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

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ABSTRACT
A flexible stochastic approach is described to model separation processes, in which air-borne particles are separated via a setup of one or more 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 with distinct aerodynamic properties on the central axis. In this modeling approach a bivariate transfer function is used to describe the passage probability of particles depending on their size and mass. The distribution of feed particles and the changes of the distribution due to the separation process is described via probability densities. The modeling procedure is applicable to various kinds of separation methods and allows optimization of geometric and operation parameters. To this end, the model utilizes flexibly defined separation performance measures which are illustrated in a case study that 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.

KEYWORDS
aerodynamic sizing; material separation; aerosol; stochastic modeling; classifying aerodynamic lens

1. Introduction

The technique of aerodynamic focusing has applications in concentrating particles to a focused beam in low pressure environments (Klimešová et al., 2019), in mass spectrometry (Drewnick et al., 2005; Schreiner et al., 1999) and in synthesizing nanostructured materials (Dong et al., 2004; Piseri et al., 2004). Early works on aerodynamic focusing conclude that it might be the basis for new aerosol measurement techniques (de La Mora and Riesco-Chueca, 1988). Furthermore, 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. Focusing is often achieved by utilizing aerodynamic lenses, consisting of radial symmetrical pipes with an orifice (Liu et al., 1995),

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into which an aerosol is injected at the center of the pipe’s end. Then, the orifice leads to a temporary flow contraction which results in a focused stream of aerosol. Liu et al. (1995) characterized the focusing quality of aerodynamic lenses by a dimensionless contraction factor which in detail describes the features that contribute to the broadening of particle beams. Aerodynamic focusing of particles is the basis for various characterization techniques. For example, 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 for Stokes numbers smaller, yet close to one. On the other hand, for larger Stokes numbers, significant impact losses occurred. Wang et al. (2005) propose 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 which is introduced by limitations of the available equipment. Then, Wang and McMurry (2006) released a tool for designing aerodynamic lenses for focusing nanoparticles. Therefore, they computed optimal Stokes numbers beforehand via CFD simulations. Later on, as part of a project on multiparameter characterization of aerosols, a new device, namely the Differential Aerodynamic Particle Sizer (DAPS) was described. The DAPS allows to measure the aerodynamic diameter of nanoparticles by focusing various particle sizes in order to investigate specific, nearly monodisperse particle fractions (Babick et al., 2018).

The DAPS is based on the principle of classifying aerodynamic lenses. In contrast to aerodynamic lenses a classifying aerodynamic lens (CAL), see Figure 1, behaves more like a prism than a lens. More specifically, the aerosol is injected at a well-defined radial region offside the center line of the pipe, which results in the separation of particles when passing through the lens due to their distinct relaxation time $\tau_p$. Before passing through the lens the aerosol must follow the contracting streamlines which widen again after the orifice to accommodate the available space. Inertial and drag forces play vital roles here, because a particles path depends on its Stokes number: It either stays on its original streamline, which is the direction determined while passing through the orifice, or it adapts partially or fully to a new streamline. The consequence is that particles possessing a specific relaxation time $\tau_L$, as a result of the flowing conditions and the design of the lens, will be focused 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 portion of the aerosol which is focused on the centerline, however, is collected via an orifice, which we will call the sampler. This separation process results in a transfer function which shows a differential, classifying behavior which motivates the wording “classifying aerodynamic lens”. Using this approach, it is possible to yield a “mono-aerodynamic” aerosol. More precisely, a CAL separates particles whose relaxation times $\tau_p$ are approximately equal to a characteristic value $\tau_L$, called lens relaxation time, which depends on the CAL’s operating parameters. Since a particle’s relaxation time $\tau_p$ depends on its size $d_p$ and its mass density $\rho_p$, CALs can be used to achieve separation with respect to multidimensional particle characteristics. Therefore, the present paper introduces a stochastic model, which describes the separation processes of particle mixtures. For any distribution of feed particle characteristics, which can be freely chosen, the model describes the distribution of product particle characteristics depending on operating parameters. The general approach can be described by the following steps:
(i) Define the governing equations which describe the influence of particle characteristics and operating parameters on the separation process (Section 2.1).

(ii) Describe these relationships stochastically in form of a transfer function which describes the separation probability of a particle based on its physical characteristics (Section 2.2).

(iii) Define the distribution of characteristics of the considered particle mixture (Section 2.3).

(iv) Combine the last two steps into a stochastic model which describes the distribution of particle characteristics after separation in dependence of operating parameters (Section 2.4).

(v) Define the operating parameters to be optimized and their respective physical and technical limitations (Section 2.5).

(vi) Define performance measures suitable for the process which characterize separation process (Section 2.6).

(vii) Apply optimization algorithms to obtain operating parameters which lead to in a reasonable separation in accordance with the performance measures defined in the previous step (Section 3).

These steps can be used to virtually optimize any separation process for which the particle systems and the relationships between particle characteristics, operating parameters and separation probabilities are known. In the present paper, we demonstrate these steps in detail for the separation of particles from an aerosol based on their mass density and size using CALs.

2. Methods

There are several challenges to overcome when setting up a separation experiment based on a classifying aerodynamic lenses. The most important parameters are focusing pressure $p$, which is the pressure before the orifice, mass flow $Q_m$ and the diameter of the CAL orifice $d_L$. Even when the importance of additional details, such as the geometric shape of nozzles and sampler and the radial position of the aerosol inlet, is neglected, the interdependence of pressure $p$, mass flow $Q_m$ and orifice diameter $d_L$ creates a complex optimization problem for separation processes. Once a configuration of lens geometry and operating parameters is chosen, the manufacturing and testing of the prototype is costly in time and money. To minimize the risk it is good practice to simulate the separation process, using numerical fluid dynamics and particle trajectory analysis. However, CFD simulations of CALs are difficult, because they make use of critical orifices\(^1\). These possess high aspect ratios and creating appropriate meshes is an elaborate process. Therefore, there is a need for a fast, reliable prediction method. The present paper utilizes stochastic models for predicting the most promising set-up. For that purpose we propose a stochastic description of CALs, which decorates each vector of particle characteristics with a realistic probability for passing through a lens.

Then, we describe the 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 performance measures, such that fast numerical computation of these performance measures is possible.

\(^1\)Critical orifices are used to define the mass flow rate into the lens.
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.

2.1. Particle and lens relaxation times

A CAL focuses particles of a certain optimal Stokes number on the central axis, where they are collected via a sampling orifice. The optimal Stokes number $Stk_o$ is a function of Mach and Reynolds number, but is usually close to unity, see Wang et al. (2005). In the present paper we make the general assumption that $Stk_o = 1$. The Stokes number of a particle is calculated by

$$Stk = \frac{\tau_p u}{\ell}, \quad (1)$$

where $\ell$ is the diameter of the lens, $u$ 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 mass density $\rho_p$ and the volume equivalent diameter $d_p$, and is given by

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

where $\eta$ is the viscosity of the gas, $p$ is the pressure and $C_c$ is the Cunningham correction. (Friedlander (2000); Willeke (2011)).

Assuming that the velocity field and the diameter of the orifice are constant, it is deduced that a particle is focused, when its particle relaxation time $\tau_p$ equals a lens specific specific relaxation time $\tau_L$. This characteristic value of the lens is given by

$$\tau_L(d_L, \dot{Q}_v, p) = Stk_o \cdot \frac{\pi d_L^3}{\dot{Q}_v(p)}, \quad (3)$$

where $d_L$ is the diameter of the lens, $\dot{Q}_v$ is the volume flow through it and $p$ is the pressure. In order to focus particles with given size and mass 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 (3) the following formula is obtained:

$$d_L = \left( \frac{2\rho_p d_p^2 C_c(p, d_p) \dot{Q}_m}{9\pi \rho_g \eta Stk_o} \right)^{\frac{1}{3}}, \quad (4)$$

where $\rho_g$ is the gas density. Note that for every particle of volume equivalent diameter $d_p$ and mass 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 mass density.

There is an additional ambiguity involved: Equation (2) is not bijective, such that there will be cases where particles with distinguishable size and mass density possess

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2 the length of the relevant dimension of the obstacle
equal particle relaxation times and thus the same aerodynamic properties, described by the aerodynamic diameter $d_a$ given by

$$d_a = d_p \sqrt{\frac{\rho_p}{\rho_0}},$$  \hspace{1cm} (5)

where $\rho_0$ is the unit mass density (Willeke, 2011).

### 2.2. Transfer functions of CALs

As stated above particles are focused by a CAL if their relaxation time fulfills the following equation:

$$\tilde{\tau}(d_p, \rho_p) = \frac{\tau(d_p, \rho_p)}{\tau_L} = 1.$$  \hspace{1cm} (6)

We call $\tilde{\tau}(d_p, \rho_p)$ the normalized relaxation time of the particle. The set of configurations $\{(d_p, \rho_p) \in \mathbb{R}^2_+ : \tilde{\tau}(d_p, \rho_p) = 1\}$ form a curve in the two-dimensional parameter space of particle sizes and mass densities. These so-called iso-$\tau$ lines are visualized in Figure 2a for three different pressures $p$, while the remaining lens parameters $\dot{Q}_m$ 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-$\tau$ line, i.e., which fulfill Equation (6). 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

\[
\Omega(\tilde{\tau}) = \frac{1}{2\beta(1-\delta)} \left( |\tilde{\tau} - (1+\beta)| + |\tilde{\tau} - (1-\beta)| - |\tilde{\tau} - (1+\beta\delta)| - |\tilde{\tau} - (1-\beta\delta)| \right),
\]

where \( \beta, \delta \) are model parameters. The transfer function \( \Omega \) is taken from Stolzenburg and McMurry (2008), where it is used to describe the behavior of differential mobility analyzers. Figure 2b shows such a transfer function \( \Omega \) with parameters \( \beta = 0.4 \) and \( \delta = -0.25 \). The value of \( \Omega(\tilde{\tau}) \) 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. The transfer function depicted in Figure 2b was specifically chosen to replicate the observations made from CFD simulations reported in Babick et al. (2018). They tracked particle trajectories for a certain range of different aerodynamic diameters and computed the corresponding transfer probabilities. Equation (7) allows to mimic the general form of this transfer behavior.

In order to obtain a particle size and mass density dependent transfer function \( T_L \) of a CAL with relaxation time \( \tau_L \) and particle relaxation time dependent transfer function \( \Omega \), we combine Equations (6) and (7). This leads to the bivariate transfer function \( T_L : (0, \infty)^2 \rightarrow [0, 1] \) of a CAL given by

\[
T_L(d_p, \rho_p) = \Omega(\tilde{\tau}(d_p, \rho_p)) = \Omega \left( \frac{\tau(d_p, \rho_p)}{\tau_L} \right).
\]

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 2c. 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.
2.3. **Distribution of particle characteristics**

In the previous section we gave a stochastic description of CALs in the form of bivariate transfer 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 probability 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 number-based fraction of particles in the mixture with size $d_p \in [a, b]$ by computing

$$\mathbb{P}(D \in [a, b]) = \mathbb{P}((D, R) \in [a, b] \times \mathbb{R}) = \int_0^b \int_a^b f(d, \rho) \, d\rho \, d\rho. \quad (9)$$

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

$$f(d, \rho) = \lambda f_A(d, \rho) + (1 - \lambda) f_B(d, \rho), \quad (10)$$

where the parameter $\lambda \in [0, 1]$ describes the mixing ratio of particles of type $A$ and $B$\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., $\int_\mathbb{R} \int_\mathbb{R} f_X(x_1, x_2) \, dx_2 \, dx_1 = 1$ holds.}. We make the assumption that particle characteristics are not correlated. However, note that the stochastic description introduced in the present paper does not require independence of particle size $d_p$ and mass density $\rho_p$ for the considered particle systems. Figure 3a depicts the probability density of a particle mixture of Cu and SiO$_2$ particles. Note that Figure 3a shows a bimodal probability density, where the task of a CAL will be to separate the desired Cu particles from SiO$_2$ particles. The red line depicts an iso-$\tau$ line of a CAL. Since the iso-$\tau$ line does not pass through the mode of the probability density belonging to the SiO$_2$ particles, it can be expected that the separation task will be performed rather well.

2.4. **Stochastic modeling of the separation process**

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 bivariate transfer function $T_L$ of a CAL takes this effect into account.

Using the bivariate transfer 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 $\mathbf{x} = (d_p, \rho_p) \in \mathbb{R}^2$ is located in some region $\Omega \subset \mathbb{R}^2$. For example, the number of particles in the region $\Omega$ can be computed as

$$\mathbb{P}(\mathbf{x} \in \Omega) = \int_\Omega f_X(\mathbf{x}) \, d\mathbf{x}.$$

The mixing ratio $\lambda$ describes the mixture on the basis of particle numbers. Thus, the mass ratio of the mixture is in favor of the heavier particle species.
a) Two-dimensional probability density $f$ of particle size-mass density vectors of an exemplary Cu-SiO$_2$ particle mixture. The red line is the iso-$\tau$ line of a CAL with lens parameters $p = 10$ Pa, $d_L = 0.07$ m, $Q_m = 0.02$ slm. b) The two-dimensional probability density $\tilde{f}$ of size-mass density vectors of particles which pass through the CAL.

$(D, R)$ 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 probability of the event that the random particle passes the CAL is equal to the probability of the event that the inequality

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

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

$$c_L = \mathbb{P}(T_L(D, R) \geq U) = \int_0^\infty \int_0^\infty f(d, \rho) T_L(d, \rho) \, d\rho \, dd.$$  \hspace{1cm} (12)

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 $(\tilde{D}, \tilde{R})$ belongs to a rectangle $C_1 \times C_2 \subset \mathbb{R}^2$, where $C_1, C_2 \subset \mathbb{R}^2$ are some given 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

\[ \tilde{f}(d, \rho) = \frac{1}{c_L} f(d, \rho) T_L(d, \rho). \]  
(13)

The conditional probability density \( \tilde{f} \) is visualized in Figure 3b for the input probability density \( f \) shown in Figure 3a.

### 2.5. Constraints on lens geometry and operating parameters

In the previous section we described the relative amount \( c_L \) of particles which pass through the CAL by Equation (12) and the probability density \( \tilde{f} \) of their particle characteristics in dependence of the CAL’s bivariate transfer function \( T_L \), see Equations (12) and (13), respectively. Since the bivariate transfer function \( T_L \) depends on the lens parameters \( p, Q_m, d_L \), see Equations (2), (3) and (8), we can modify the lens geometry and operating to influence the separation results. However, there are certain physical constraints on the lens parameters \( p, Q_m, d_L \) which we want to discuss in order to describe the space of valid parameter configurations. To reduce the complexity of the problem, the following deductions and assumptions are used:

(i) Particles do not affect the flow of the carrier gas.
(ii) The particle relaxation time is based on the pressure before passing the orifice\(^5\).
(iii) All particles start in the same region of the lens, such that they experience the same velocity when going through the orifice.
(iv) Only subsonic and continuum flow conditions are considered.
(v) Particle mass load is small, to avoid coagulation which could change the size-distribution in the lens setup.

As stated in Wang et al. (2005) focusing of submicron 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 in Wang et al. (2005) are provided below. The Reynolds number \( Re \) is calculated via the mass flow rate of the gas \( Q_m \) by

\[ Re = \frac{\rho_g(p) \cdot \bar{u} \cdot d_L}{\mu_g} = \frac{4 \cdot Q_m}{\pi \mu_g d_L} < 200 = Re_c, \]  
(14)

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

\[ Ma = \frac{u}{c_g} < 1 = Ma_c, \]  
(15)

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

\[ Kn = \frac{2 \cdot \lambda_g(p)}{d_L} < 0.1 = Kn_c, \]  
(16)

\(^5\)For CALs in use, mass flow rate of the carrier gas is fixed via mass flow control devices or critical orifices, thus the pressures in the CAL depend on the adjustable suction rate of the chosen pumping system. The pressure drop over the lens is small (< 10 Pa) in comparison to the pressure drop over the lens exits, and can be calculated.
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. There exists an optimal pressure for which the pump evacuates at a maximum volume flow rate. In the present paper we use measurements from a rotary vane pump (1001 Leybold) as exemplary data. More precisely, the function we use to describe the pressure-dependent volume pump rate \( S_{slm} \) in slm is given by

\[
S_{slm}(p) = 60 \cdot 10^{y(p)} \cdot \rho_g \cdot (p/p_0) \cdot (T_0/T),
\]

where \( p_0 = 101325 \text{ Pa} \) is the standard pressure, \( T_0 = 273.15 \text{ K} \) is the standard temperature and \( y \) denotes a polylogarithmic fit to the volume pump rate data provided in Leybold GmbH (2018) which is given by

\[
y(p) = \sum_{k=0}^{8} x_k \log^k(p),
\]

with fitted regression parameters

\[(x_0, x_1, \ldots, x_8) = (2.908, -0.016, -0.082, 0.050, 0.010, -0.025, -0.002, 0.006, -0.001).\]

Furthermore, the available pressure range is constrained by the pumping capacity:

\[10 \text{ Pa} \leq p \leq 101325 \text{ Pa}.\]

When we apply the constraints that result from the calculation of the critical values for Re\(_c\), Ma\(_c\), Kn\(_c\) and the pumping capacity, we can locate all feasible combinations of pressure, flow rate and lens diameter. Using Equation (3) we can calculate the values of \( \tau_p \) belonging to the constrained parameter space. For every particle with mass density \( \rho_p \) and diameter \( d_p \), there exists a surface, see Equation (4), 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 Inequalities (14)-(16) and (19) 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.

### 2.6. Performance measures

In Section 2.4 we described how to obtain the probability density \( \tilde{f} \) of size and mass density for feed particles which pass through a CAL with bivariate transfer function \( T_L \). Since \( T_L \) depends on CAL operating parameters, the latter can be varied while respecting the constraints discussed in Section 2.5 in order to modify separation results. Therefore, we introduce quantities, which we refer to as performance measures, to evaluate the quality of a separation process. Furthermore, we derive some formulas which allow a quick numerical computation of performance measures. To do so, we analyze mass fractions in the feed, product and waste and differentiate between value and non-value materials. Figure 4 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 \( nv \). 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 \( m_{nv,F} \) of the non-value material. The feed is separated in product and waste fractions denoted by \( P \) and \( W \), respectively.

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

**Figure 4.** The feed \( F \) is separated into the product \( P \) and the waste \( W \). Desired fractions are marked by \( v \) and undesired fractions by \( nv \). 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:

\[
\begin{align*}
P_F &= \frac{m_{v,F}}{m_F} = \frac{m_{v,F}}{m_{nv,F} + m_{v,F}}, \quad (20) \\
P_P &= \frac{m_{v,P}}{m_P} = \frac{m_{v,P}}{m_{nv,P} + m_{v,P}}, \quad (21) \\
Y_P &= \frac{m_P}{m_F} = \frac{m_{nv,P} + m_{v,P}}{m_{nv,F} + m_{v,F}}. \quad (22)
\end{align*}
\]

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.,

\[
E = \frac{P_P}{P_F}. \quad (23)
\]

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

\[
Y_v = EY_P = \frac{m_{v,P}}{m_{v,F}}. \quad (24)
\]

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 \([0, 1]\).

Having in mind the stochastic description of both the in-going particle mixtures and the CAL introduced in Sections 2.2 and 2.4, 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

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

(25)

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

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

(26)

To decide whether the \(i\)-th random particle goes through the considered CAL with bivariate transfer function \(T_{L_i}\), 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 (11). Thus, the (random) mass \(m_P\) of particles in the product is given by

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

(27)

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

\[
\mathbb{1}_{U_i \leq T(D_i, R_i)} = \begin{cases} 
1, & \text{if } U_i \leq T(D_i, R_i), \\
0, & \text{if } U_i > T(D_i, R_i).
\end{cases}
\]

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

\[
m_{v,F} = \frac{\pi}{6} \sum_{i=1}^{n} D_i^3 R_i \mathbb{1}_{R_i \in C_v},
\]  

(28)

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

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

(29)

By inserting the formulas given in Equations (26) - (29) into the definitions considered in Equations (20) - (24) 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

\[
\hat{Y}_P = \frac{\sum_{i=1}^{n} R_i D_i^3 \mathbb{1}_{U_i \leq T(D_i, R_i)}}{\sum_{i=1}^{n} R_i D_i^3},
\]  

(30)
which can be computed 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 \(p, d, \dot{Q}_m\) 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 Section 2.4, in order to derive theoretical formulas for the computation of performance measures in the case of an unboundedly increasing number \(n\) incoming random particles. Due to the law of large numbers (Jacod and Protter (2003); Karr (1993)) we have

\[
\frac{1}{n} m_F = \frac{1}{n} \sum_{i=1}^{n} m(D_i, R_i) \xrightarrow{n \to \infty} \mathbb{E} [m(D, R)] = \int_0^\infty \int_0^\infty m(d, \rho) f(d, \rho) \, d\rho \, dd, \tag{31}
\]

and, analogously,

\[
\frac{1}{n} m_P \xrightarrow{n \to \infty} \mathbb{E} \left[ m(D, R) 1_{T_L(D, R) \geq U} \right] = \int_0^\infty \int_0^\infty m(d, \rho) f(d, \rho) T_L(d, \rho) \, d\rho \, dd, \tag{32}
\]

\[
\frac{1}{n} m_{v,F} \xrightarrow{n \to \infty} \mathbb{E} \left[ m(D, R) 1_{R \in C_v} \right] = \int_{C_v} \int_0^\infty m(d, \rho) f(d, \rho) \, d\rho \, dd, \tag{33}
\]

\[
\frac{1}{n} m_{v,P} \xrightarrow{n \to \infty} \mathbb{E} \left[ m(D, R) 1_{T_L(D, R) \geq U} 1_{R \in C_v} \right] = \int_{C_v} \int_{C_v} m(d, \rho) f(d, \rho) T_L(d, \rho) \, d\rho \, dd, \tag{34}
\]

where \(\mathbb{E}\) denotes the expectation. Thus, the random variables considered in Equations (31) - (34) converge to deterministic limits. The integral representations of the limits in Equations (31) - (34) allow the numerical computation of the mass values of the feed and the product. Similarly, we can represent the limits of the separation performance measures given in (20) - (24) via integrals. For example, the limit or, equivalently, the expected value of the product purity \(P_P\) for an unboundedly increasing number \(n\) of particles is given by

\[
P_P = \frac{m_{v,P}}{m_P} = \frac{1}{n} m_{v,P} \xrightarrow{n \to \infty} \frac{1}{n} \int_{C_v} \int_0^\infty m(d, \rho) f(d, \rho) T_L(d, \rho) \, d\rho \, dd \xrightarrow{n \to \infty} \mathbb{E} P_P, \tag{35}
\]

for \(n \to \infty\). The expected values for the remaining performance measures can be derived analogously to (35). In the following, we will denote the expected values \(\mathbb{E} P_F, \mathbb{E} P_P, \mathbb{E} Y_P, \mathbb{E} E, \mathbb{E} Y_v\) simply by \(P_F, P_P, Y_P, E, Y_v\), respectively.

The formulas given in Equations (31) - (34) allow the numerical computation of expected performance measures for feed particle mixtures. More precisely, for any two-dimensional probability density \(f\), which describes the number-based distribution of size-mass density of feed particles going through a CAL with bivariate transfer function \(T_L\), we can numerically compute the measures \(P_F, P_P, Y_P, E\) and \(Y_v\). 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.

3. Optimization of performance measures: A case study

In Section 2.6, 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 2.5 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.

3.1. Description of considered cases \& 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

\[
f_A(d, \rho) = f_1(d)f_2(\rho), \tag{36}
\]

where \( f_1 \) is the probability density of a log-normal distribution with mean \( d_A \) and standard deviation\(^6\) 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 (36) 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, physically unrealistic particles could occur. Furthermore, truncating distributions limits the range of integration in the formulas for the performance measures given in (26) - (29) to bounded sets, which in return makes numerical integration more viable.

We also remark that in Equation (36) 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 using the mixing ratio introduced in Equation (10). 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.

---

\(^6\)The mean (or expectation) \( \mu \) and standard deviation \( \sigma \) of a real-valued 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.

<table>
<thead>
<tr>
<th>A1</th>
<th>target mode of value material</th>
</tr>
</thead>
<tbody>
<tr>
<td>A2a</td>
<td>optimize performance measure: Product purity</td>
</tr>
<tr>
<td>A2b</td>
<td>optimize performance measure: Product yield</td>
</tr>
<tr>
<td>A2c</td>
<td>optimize performance measure: Cost function</td>
</tr>
<tr>
<td>A3</td>
<td>second CAL for enhanced product yield</td>
</tr>
</tbody>
</table>

In the present paper, we consider mixtures of Cu and SiO\(_2\) particles as feed material, where we assume that Cu has a mean mass density of \( \rho_{Cu} = 8900\, \text{kg}\,\text{m}^{-3} \) and SiO\(_2\) has a mean mass density of \( \rho_{SiO_2} = 2190\, \text{kg}\,\text{m}^{-3} \). 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 \( d_a \), see Equation (5). Table 1 indicates that, for each particle size constellation C1-C4, the aerodynamic diameters \( d_a \) 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 \( f_{Cu} \) and \( f_{SiO_2} \) of Cu and SiO\(_2\) particles are assumed to have the form given in Equation (36). The joint probability densities \( f_{Cu, SiO_2} \) of characteristics of the mixtures are modeled by Equation (10), see Figure 5 (left column), with an equal (number-based) mixing ratio \( \lambda = 0.5 \). The corresponding resulting feed purities \( P_F \) are given in Table 1. For each of the considered feed materials C1-C4 we optimize the lens parameters \( p, d_L, Q_m \) with respect to performance measures introduced in Section 2.6, on the basis of several approaches, which will be denoted by A1, A2a, A2b, A2c and A3 in the following. For an overview of these approaches, see Table 2.

3.2. Target mode of value material (A1)

For each case stated in Table 1, lens parameters \( p, d_L, Q_m \) are determined such that the constraints given in (14) - (16) and (19) 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 5 (left column, red line) shows the iso-\( \tau \) lines of the CALs based on this approach. Heuristically speaking, this choice 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 minimize SiO\(_2\) in the product which can lead to a low product purity \( P_F \). Approach A1 serves as a reference to which the other approaches are compared to.
Figure 5. 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.
3.3. 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 distribution $f_{\text{Cu,SiO}_2}$ of feed material described by the cases C1-C4. This approach (denoted by A2a) is equivalent to maximizing the enrichment $E = \frac{P_v}{P_F}$, since the values of feed purity $P_F$, given in Table 1, do not depend on the CAL parameters.

To be more precise, for each feed material distribution $f_{\text{Cu,SiO}_2}$ 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 $(p, d_L, \dot{Q}_m)$, i.e., $(p, d_L, \dot{Q}_m) \in D$ if and only if $(p, d_L, \dot{Q}_m)$ satisfies the constraints given by (14)-(16) and (19). The values of the cost function are given by

$$g_{A2a}(p, d_L, \dot{Q}_m) = -E(p, d_L, \dot{Q}_m),$$

where $E(p, d_L, \dot{Q}_m)$ is the enrichment $E$ obtained by a CAL with parameters $p, d_L, \dot{Q}_m$ for the feed material distribution $f_{\text{Cu,SiO}_2}$. Note that the performance measure $E(p, d_L, \dot{Q}_m)$ can be computed numerically using the integral representation introduced in Section 2.6. The optimal parameter constellation $(p_{\text{opt}}, d_{L,\text{opt}}, \dot{Q}_{m,\text{opt}})$ of the CAL minimizes the cost function $g_{A2a}$ (thus maximizes the enrichment $E$) and is given by

$$(p_{\text{opt}}, d_{L,\text{opt}}, \dot{Q}_{m,\text{opt}}) = \arg\min_{(p, d_L, \dot{Q}_m) \in D} g_{A2a}(p, d_L, \dot{Q}_m).$$

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 $Y_F, P_F$ 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: $g_{A2b}(p, d_L, \dot{Q}_m) = -Y_F(p, d_L, \dot{Q}_m)$, which optimizes the product yield $P_F$ (approach A2b), the product purity can suffer, see case C4 in Table 3.

Therefore, neither the optimization of the product purity $P_F$ nor the product yield $Y_F$ seem to be suitable as possible goals. As an alternative approach (A2c) we thus propose the cost function $g_{A2c}(p, d_L, \dot{Q}_m) = -Y_v(p, d_L, \dot{Q}_m)E(p, d_L, \dot{Q}_m)$. This approach tries to maximize both the yield of the value material $Y_v$ 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 $Y_v$), 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 $Y_v$ 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 5 (right column).

The iso-$\tau$ lines obtained with the optimization approaches A2a, A2b and A2c are also depicted in Figure 5 (left column). It indicates that the iso-$\tau$ lines obtained by the optimization approaches A2a and A2c avoid the mode of 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 A2c 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 $Y_P$.

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

Even though approach A2c leads 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.
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>

Figure 6 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 separated fractions. 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. Results & conclusions

4.1. 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 $Y_P$. 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 boundary of the parameter space. Almost all of the optimized parameter combinations have values close to the lower constraint for the pressure which is
given by $10\text{Pa}$, see Inequality (19). The tendency to low pressure values is no surprise because for lower pressures the Cu and SiO$_2$ particles become less similar aerodynamically. This is due to the difference in the 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.

### 4.2. Conclusions

Classifying aerodynamic lenses offer an adjustable, differential transfer function which enables them to separate particles by size and mass density. Stochastic modeling provides a highly adjustable tool for choosing the best preconditions in a design process.

For the goal of aerodynamic classification, it was possible to make reasonable predictions regarding the influence of various process parameters on the separation performance. 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 mixtures 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 optimized 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 parameters 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>
<thead>
<tr>
<th>Symbol</th>
<th>Dimension</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$</td>
<td>[kg]</td>
<td>mass</td>
</tr>
<tr>
<td>$d_p$</td>
<td>[m]</td>
<td>volume equivalent particle diameter</td>
</tr>
<tr>
<td>$\tau_p$</td>
<td>[s]</td>
<td>particle relaxation time</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>[kg/m$^3$]</td>
<td>particle mass density</td>
</tr>
<tr>
<td>$d_L$</td>
<td>[m]</td>
<td>orifice diameter</td>
</tr>
</tbody>
</table>
\( \tau_l \quad [s] \quad \text{lens relaxation time} \\
\( l \quad [m] \quad \text{length} \\
\( \rho_g \quad [kg/m^3] \quad \text{gas density} \\
\( \rho_0 \quad [kg/m^3] \quad \text{unity density} \\
\( \lambda_g \quad [m] \quad \text{gas mean free path} \\
\( \eta_g \quad [Pa \cdot s] \quad \text{dynamic gas viscosity} \\
\( u_g \quad [m/s] \quad \text{mean gas velocity} \\
\( C_C \quad \text{Cunningham correction} \\
\( \dot{Q}_m \quad [kg/s] \quad \text{gas mass flow rate} \\
\( \dot{Q}_v \quad [m^3/s] \quad \text{gas volume flow rate} \\
\( \dot{Q}_{slm} \quad [slm] \quad \text{volume flow rate in standard litre per minute} \\
\( S \quad [m^3/s] \quad \text{pumping speed} \\
\( p \quad [Pa] \quad \text{pressure} \\
\( T \quad [K] \quad \text{temperature} \\
\( Stk \quad \text{Stokes number} \\
\( Re \quad \text{Reynolds number} \\
\( Ma \quad \text{Mach number} \\
\( Kn \quad \text{Knudsen number} \\
\( Y \quad \text{yield} \\
\( P \quad \text{purity} \\
\( E \quad \text{enrichment} \\
\( \mathbb{1} \quad \text{indicator function} \\
\( f \quad \text{probability density function} \\
\( \mathbb{P} \quad \text{probability measure} \\
\( \mathbb{E} \quad \text{expectation} \\
\( D \quad \text{random volume equivalent particle diameter} \\
\( R \quad \text{random mass density} \\
\( \lambda \quad \text{mixing ratio of particle species} \\

\textbf{Index} \quad \textbf{Description} \\
a \quad \text{aerodynamic} \\
p \quad \text{particle} \\
L \quad \text{lens} \\
g \quad \text{gas} \\
c \quad \text{critical} \\
o \quad \text{optimal} \\
o \quad \text{standard conditions} \\
F \quad \text{feed} \\
P \quad \text{product} \\
W \quad \text{waste}
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References


