\end{align*}
\]

**Figure 5.** The feed \( F \) is separated into the product \( P \) and the waste \( W \). Desired fractions are marked by \( v \) and undesired fractions by \( \text{nv} \). The terms “product” and “waste” are used only to better distinguish the two separated fractions by name.

Furthermore, we consider the feed purity \( P_F \), product purity \( P_P \) and product yield \( Y_P \) which are defined as follows:

\[
P_F = \frac{m_{v,F}}{m_F} = \frac{m_{v,F}}{m_{\text{nv},F} + m_{v,F}}, \quad (18)
\]

\[
P_P = \frac{m_{v,P}}{m_P} = \frac{m_{v,P}}{m_{\text{nv},P} + m_{v,P}}, \quad (19)
\]

\[
Y_P = \frac{m_P}{m_F} = \frac{m_{v,P} + m_{\text{nv},P}}{m_{\text{nv},F} + m_{v,F}}, \quad (20)
\]

The ratio of product purity \( P_P \) divided by feed purity \( P_F \) describes the gain in purity, or, in other words, the enrichment \( E \) of value material in the product \( P \), i.e.,

\[
E = \frac{P_P}{P_F}. \quad (21)
\]

Multiplying the enrichment \( E \) with the product yield \( Y_P \) gives a measure for the yield of value material \( Y_v \), i.e.,

\[
Y_v = EY_P = \frac{m_{v,P}}{m_{v,F}}. \quad (22)
\]

In the present paper, we will quantify the separation performance by mainly considering the product yield \( Y_P \) and the yield of value material \( Y_v \). These quantities are
normalized and take values in the interval $[0, 1]$, where values close to 1 indicate good separation results.

Having in mind the stochastic description of both the in-going particle mixtures and the CAL introduced in Sections 3.1 and 3.2, it is possible to estimate performance measures using Monte Carlo simulation (Asmussen and Glynn (2007); Kroese et al. (2013)). Therefore, for some $n > 1$, we consider the random vectors $(D_1, R_1), (D_2, R_2), \ldots, (D_n, R_n)$ with joint probability density $f$ which represent $n$ in-going random particles. Note that the mass $m(D_i, R_i)$ of the $i$-th random particle described by the random size-mass density vector $(D_i, R_i)$ is given by

$$m(D_i, R_i) = \frac{\pi}{6} D_i^3 R_i$$

for each $i = 1, \ldots, n$ and thus the (random) mass $m_F$ of the $n$ ingoing random particles is given by

$$m_F = \sum_{i=1}^{n} m(D_i, R_i) = \frac{\pi}{6} \sum_{i=1}^{n} D_i^3 R_i.$$  (24)

To decide whether the $i$-th random particle goes through the considered CAL with transfer probability function $T_L$, we consider an additional uniformly distributed random variable $U_i$ on the unit interval $[0, 1]$. Recall that the particle passes the CAL if $U_i \leq T(D_i, R_i)$ holds, see Inequality (16). Thus, the (random) mass $m_P$ of particles in the product is given by

$$m_P = \frac{\pi}{6} \sum_{i=1}^{n} D_i^3 R_i \mathbb{1}_{U_i \leq T(D_i, R_i)}.$$  (25)

To measure the separation performance we have to distinguish between particles comprised of value and non-value materials. Therefore, we consider a predefined interval $C_v \subset (0, \infty)$, which describes the range of mass densities associated to the value material. Therefore, a random particle with size and density $(D_i, R_i)$ is considered to be comprised of the value material if $R_i \in C_v$. With this definition of the value material, we can formulate the mass $m_{v,F}$ of value material in the feed as

$$m_{v,F} = \frac{\pi}{6} \sum_{i=1}^{n} D_i^3 R_i \mathbb{1}_{R_i \in C_v},$$  (26)

and, analogously, the mass $m_{v,P}$ of value material in the product is given by

$$m_{v,P} = \frac{\pi}{6} \sum_{i=1}^{n} D_i^3 R_i \mathbb{1}_{R_i \in C_v, U_i \leq T(D_i, R_i)}.$$  (27)

By inserting the formulas given in Equations (24) - (27) into the definitions considered in Equations (18) - (22) of our performance measures, we can estimate the separation performance. For instance, an estimator $\hat{Y}_P$ for the product yield $Y_P$ is given by

$$\hat{Y}_P = \frac{\sum_{i=1}^{n} R_i D_i^3 \mathbb{1}_{U_i \leq T(D_i, R_i)}}{\sum_{i=1}^{n} R_i D_i^3},$$  (28)
which can be used via Monte Carlo simulation of the random vectors 
\((D_1, R_1), \ldots, (D_n, R_n)\). However, this approach can be relatively expensive, especially if the lens parameters \(p, d_L, \dot{Q}_m\) have to be optimized to maximize some performance measure, like the enrichment \(E\), for a given distribution \(f\) of size-mass density vectors of incoming particles. To overcome this, we utilize the stochastic model of CALs described in Sections 3.1 and 3.2, in order to derive theoretical formulas for the computation of performance measures in the case of infinitely many incoming random particles. Due to the law of large numbers (Jacod and Protter (2003); Karr (1993)) we have

\[
\frac{1}{n} \sum_{i=1}^{n} m(D_i, R_i) \xrightarrow{n \to \infty} \mathbb{E}[m(D, R)] = \int_{0}^{\infty} \int_{0}^{\infty} m(d, \rho) f(d, \rho) d\rho dd, \tag{29}
\]

and, analogously,

\[
\frac{1}{n} \sum_{i=1}^{n} m(D_i, R_i) \mathbb{1}_{T_L(D, R) \geq U} \xrightarrow{n \to \infty} \mathbb{E}[m(D, R) \mathbb{1}_{T_L(D, R) \geq U}] = \int_{0}^{\infty} \int_{0}^{\infty} m(d, \rho) f(d, \rho) T_L(d, \rho) d\rho dd, \tag{30}
\]

\[
\frac{1}{n} \sum_{i=1}^{n} m_{v,F} \xrightarrow{n \to \infty} \mathbb{E}[m(D, R) \mathbb{1}_{R \in C_v}] = \int_{0}^{\infty} \int_{C_v} m(d, \rho) f(d, \rho) d\rho dd, \tag{31}
\]

\[
\frac{1}{n} \sum_{i=1}^{n} m_{v,P} \xrightarrow{n \to \infty} \mathbb{E}[m(D, R) \mathbb{1}_{T_L(D, R) \geq U} \mathbb{1}_{R \in C_v}] = \int_{0}^{\infty} \int_{C_v} m(d, \rho) f(d, \rho) T_L(d, \rho) d\rho dd, \tag{32}
\]

where \(\mathbb{E}\) denotes the expectation. Thus, the random variables considered in Equations (29) - (32) converge to deterministic limits. The integral representations of the limits in Equations (29) - (32) allow the numerical computation of the mass values of feed and product. Similarly, we can represent the limits of the separation performance measures given in (18) - (22) via integrals. For example, the limit or, equivalently, the expected value of the product purity \(P_P\) for infinitely many particles is given by

\[
P_P = \frac{m_{v,P}}{m_P} = \frac{1}{n} \sum_{i=1}^{n} m_{v,P} \xrightarrow{n \to \infty} \frac{1}{n} \int_{0}^{\infty} \int_{C_v} m(d, \rho) f(d, \rho) T_L(d, \rho) d\rho dd = \mathbb{E}P_P, \tag{33}
\]

for \(n \to \infty\). The expected values for the remaining performance measures can be derived analogously to (33). In the following, we will denote the expected values \(\mathbb{E}P_F, \mathbb{E}P_P, \mathbb{E}Y_F, \mathbb{E}E, \mathbb{E}Y_v\) simply by \(P_F, P_P, Y_F, E, Y_v\), respectively.

The formulas given in Equations (29) - (32) allow the numerical computation of expected performance measures for feed particle mixtures. More precisely, for any two-dimensional probability density \(f\), which describes the distribution of size-mass density of feed particles going through a CAL with transfer probability function \(T_L\), we can numerically compute the measures \(P_F, P_P, Y_F, E, Y_v\). By varying the lens parameters we can find suitable choices of operating parameters \(p, d, \dot{Q}_m\) which optimize the separation quality with respect to one or several performance measures. In the following section we discuss this approach for various hypothetical separation problems.
4. Results & discussion

In Section 3, we defined several quantities for measuring the separation performance of a CAL for mixtures having identical mean aerodynamic diameter and introduced analytical representations of these measures for numerical evaluation. Furthermore, in Section 2.1 we confined a reasonably sized space of viable operating parameters of a CAL. Thus, we can now conduct a case study for various distributions of feed particles, for which we search optimized initial parameters to be used later on in physical laboratory experiments.

4.1. Case studies & approaches

Therefore, we consider various cases of particle mixtures which will be described by their joint probability density \( f: \mathbb{R}^2 \rightarrow [0, \infty) \) as a function of size and mass density.

For nanoparticles of one single type of material \( A \) with mean particle size \( d_A \) and mean mass density \( \rho_A \) such a joint probability density \( f_A \) will be modeled by

\[
 f_A(d, \rho) = f_1(d) f_2(\rho), \tag{34}
\]

where \( f_1 \) is the probability density of a log-normal distribution with mean \( d_A \) and standard deviation\(^3\) of 200 nm, which is truncated at 3000 nm such that only particle sizes below that threshold can occur. The function \( f_2 \) considered in (34) is the probability density of a normally distributed random variable with mean \( \rho_A \) and standard deviation 0.1\( \rho_A \), which is truncated such that only mass densities between 0 and 22 000 kg m\(^{-3} \) can occur. Note that without truncating these distributions, arbitrarily large and dense particles could occur. Furthermore, truncating distributions limits the integration area in the formulas for the performance measures given in (24) - (27) to bounded sets, which in return makes numerical integration more viable. We also remark that in Equation (34) the particle size and mass density are modeled by stochastically independent random variables. On the other hand, note that it is possible to model such two-dimensional distributions for correlated particle size and mass density. For example the components \( \exp(X_1) \) and \( X_2 \) of the random vector \( (\exp(X_1), X_2) \) are log-normally and normally distributed and are in general correlated if \( (X_1, X_2) \) is a bivariate normally distributed random vector.

Recall that for mixtures of particles of type \( A \) and \( B \) with two-dimensional probability densities \( f_A \) and \( f_B \), respectively, we can describe the joint density \( f_{A,B} \) of such particle systems by

\[
 f_{A,B}(d, \rho) = \lambda f_A(d, \rho) + (1 - \lambda) f_B(d, \rho), \tag{35}
\]

where \( \lambda \in [0, 1] \) is the mixing ratio, see Equation (15). In the present paper we only consider the case \( \lambda = 0.5 \). Thus, the probability density \( f_{A,B} \) models a particle mixture with equal numbers of particles of type \( A \) and \( B \). However, this does not imply mass equality between particles of both types since their mass distributions can differ quite significantly.

\(^3\)The mean (or expectation) \( \mu \) and standard deviation \( \sigma \) of a random variable \( X \) with probability density \( f \) are given by \( \mu = \mathbb{E}X = \int_{-\infty}^{\infty} x f(x) \, dx \) and \( \sigma = \sqrt{\mathbb{E}[(X - \mu)^2]} = \left( \int_{-\infty}^{\infty} (x - \mu)^2 f(x) \, dx \right)^{0.5} \), respectively (Jacod and Protter (2003); Karr (1993)).
Table 1. Feed properties of the considered cases including means of particle sizes and feed purities $P_F$. In each case both Cu and SiO$_2$ have the same mean aerodynamic diameter $d_a$.

<table>
<thead>
<tr>
<th>cases</th>
<th>$d_a$ [nm]</th>
<th>$d_{Cu}$ [nm]</th>
<th>$d_{SiO_2}$ [nm]</th>
<th>$P_F$ [ ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>500</td>
<td>168</td>
<td>307</td>
<td>0.82</td>
</tr>
<tr>
<td>C2</td>
<td>1000</td>
<td>335</td>
<td>614</td>
<td>0.68</td>
</tr>
<tr>
<td>C3</td>
<td>1500</td>
<td>503</td>
<td>921</td>
<td>0.62</td>
</tr>
<tr>
<td>C4</td>
<td>2000</td>
<td>670</td>
<td>1230</td>
<td>0.79</td>
</tr>
</tbody>
</table>

Table 2. Overview of approaches conducted in the case study.

|---|-------------------------------|----------------------------------------------|--------------------------------------------|---------------------------------------------|-------------------------------------|

In the present paper, we consider mixtures of Cu and SiO$_2$ particles, where we assume that Cu has a mean mass density of $\rho_{Cu} = 8900 \text{ kg m}^{-3}$ and SiO$_2$ has a mean mass density of $\rho_{SiO_2} = 2190 \text{ kg m}^{-3}$. In this case study we consider four different constellations, denoted by C1-C4, of mean particle sizes $d_{Cu}$ and $d_{SiO_2}$ which can be found in Table 1. Each case of volume equivalent diameters $d_{Cu}$ and $d_{SiO_2}$ corresponds, together with the mass densities $\rho_{Cu}, \rho_{SiO_2}$, to a respective aerodynamic diameter $d_a$. Table 1 indicates that, for each particle size constellation C1-C4, the aerodynamic diameters $d_a$, given by Equation (3), of Cu and SiO$_2$ particles are equal, which constitutes similar aerodynamic behavior of particles for a given constellation. For each of the considered cases the probability densities $f_{Cu}, f_{SiO_2}$ of Cu and SiO$_2$ particles are assumed to have the form given in Equation (34). Figure 6(left column) visualizes the corresponding joint probability densities $f_{Cu, SiO_2}$ of the mixtures given by Equation (35). For each of the considered feed materials C1-C4 we optimize the lens parameters $p, d_L, \dot{Q}_m$ with respect to performance measures introduced in Section 3.3, on the basis of several approaches, which will be denoted by A1, A2a, A2b, A2c and A3. For an overview of these approaches see Table 2.

4.1.1. Target mode of value material (A1)

For each case stated in Table 1, lens parameters $p, d_L, \dot{Q}_m$ are determined such that the constraints given in (6) - (8) are satisfied and the corresponding iso-$\tau$ line of the CAL goes through the mode of the probability density $f_{Cu}$. For each of the cases C1-C4, Figure 6 (left column, red line) shows the iso-$\tau$ lines of the CALs calibrated with this approach. Heuristically speaking, this calibration of the CAL parameters tries to maximize the number of Cu particles in the product $P$. However, this approach ignores the fact that larger particles carry more mass of value material which is reflected by the relatively low product yield $Y_P$, since it considers the mass of particles, see Table 3 (constellation C1). Moreover, the approach A1 does not try to avoid SiO$_2$ in the product which can lead to a low product purity $P_F$.

4.1.2. Optimize performance measures (A2)

In order to remedy the low product purity obtained by approach A1, we now choose CAL parameters, which maximize the product purity $P_F$, for each probability distri-
feed material distribution  

A2c: product material distribution

![Diagram of material distributions](image)

**Figure 6.** Left column: probability densities $f$ of the Cu-SiO$_2$ particle mixtures in feed of cases C1-C4. The lines indicate the iso-$\tau$ lines of CALs optimized with the approaches A1, A2a, A2b and A2c, respectively. Right column: probability density $f$ of the feed material considered in C1-C4 after passing through a CAL which was optimized using approach A2c.
To be more precise, for each feed material distribution \( f_{\text{Cu,SO}_2} \) considered in C1-C4, we define a cost function \( g_{A2a}: D \rightarrow \mathbb{R} \) where \( D \subset \mathbb{R}^3 \) is the set of valid lens parameter constellations \((p, d_L, Q_m)\), i.e., \((p, d_L, Q_m) \in D \) if and only if \((p, d_L, Q_m)\) satisfies the constraints given by (6)-(8), see also Figure 2. The values of the cost function are given by

\[
g_{A2a}(p, d_L, Q_m) = -E(p, d_L, Q_m),
\]

where \( E(p, d_L, Q_m) \) is the enrichment \( E \) obtained by a CAL with parameters \( p, d_L, Q_m \) for the feed material distribution \( f_{\text{Cu,SO}_2} \). Note that the performance measure \( E(p, d_L, Q_m) \) can be computed numerically using the integral representation introduced in Section 3.3. The optimal parameter constellation \((p_{opt}, d_{L, opt}, Q_{m, opt})\) of the CAL minimizes the cost function \( g_{A2a} \) (thus maximizes the enrichment \( E \)) and is given by

\[
(p_{opt}, d_{L, opt}, Q_{m, opt}) = \arg\min\limits_{(p, d_L, Q_m) \in D} g_{A2a}(p, d_L, Q_m).
\]

This constrained optimization was performed using the particle swarm optimization algorithm in Matlab, see Eberhart and Kennedy (1995) and Mezura-Montes and Coello (2011), which, however, does not necessarily provide a global minimum. The CAL parameters determined in this way are given in Table 3 and the corresponding values of the performance measures \( Y_P, P_P \) are listed in Table 3. In comparison to the results obtained by approach A1, the product purity increased significantly. However, this optimization can lead to a rather poor yield, see, for example, case C1. This is due to the fact that the maximization of the enrichment would be achieved if the CAL would solely separate one single particle comprised of the value material.

On the other hand, if we chose the following cost function: \( g_{A2b}(p, d_L, Q_m) = -Y_P(p, d_L, Q_m) \), which optimizes the product yield \( P_P \) (approach A2b), the product purity suffers, see Table 3, case C4.

Therefore, neither the optimization of the product purity \( P_P \) nor the product yield \( Y_P \) seem to be suitable as possible goals. As an alternative approach (A2c) we propose the cost function \( g_{A2c}(p, d_L, Q_m) = -Y_e(p, d_L, Q_m)E(p, d_L, Q_m) \). This approach tries to maximize both the yield of the value material \( Y_e \) and the enrichment \( E \). Note that the best separation result would be achieved if the CAL would separate the entire fraction of the value material (maximizes \( Y_e \)), but moreover, if it only separates the value material (maximizes \( E \)). In comparison to the previously described approaches A1, A2a and A2b, the maximization of both the yield of value material \( Y_e \) and the enrichment \( E \) leads to a good compromise between purity and yield, see Table 3. The probability densities corresponding to the products of cases C1-C4 obtained by approach A2c are visualized in Figure 6 (right column).

The iso-\( \tau \) lines obtained with the optimization approaches A2a, A2b and A2c are also depicted depicted in Figure 6(left column). It indicates that the iso-\( \tau \) lines obtained by the optimization approaches A2a and A2c avoid the mode of \( \text{SiO}_2 \) particles in the feed distributions. This is due to the fact that the cost functions in both approaches consider the enrichment \( E \). However, as it can be seen for the cases C1 and C2, the approach A2a sometimes provides iso-\( \tau \) lines indicating a separation of rather
small Cu particles which leads to a poor product yield. Approach A2b, which solely maximizes the product yield $Y_P$, often leads to iso-$\tau$ lines, see cases C2-C4, which do not avoid the mode corresponding to the non-value SiO$_2$ particles. On the other hand, the iso-$\tau$ lines obtained by approach A3c avoid the mode corresponding to SiO$_2$ particles and indicate separation of relatively large particles which leads to both a good product purity $P_P$ and product yield $Y_P$.

### 4.1.3. Utilize a second CAL (A3)

Even though approach A2c led to good results, Table 3 indicates a relatively low product yield. Note that a high yield $Y_P$ is not necessarily desired, since this could mean that no separation at all took place. However, it is still possible to increase the product yield while maintaining a good purity by introducing a second CAL, which extracts value material from the waste of the first CAL.

Figure 7 visualizes this procedure, denoted by approach A3, for case C1. Note that, similarly to a system of just one CAL, we can derive formulas for performance measures of such a system with two CALs, which measure the quality of the two

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**Figure 7.** Scheme for improving the product yield by introducing a second CAL which separates the waste fraction of the first CAL (approach A3). Top left: probability density of a Cu and SiO$_2$ particle mixture of case C1 (logarithmic color scale). The red and brown lines indicate iso-$\tau$ lines of the first and second CAL, respectively. Top right: probability density of the fraction separated by the first CAL. Bottom left: probability density of the waste fraction of the first CAL (logarithmic color scale). The brown line indicates the iso-$\tau$ line of the second CAL. Bottom right: probability density of the separated fraction after the waste of the first CAL passed through the second CAL.
Table 3. Optimized CAL parameters and computed performance measures $Y_P$ and $P_P$ for the feed materials C1-C4 and the approaches A1-A3.

<table>
<thead>
<tr>
<th>Case</th>
<th>Approach</th>
<th>$p$ [Pa]</th>
<th>$d_L$ [mm]</th>
<th>$\dot{Q_m}$ [slm]</th>
<th>$Y_P$</th>
<th>$P_P$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: $d_a = 500$ nm</td>
<td>A1</td>
<td>10</td>
<td>100</td>
<td>3</td>
<td>0.004</td>
<td>0.025</td>
</tr>
<tr>
<td></td>
<td>A2a</td>
<td>10</td>
<td>24.3</td>
<td>3.25</td>
<td>6.6e-16</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>A2b</td>
<td>10</td>
<td>23.1</td>
<td>0.001</td>
<td>0.12</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A2c</td>
<td>10</td>
<td>23.1</td>
<td>0.001</td>
<td>0.12</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A3</td>
<td>10/375</td>
<td>25.0/10.0</td>
<td>0.001/0.153</td>
<td>0.22</td>
<td>0.96</td>
</tr>
<tr>
<td>C2: $d_a = 1000$ nm</td>
<td>A1</td>
<td>42.8</td>
<td>100</td>
<td>11.2</td>
<td>0.15</td>
<td>0.067</td>
</tr>
<tr>
<td></td>
<td>A2a</td>
<td>10</td>
<td>35.0</td>
<td>1.38</td>
<td>1.4e-19</td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td>A2b</td>
<td>10</td>
<td>56.2</td>
<td>0.110</td>
<td>0.15</td>
<td>0.065</td>
</tr>
<tr>
<td></td>
<td>A2c</td>
<td>11</td>
<td>18.4</td>
<td>0.0011</td>
<td>0.11</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A3</td>
<td>10/183</td>
<td>17.4/21.1</td>
<td>0.001/0.396</td>
<td>0.2</td>
<td>0.95</td>
</tr>
<tr>
<td>C3: $d_a = 1500$ nm</td>
<td>A1</td>
<td>10</td>
<td>100</td>
<td>0.32</td>
<td>0.13</td>
<td>0.34</td>
</tr>
<tr>
<td></td>
<td>A2a</td>
<td>10</td>
<td>18.9</td>
<td>0.0011</td>
<td>0.13</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A2b</td>
<td>10.6</td>
<td>70.0</td>
<td>0.185</td>
<td>0.22</td>
<td>0.031</td>
</tr>
<tr>
<td></td>
<td>A2c</td>
<td>10</td>
<td>18.2</td>
<td>0.001</td>
<td>0.13</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A3</td>
<td>10/237</td>
<td>19.5/20.5</td>
<td>0.001/0.952</td>
<td>0.22</td>
<td>0.95</td>
</tr>
<tr>
<td>C4: $d_a = 2000$ nm</td>
<td>A1</td>
<td>10</td>
<td>17</td>
<td>0.001</td>
<td>0.11</td>
<td>0.72</td>
</tr>
<tr>
<td></td>
<td>A2a</td>
<td>10</td>
<td>19.0</td>
<td>0.001</td>
<td>0.15</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A2b</td>
<td>10</td>
<td>14.9</td>
<td>0.0013</td>
<td>0.26</td>
<td>0.014</td>
</tr>
<tr>
<td></td>
<td>A2c</td>
<td>10.4</td>
<td>18.8</td>
<td>0.0011</td>
<td>0.15</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>A3</td>
<td>10/320</td>
<td>18.7/17.5</td>
<td>0.001/0.691</td>
<td>0.23</td>
<td>0.95</td>
</tr>
</tbody>
</table>

Therefore, it is possible to optimize both the lens parameters of the first and second lens, which improves the separation performance even further, see Table 3. For example, for the case C1 the product yield improved from 0.12 to 0.21 while maintaining a purity of 0.96.

### 4.2. Interpretation of the results

The results given in Table 3 show some trends. For instance: When comparing the product yield $Y_P$ of the considered cases, it is found that a greater value of the aerodynamic diameter is linked to a higher product yield. An explanation for this is that the performance measure is biased towards mass, and particle mass is strongly influenced by the particle size. This bias can be seen in the product purity $P_P$ as well, but it is not nearly as pronounced as in the product yield. In general, the more complex approaches A3/A2c lead to better performance than the approaches which target the mode (A1) or optimize a single performance measure (A2a and A2b). Another observation is that the cost function introduced in approach A2c favors the product purity over the product yield. An interesting quality emerges when comparing the optimized parameter sets of different approaches: They display remarkable similarity and seem to approach the lower boundaries of the parameter space. Almost all of the optimized parameter combinations can be found in the upper left corner of Figure 2b. The tendency to low values is no surprise, because the lower the pressure the less similar the Cu and SiO$_2$ particles become aerodynamically, because of the difference in particle slip, which depends only on particle size but not on the mass density. Due to limitations of pumping capacity, the low pressure reduces the maximum mass flow rate which the system is able to handle. This is problematic, because we intuitively expected that one optimized parameter set would be found between pressure values from 100 to 1000 Pa, because
this domain inhabits the highest pumping capacities. Thus, making higher mass flow
rates possible, which should in turn lead to higher product yield, given that the mass
load - the mass of particles per volume of gas flow - stays equal. But surprisingly this
expected trend is not really found in the simulations.

5. Conclusions

Classifying aerodynamic lenses offer an adjustable, differential transfer function which
enables them to separate particles by size and mass density. When CALs are used
sequentially at different pressures, they can even overcome the problem of ambiguity
in aerodynamic sampling. Stochastic modeling provides a highly adjustable tool for
choosing the best preconditions in a design process.

For our goal of aerodynamic classification, it was possible to make reasonable pre-
dictions regarding the influence of various process parameters on the separation perfor-
mance. These predictions reduce the risks that can occur while making certain design
decisions. Therefore, we introduced different quantities for measuring the separation
performance, such that it was possible to analyze and optimize the performance of the
separation process. These performance measures are applicable for different forms of
separation processes and are based on practicability.

We selected a few interesting virtual particle mixtures for a case study, namely mix-
tures of Cu and SiO$_2$, for which the valuable Cu particles should be extracted. For
these particle systems, the CAL geometry and the operating parameters were opti-
mized with respect to several performance measures in order to obtain large quantities
of pure separation products. We have seen that some particle mixtures are rather easy
to separate while others are more challenging in this regard. When the design param-
eters are carefully chosen, yield and purity are improved by two to three orders of
magnitude. Additionally, it is possible to further enhance the separation performance,
by repeating the separation process on the waste of the first CAL (in order to improve
the product yield).

The described methods can be easily transferred to different separation processes, for
which the influence of process parameters on the transfer functions are well understood.
Then, process parameters can be optimized with respect to performance measures for
arbitrary feed materials.

List of Symbols

<table>
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<tr>
<th>Symbol</th>
<th>Dimension</th>
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</table>

**Index**

- **a**: aerodynamic
- **p**: particle
- **L**: lens
- **g**: gas
- **c**: critical
- **o**: optimal
- **0**: standard conditions
- **F**: feed
- **P**: product
- **W**: waste

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References


