ABSTRACT

Triboelectrostatic separation of coal is a dry beneficiation process that relies on electric forces to separate carbon from impurities by application of an external electric field on particles. The technique is highly efficient in terms of energy consumption because it targets individual particles, in contrast to other cleaning techniques, which operate on bulk fluids. Furthermore, it is very efficient in processing fine particles because as particles become smaller, the electric force, which acts at the surface, becomes more dominant than the buoyant force, which acts at the volume.

The idea of dry coal cleaning by means of electro-separation has been around for quite some time. Indeed, bench-scale triboelectric separation units have been built and tested successfully; however, scale up and commercialization of these units have not met with the same level of success because the design of those devices, for the most part, has been based on a trial and error approach while understanding of basic principles of the process has been widely overlooked. Such an understanding is needed if the design of these devices is ever going to move beyond the trial and error stage.

In this project, a computational methodology was developed to simulate the cleaning of Illinois coal in a triboelectrostatic separator and gain “detailed” understanding of the phenomenon. To this end, the governing equations of fluid flow, electric fields, and particles were solved using FLUENT software and in-house computer codes. The governing nondimensional parameters of the phenomenon were identified and extensive parametric studies were performed to explore the effect of these parameters on separation efficiency. Results were analyzed and justified by inspection of particle trajectories and the flow field. While computer simulations yielded a wealth of information concerning the subtle interplay of governing parameters in determining separation efficiency, separation efficiencies achieved with simulation were generally higher than those found by actual experimentation. This suggests the necessity of refining computational modeling of tribocharging in an effort to mimic reality more closely, which will be proposed in the future.
EXECUTIVE SUMMARY

Beneficiation of coal is a vitally important process in reducing environmental hazards associated with combustion of run-of-mine coal. To scale down energy consumption and improve on environmental impacts of wet cleaning processes, a promising alternative is dry beneficiation of coal by triboelectrostatic separation. In this technique, coal is finely pulverized first so that all its constituents are liberated. Particles are then charged by rubbing them against each other and/or a wall, such as forcing them to move inside a spiral channel. Charged particles are subsequently exposed to an electric field for electrostatic separation. The technique is highly efficient in terms of energy consumption because it targets individual particles, in contrast to other dry cleaning techniques that operate on fluid bulk. Furthermore, it is very efficient in processing fine particles because as the particles become smaller, the electric force, which acts at the surface, becomes more dominant than the buoyant force, which acts at the volume.

The aim of this project was to gain a “detailed” understanding of the triboelectrostatic separation of the Illinois coal by computer simulations. To this end, the governing equations of fluid flow, electric fields, and particles were solved using an Eulerian/Lagrangian approach, where fluid was treated as a continuum and particle trajectories were found using Newton’s second law. The two-way coupling between fluid and particles was also accounted for. The computer methodology was validated by comparing results with solutions from benchmark problems.

The governing nondimensional parameters of the problem were identified and extensive parametric studies were performed to explore the effect and interplay of these parameters on separation efficiency. It was shown that co-flow is necessary to stabilize the carrier fluid flow and that its inclusion generally leads to an increase in separation efficiency because of better adjustment of particle trajectories. Computations showed that for a fixed geometry, the particle charge to mass ratio, its residence time, and the particle/wall incidence/reflection angle were among the most influential parameters in controlling separation efficiency.

The effect of channel geometry was explored and it was shown that by making electrodes slightly divergent, it is possible to reduce angles of incidence and reflection. This in turn prevents particles from moving toward the electrode of the same charge. The result is an increase in separation efficiency.

While computational simulations yielded a wealth of information that was in line with intuition and limited available experimental results, separation efficiencies achieved with modeling tended to be higher than those measured through experiments. It is thought that this discrepancy is due to utilization of “assigned” particle charging instead of modeling tribocharging. Similarly, a possible charge transfer due to particle/particle collision in the separation chamber must also be accounted for.
OBJECTIVES

The overall goal of this project was to study beneficiation of coal by triboelectrostatic separation using computer simulation. The specific objectives of the project were:

1. To develop a computational methodology for simulating separation of coal particles by electric fields.

2. To perform a detailed investigation of the triboelectrostatic separation process by exploring the effect of various controlling parameters, such as initial particle velocity, fluid flow rate, and the strength of the electric field, on separation efficiency.

3. To explore the geometric design of the triboelectrostatic separator in order to improve its separation efficiency.

INTRODUCTION AND BACKGROUND

Beneficiation of coal is a vitally important process in reducing environmental hazards associated with combustion of run-of-mine coal. Currently, the most widely used coal cleaning technologies utilize water to eliminate minerals from the coal. Wet cleaning processes consume large amounts of water and energy and have various negative environmental impacts. Furthermore, cleaned coal must be dewatered before it is burned, which is an expensive undertaking. To scale down energy consumption and to improve the environmental impact of coal cleaning processes, a promising alternative is dry beneficiation of coal using electric fields. Electro-separation techniques are highly efficient in terms of energy consumption because they target individual particles in contrast to wet cleaning techniques that operate on fluid bulk. Furthermore, these techniques are very efficient in processing fine particles. Triboelectrostatic separation, where electric force is applied on initially charged particles, is particularly attractive because it provides the largest electric force per unit volume of particle (i.e., the Coulomb force) compared to other electric forces such as electrophoretic force.

Triboelectrostatic separation of coal consists of two main processes: tribocharging of coal and separation of charged particles. To this end, coal is finely pulverized first so that all its constituents are liberated. Particles are then charged by rubbing them against each other and/or a wall, such as forcing them to move inside a spiral loop. The charging mechanism can be best understood by considering a parameter called “work function,” which is defined as the work required to remove electrons from any surface. Its unit of measurement is the electron-Volt [eV]. Work function values for many common materials are well documented (e.g. Michaelson, 1977). When two materials are brought in contact, electrons move until the energy of electrons in each material at the interface is equalized. The material with a higher work function gains electron and becomes negatively charged while the material with a lower work function loses electrons and becomes positively charged. In the case of clean coal, the work function of carbon is 4 eV while impurities have higher work functions than 4 eV. Therefore, in a mixture of carbon and impurities, carbon particles will become positively charged while impurities will
become negatively charged. The raw coal is subsequently passed through an electric field for electrostatic separation.

To improve the efficiency of the triboelectrostatic separators (TES), it is possible to increase surface charges of particles by rubbing them against an electric charger (Tao, 2010); however, there is an upper limit, $q_{\text{max}}$, on the charge that can accumulate on a particle surface due to electric breakdown of the surrounding media. This upper limit can be estimated from Gauss’s law, which relates the distribution of electric charge to the resulting electric field:

$$ q_{\text{max}} = E_{\text{max}} \varepsilon \left[ \text{C/m}^2 \right], $$

where $\varepsilon$ is the permittivity of the surrounding media and $E_{\text{max}}$ is the maximum electric field strength for the electric breakdown in the surrounding media. In the case of air, the maximum electric field strength for breakdown is about $E_{\text{max}} = 3 \times 10^6 \, \text{[V/m]}$ (Crowley, 1986) and the permittivity of the free space is about $\varepsilon_0 = 8.85 \times 10^{-12} \, \text{[F/m]}$. Substitution of these quantities in Equation 1 results in an upper limit for the surface charge density: $q_{\text{max}} = 2.6 \times 10^{-5} \, \text{[C/m}^2\text{]}$. This upper limit is sometimes referred to as the Gauss maximum charge. For simulations performed as part of this study, the particle charge used was well below the Gauss maximum charge and is within the experimental range.

Computer modeling of triboelectrostatic separation involves solving a set of coupled partial differential equations, such as the turbulent flow equations. As such, it is not possible to predict the behavior of particles at the outset; however, considerable insight can be gained by considering the behavior of an isolated particle. Figure 1 shows a schematic of a particle in a separation chamber. Here, two basic equations are needed to determine particle trajectory; namely, Newton’s second law,

$$ F_p = m_p \mathbf{a}_p, $$

and the particle kinematic equation,

$$ \frac{d \mathbf{r}_p}{dt} = \mathbf{u}_p. $$

![Figure 1. Schematic of a particle in a separation chamber.](image)
Note that these equations are in vector form. Here, \( \mathbf{F}_p = \mathbf{F}_B + \mathbf{F}_D + \mathbf{F}_E \) is the sum of buoyant, drag, and electric field forces that are exerted on the particle; \( m_p \) is particle mass; \( \mathbf{a}_p \) is particle acceleration; \( \mathbf{u}_p \) is particle velocity; and \( \mathbf{r}_p \) is particle position with respect to reference coordinates. Buoyancy is \( \mathbf{F}_B = \mathbf{g}(\rho_p - \rho_f)V_p \), where \( V_p \) and \( \rho_p \) are particle volume and density. The electric force is due to Coulomb forces and is \( \mathbf{F}_E = \mathbf{E}_p q_p \), where \( \mathbf{E}_p \) is the strength of the electric field at the particle position. The drag force depends on the relative velocity of the particle and the fluid and can be formulated as \( \mathbf{F}_D = (\mathbf{u}_f - \mathbf{u}_p)/\tau_p \) where \( \mathbf{u}_f \) is the fluid viscosity at the particle position and \( \tau_p \) is the particle response time. Substitution for these forces in Equations 2 and 3 results in:

\[
\frac{\mathbf{u}_{n+1} - \mathbf{u}_n}{\tau_p} + \frac{g(\rho_p - \rho_f)}{\rho_p} + \frac{\mathbf{E}_p q_p}{m_p} = \frac{d\mathbf{u}_p}{dt}. \tag{4}
\]

As is evident from Figure 1, the electric field strength is zero in the vertical direction and gravitational acceleration is zero in the horizontal direction. Furthermore, the electric field strength is uniform in the horizontal direction. Therefore, Equation 4 in both horizontal and vertical directions can be written as:

\[
\frac{u_{n+1} - u_n}{\tau_p} + \frac{E_p}{m_p} = \frac{du_p}{dt}, \tag{5}
\]

\[
\frac{v_{n+1} - v_n}{\tau_p} - \frac{g(\rho_p - \rho_f)}{\rho_p} = \frac{dv_p}{dt}.
\]

If the fluid velocity \( \mathbf{u}_f = (u_f, v_f) \) is spatially uniform, independent of time, and the fluid inertia can be ignored (i.e., Stokes flow) the only time-dependent terms in Equation 5 will be particle velocity in horizontal and vertical directions; therefore, this equation can be integrated analytically with respect the time. However, if the fluid velocity is independent of time but nonuniform (such as Poiseuille flow), or the fluid inertia cannot be ignored, then this equation should be integrated over a time step \( \Delta t \) to account for variations of the drag force with particle motion:

\[
\begin{align*}
    u_{n+1} &= u_f + \exp(-\Delta t/\tau_p)(u_n - u_f) - C_x \tau_p[\exp(-\Delta t/\tau_p) - 1], \\
    v_{n+1} &= v_f + \exp(-\Delta t/\tau_p)(v_n - v_f) - C_y \tau_p[\exp(-\Delta t/\tau_p) - 1],
\end{align*} \tag{6}
\]

where \( C_x = E_x q_p/m_p \), \( C_y = -g(\rho_p - \rho_f)/\rho_p \), \( E_x \equiv E \), and superscripts \( n \) and \( n+1 \) refer to current and future time. Once the velocity of the particle is found at the new time step, its new location can be computed from Equation 3 by using the particle velocity found in Equation 6, yielding:
\[ x_{p}^{n+1} = x_{p}^{n} + \Delta t(u_{t} + C_{x}\tau_{p}) + \tau_{p}[1 - \exp(-\Delta t/\tau_{p})](u_{p}^{n} - u_{t} - C_{x}\tau_{p}), \]
\[ y_{p}^{n+1} = y_{p}^{n} + \Delta t(v_{t} + C_{y}\tau_{p}) + \tau_{p}[1 - \exp(-\Delta t/\tau_{p})](v_{p}^{n} - v_{t} - C_{y}\tau_{p}), \]  

(7)

Figure 2 shows trajectories of particles of different sizes in creeping flow where the Stokes drag law has been used. An observation that can be made from this figure is that compared to larger particles, smaller particles deflect more readily toward the electrode of the opposite polarity. Thus, particle charge to mass (volume) ratio is perceived to be an important parameter in electrostatic separation.

![Figure 2. Trajectories of different diameter particles in an electric field.](image)

THEORETICAL AND COMPUTATIONAL APPROACH

The separation of coal particles from impurities in the separation chamber involves tracking the motion of coal particles and solving fluid flow and electric field equations while accounting for interactions between particles and fluid. The phenomenon falls into the category of dispersed multiphase flow problems where there are two main approaches for finding solutions. In one approach, both carrier fluid and particulates are considered as continuum and are represented by two sets of mass conservation and momentum equations. This is called the Eulerian/Eulerian approach. In the other approach, the fluid is considered to be continuum while particles are treated as discrete points and their trajectories are calculated using Newton’s second law. This is called the Eulerian/Lagrangian approach. Each approach has its own advantages and disadvantages. The Eulerian/Lagrangian approach is more accurate since it tracks the motion of individual particles; however, it becomes computationally more expensive as particle mass flow rate is increased. On the other hand, the Eulerian/Eulerian approach is less accurate, but is well suited for flows with high volumes of particle loading.

In this project, an Eulerian/Lagrangian approach as implemented in the Discrete Phase Model (DPM) of FLUENT has been used. This technique has no restriction on the mass loading of particles; however, the particle volume fraction (i.e., particle volume over the volume of the whole domain) should be less than 10-12%, which is typically the case in
triboelectrostatic separation. There are several different options in solving flow field equations and tracking particles under the DPM, depending on whether one accounts for the influence of particles on fluid flow (i.e., two-way coupling) or does not (i.e., one-way coupling), as well as treating particles in a steady or unsteady fashion. In this project, steady-state particle tracking and two-way coupling have been used for most simulations; however, transient particle tracking was used for selected cases to make animations.

A. Fluid Flow Equations

The carrier fluid is air, which is a compressible fluid. However, since the geometric dimensions of the separation chamber are relatively small, air will not go through any significant pressure change. Therefore, it is reasonable to treat fluid flow as incompressible. This leads to simplification of the mass conservation equation to $\nabla \cdot \mathbf{u} = 0$, where $\mathbf{u}(\mathbf{x}, t)$ is the instantaneous fluid velocity.

Based on limited experimental data, it can be conjectured that the flow field in TES units under normal operating conditions will be turbulent. Thus, a turbulence model should be used to solve flow field equations. To this end, Reynolds-averaged Navier-Stokes (RANS) equations have been used in conjunction with a standard $k-\varepsilon$ model, $k$ and $\varepsilon$ being kinetic energy and dissipation energy of the turbulence. The essence of RANS is to work with equations of mass and momentum in a statistically-averaged form in order to remove small velocity scales, and therefore, to work with a modified set of equations that are computationally less expensive. To do so, the instantaneous velocity field $\mathbf{u}(\mathbf{x}, t)$ is decomposed into its mean (statistically-averaged) $\mathbf{\bar{u}}(\mathbf{x}, t)$ and fluctuation parts $\mathbf{u}'(\mathbf{x}, t)$; i.e., $\mathbf{u} = \mathbf{\bar{u}} + \mathbf{u}'$, and averaged equations are derived for mass and momentum equations. Averaging, however, introduces some unknown terms that must be modeled to close the equations. Equations are further closed by deriving an equation for fluctuation kinetic energy $k$ and dissipation energy $\varepsilon$. Mass and momentum conservation equations for mean flow are:

$$\nabla \cdot \mathbf{\bar{u}} = 0$$

(8)

$$\rho \left( \frac{\partial \mathbf{\bar{u}}}{\partial t} + \nabla \cdot (\mathbf{\bar{u}} \mathbf{u}) \right) = -\nabla \mathbf{p} + \rho \mathbf{g} + \nabla \cdot \mu \left[ \nabla \mathbf{\bar{u}} + (\nabla \mathbf{\bar{u}})^T \right] - \nabla \cdot \mathbf{R} + \mathbf{S}_m$$

(9)

where

$$\mathbf{R} = \mu \left( \nabla \mathbf{\bar{u}} + (\nabla \mathbf{\bar{u}})^T \right) - \frac{2}{3} \rho \mathbf{I}$$

(10)

is the Reynolds stress tensor according to the Boussinesq hypothesis. Here the following conventional notations have been used: $\mathbf{p}$ is averaged pressure, $\mathbf{g}$ is gravity, $\rho$ is density, and $\mu$ is viscosity. The momentum source term $\mathbf{S}_m$ is added to account for the influence of particles on the fluid flow (i.e., two-way coupling). Equations for turbulent kinetic energy $k$ and dissipation $\varepsilon$ are:
\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{u}) \right) = \nabla \cdot \left( \left[ \mu + \frac{\mu_t}{\sigma_k^2} \right] \nabla \mathbf{u} \right) + G_k + G_b - \rho \varepsilon - Y_m + S_k, \quad (11) \]

\[ \rho \left( \frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}) \right) = \nabla \cdot \left( \left[ \mu + \frac{\mu_t}{\sigma_k^2} \right] \nabla \varepsilon \right) + C_{1e} \varepsilon \left( G_k + C_3 \varepsilon G_b \right) - C_{2e} \rho \varepsilon^2 \varepsilon_k + S_c. \quad (12) \]

Here, \( \mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \) is called turbulence viscosity, \( G_k \) and \( G_b \) are called generation of turbulent kinetic energy and buoyancy, respectively, \( Y_m \) is called fluctuation dilation in compressible turbulence to the overall dissipation rate, and \( \sigma_k = 1, \sigma_e = 1.3 \) are called turbulent Prandtl numbers. Turbulent constants are \( C_{1e} = 1.44, C_{2e} = 1.92, C_\mu = 0.09 \).

Solving Equations 8-9 and 10-11 determine the velocity field, which can be used to calculate drag force on particles.

**B. Electric Field**

The governing equations of the electric field are Maxwell’s equations (Stratton, 2007). The charge conservation equation, along with the fact that the electric field \( \mathbf{E} \) is irrotational \((\nabla \times \mathbf{E} = 0)\) and divergence free \((\nabla \cdot \mathbf{E} = 0)\), leads to the Laplace equation for electric potential:

\[ \nabla^2 \phi = 0. \quad (13) \]

Once electric potential is calculated, electric field strength is found using \( \mathbf{E} = -\nabla \phi \). It should be noted that for cuboid separation chambers there is no need to solve the electric field equation as \( \mathbf{E} \) can be found directly from the electric potential difference of electrodes divided by their separation distance; i.e., \( E_x = \Delta \phi / H, E_y = 0 \).

**C. Equations of Motion of Particles**

The governing equations of particles are formally the same as Equations 3 and 5; however, a number of modifications must be made in Equation 5. Fluid velocity now evolves with both time and space, and therefore, it should be evaluated at each time step. Furthermore, a drag law should be adopted to calculate particle response time. It can be shown that the particle response time, in general, is:

\[ \tau_p = \frac{\rho_p d_p^2 C_{D_p}}{18 \mu_t C_D}, \quad (14) \]

where \( C_{D_p} = 24 / \text{Re} \) is the Stokes drag coefficient and \( \text{Re} = \rho_f d_p \left| \mathbf{u}_p - \mathbf{u}_f \right| / \mu_t \) is the Reynolds number based on the relative velocity of the particle and the fluid. Here, \( C_D = F_D / (1/2) \rho_f \left| \mathbf{u}_f - \mathbf{u}_p \right|^2 A_p \) is the drag coefficient and \( A_p = \pi d_p^2 / 4 \) is the projected
area of particles (assumed spherical). The drag coefficient can be calculated using empirical relations. Here, the spherical drag law suggested by Morsi and Alexander (1972) has been used:

\[
C_D = \alpha_1 + \frac{\alpha_2}{Re} + \frac{\alpha_3}{Re^2},
\]

(15)

where \(\alpha_1, \alpha_2,\) and \(\alpha_3\) are functions of the Reynolds number. Once velocities of particles are found, their trajectories can be found by numerical integration of Equation 3. To account for fluctuation velocities on particle trajectories particles, a “stochastic tracking” model has been used.

D. Numerical Method

The governing fluid flow equations are discretized using the finite volume technique and are solved using a projection algorithm in conjunction with SIMPLE for pressure solution. If the effect of particles on the flow field is neglected (i.e., one-way coupling), then particle trajectories will be found once fluid flow equations are solved. However, if disturbances caused by particles on the flow field is accounted for (i.e., two-way coupling), then the method will be iterative, comprising the following steps (Crowe et al., 1977): (1) Fluid flow equations are solved in the absence of particles; (2) Particles are introduced and their trajectories found using the flow field drag force that was just found; (3) Using particle trajectories, the momentum source term \(S_m\) is found and added to the right-hand side of Equation 9, which accounts for particle influence on the flow; (4) Trajectories of particles are found based on the updated flow field; and finally (5) Steps (3) and (4) are repeated until a converged solution is achieved where both flow field and particle trajectories are unchanged with additional calculations. In this project, a two-way coupling algorithm was used.

E. The Computational Setup and Boundary Conditions

The computational domain is shown in Figure 3 depicting a cuboid comprised of four walls. The top and the bottom surfaces are open, the left wall is grounded, and a known electric potential is imposed on the right wall. The front and the back are solid walls. Air as a carrier fluid brings coal particles into the separation chamber through the central opening at the top, and a co-flowing air enters the domain through the larger opening that encloses the central opening. The co-flow is used to prevent sudden expansion of the carrier fluid, and therefore, to stabilize the flow field. Furthermore, by adjusting the co-flow, particle residence time can be controlled more efficiently. Boundary conditions for the velocity field are no-slip and no-through at walls, imposed inlet velocity at the top, and imposed pressure at the outlet. Boundary conditions for particles are “scape” at both top and bottom, where particles can cross the computational domain, and “charge decay” at walls. Therefore, particles lose a percentage of their charges with each impact with a wall. Initially, “trap” boundary conditions were explored for particles, where the particles would be trapped at the wall once they collided with it; however, computer simulation
results showed that “charge decay” is conceptually and practically a more appropriate boundary condition. For particles with charge decay, the particle collision was considered elastic; i.e., the particle will bounce back with a restitution factor of one. It should be mentioned that the angle of reflection is taken to be the same as the angle of incidence. For the electric field, electric potential was specified at the surface of electrodes and its derivative in the normal direction was set to zero on the other surfaces.

![Figure 3. Problem setup.](image)

RESULTS AND DISCUSSION

A. Governing Nondimensional Numbers of the Problem

The advantages of presenting results in nondimensional form cannot be underestimated. Nondimensionalization not only leads to considerable savings in effort, time, and computations, but also enables one to extract trends from data that would otherwise remain disorganized and incoherent. To this end, dimensional analysis was performed to find governing nondimensional parameters of the problem. While in some simulations a broader distribution of particle sizes and charges was considered, to better understand the effect of charge and size distribution, several simulations were performed using only a binary distribution of sizes and charges.

On dimensional ground, controlling parameters of the problem are maximum and minimum diameters of particles \(d_{\text{max}}, d_{\text{min}}\) [m], maximum and minimum charges \(q_{\text{max}}, q_{\text{min}}\) [C], densities of ash \(\rho_a\) [kg/m\(^3\)] and fixed carbon \(\rho_c\) [kg/m\(^3\)], fluid density \(\rho_f\) [kg/m\(^3\)], fluid viscosity \(\mu_f\) [Pa.s], gravitational acceleration \(g\) [m/s\(^2\)], the strength of the electric field \(E\) [V/m], mass flow rate of particles \(m_p\) [kg/s], inlet velocity of the carrier fluid \(u_i\) [m/s], inlet velocity of the co-flow fluid \(u_c\) [m/s], and hydraulic...
diameters of openings for main flow and co-flow \( D_{hw}, D_{hc} [m] \). The aforementioned parameters constitute fifteen individual numbers and four basic dimensions, M (mass), L (length), T (time), and I (current) are needed to present these parameters in the SI system. Therefore, according to Buckingham PI theorem, there are eleven independent nondimensional or \( \Pi \) numbers that are found to be:

\[
\begin{align*}
\Pi_1 &= \text{St} = \frac{\rho_c u_t d^2_{max}}{\mu_t D_{n}}, \\
\Pi_2 &= \text{Re} = \frac{\rho_c u_t D_{b_n}}{\mu_t}, \\
\Pi_3 &= \frac{\rho_c}{\rho_f}, \\
\Pi_4 &= \frac{\dot{m}_p}{\rho_f u_t D^2_{b_n}}, \\
\Pi_5 &= \frac{\text{Eq}_{max}}{(\rho_c - \rho_f)gd^3_{max}}, \\
\Pi_6 &= \frac{\text{Eq}_{max}}{\mu_t u_t d_{max}}, \\
\Pi_7 &= \frac{q_{max}}{q_{min}}, \\
\Pi_8 &= \frac{\rho_a}{\rho_f}, \\
\Pi_9 &= \frac{u_c}{u_f}, \\
\Pi_{10} &= \frac{d_{max}}{d_{min}}, \\
\Pi_{11} &= \frac{A_c}{A_m}.
\end{align*}
\]

(16)

Here, nondimensional numbers that are simply the ratio of two individual parameters such as \( \Pi_3 \) are perceived as “secondary” numbers. Interpretations of “primary” nondimensional numbers are as follows: \( \Pi_1 \) resembles the well-known Stokes number and is essentially the ratio of particle response time \( \tau_p \equiv \rho_d d^2_p / \mu_t \) to the convective time scale of the flow \( \tau_c \equiv D_{b_n} / u_f \), \( \Pi_2 \) is the Reynolds flow number characterizing the strength of the main flow field, \( \Pi_4 \) is the ratio of particle mass flow rate over carrier fluid mass flow rate, \( \Pi_5 \) is the ratio of electric force over buoyancy force for fixed carbon, and \( \Pi_6 \) is the ratio of electric force to viscous force (drag).

B. Procedure Used in Construction of Separation Efficiency (SE) Curves

Separation efficiency (SE) curves are perhaps the most important results of simulations. To construct these curves, \( F \), \( C \), and \( T \) represent masses of feed (sample), concentrate (product), and tailings (refuse), respectively. Similarly, \( f, c, \) and \( t \) represent percentages of ash in feed, concentrate, and tailing, respectively. Therefore, conservation of total mass and mass of ash yield:

\[
\begin{align*}
F &= C + T, \\
fF &= cC + tT.
\end{align*}
\]

(17)

In SE curves, the horizontal axis is usually the percent ash of the concentrate, which is the ratio of the mass of ash in the concentrate over that in the feed:

\[
AC = \frac{cC}{fF} \times 100.
\]

(18)

Some researchers instead use ash rejection (AR) rate, which is the ratio of the mass of ash in the tailings over that in the feed by percentage:
\[
AR = \frac{\text{tT}}{\text{fF}} \times 100.
\]  

(19)

In this study, AC is used for the horizontal axis. The vertical axis is normally combustible recovery (CR), which is the ratio of the mass of fixed carbon in the concentrate over the mass of fixed carbon in the feed by percentage:

\[
CR = \frac{C(1-c)}{F(1-f)} \times 100.
\]  

(20)

To construct these curves, the outlet of the separator chamber was divided into five parts as shown in Figure 3, resulting in five points on the SE curve. Since carbon and ash acquire positive and negative charges, respectively, they will move toward negative (left) and positive (right) electrodes, respectively. Here, the first point on the SE curve will be the result of accounting for carbon and ash in the first bin, the second point is the result of accounting for carbon and ash in the first and second bins, and so on. Obviously, AC and CR for the fifth point are always theoretically 100% because of mass conservation; however, AC and CR of the last point was actually calculated as a further validation of the methodology and was found to match the theoretical value exactly.

C. Accounting for Particle Size and Charge Distributions

To account for particle size distribution, a “Rosin-Rammler” model as shown in Figure 4 was used. The essence of the model is to calculate the mass fraction \( Y_d \) of particles whose diameters are greater than a certain diameter \( d \), using the following equation:

\[
Y_d = \exp \left[ -\left( \frac{d}{\bar{d}} \right)^n \right],
\]  

(21)

where \( \bar{d} \) is the mean diameter of particles and \( n \) is called the spread parameter. These two parameters must be calculated to use this model.

Figure 4. Size distribution of particles using Rosin-Rammler model.
To implement this model, a distribution of particles in the range of 41-102 microns was used with $d = 70$ micron and $n = 4$. Given these two parameters and the total mass flow rate of particles, the software would then calculate corresponding mass fractions $Y_d$ for each group of particles according to the above equation.

The charge distribution was accounted for by using the size distribution of particles. Briefly, considering that the minimum and maximum size of particles are $d_{\text{min}} = 41$ and $d_{\text{max}} = 102$ microns, and corresponding minimum and maximum charges are $q_{\text{min}} = 1 \times 10^{-13}$ C and $q_{\text{max}} = 2 \times 10^{-13}$ C, a linear relation between particle charge and size was assumed yielding:

$$q = \left( \frac{d_{\text{max}} - d_{\text{min}}}{d_{\text{max}} - d_{\text{min}}} \right) d + \frac{q_{\text{min}} d_{\text{max}} - q_{\text{max}} d_{\text{min}}}{d_{\text{max}} - d_{\text{min}}}. \quad (22)$$

Using particle sizes, particle charge can be found from the above equation. This charge is then multiplied by a random number (between 0 and 1; generated using “Box-Muller” method) to account for randomness of the particle charge.

1) Validation

Mathematical formulation of particle dynamics driven by fluid flow in the presence of an electric field demands a good grasp of the laws of fluid flow and electrostatics and their interplay. While general perception about these laws may be common knowledge, unfortunately, a unified formulation of the problem does not seem to exist. Furthermore, the formulation relies on a great deal of empiricism because of its high level of complexity. For instance, it appears that there is no consensus about electric field equations that need to be solved and the manner in which the effect of charged particles on fluid flow should be implemented. The above uncertainties coupled with similar issues on how to handle boundary conditions for particle/wall interactions demand due attention. The goal has been to come up with a formulation that leads to results that closely mimic reality and avoid any unnecessary complication. To this end, all viable possibilities for solving the problem were considered and scrutinized through physical reasoning and numerical simulations. Specifically, electric field and fluid flow computations were validated as described in the next two paragraphs.

To calculate the electric field, Gauss’s law:

$$\nabla^2 \phi = -\frac{q_v}{\varepsilon_0}, \quad (23)$$

should be used, where $q_v$ is volume charge density, $\phi$ is electric potential, and $\varepsilon_0$ is the permittivity of air. Once $\phi$ is found, the electric field can be computed using $E = -\nabla \phi$. Some authors, however, have chosen to ignore the effect of particle charges on the electric field and to determine the electric field simply from $E = \Delta \phi / H$, where $\Delta \phi$ is the
electric potential difference between the two electrodes and $H$ is the separation distance between them. To examine the validity of the second approach, several computations were performed to determine electric potential $\phi$ and the strength of the electric field using the two methods for a collection of 100 charged particles, randomly distributed in a computational domain. These tests showed that for the range of particle electric charge and electric field that is common for TES systems, the simplified approach leads to reasonably accurate results. Figure 5 shows results from one of these tests. The left and right frames show contours of electric charge density and electric field potential $\phi$ along with vectors of electric field strength $E$. Here, data correspond to a realistic case (reported in pilot-scale electrostatic precipitators) comprising $\Delta \phi = 200$ kV and $H = 1$ m for a collection of 100 particles with average charge density of $q_p = 2 \times 10^{-13}$ C per particle. As can be seen, electric field potential changes linearly from the potential corresponding to the grounded (lower) electrode to that of the upper one. Electric field vectors are completely straight. These computations were done using in-house code.

![Figure 5](image.png)

Figure 5. Effect of particles on electric field with contours of electric charge density in the left frame and contours of potential electric field and vectors of electric field strength in the right frame.

Fluid flow equations for both turbulent and laminar regimes in a channel were solved in the absence of particles and fully developed mean velocity profiles were compared against the empirical profile for the former and the Poiseuille flow profile for the latter, leading to excellent agreement between the two. When particles were introduced, particle trajectories were compared qualitatively with those found by other investigators (such as Ha et al., 2003) under the same boundary conditions and excellent agreement was found between the two.

D. Reference Simulation

A large number of simulations were performed to explore the effect of governing nondimensional parameters on SE (grade recovery) curves. Three of these simulations are described in detail to put the work in perspective. Input parameters for these simulations are given in Tables 1 and 2, and pertinent nondimensional numbers are presented in Table 3. Mass percentages of ash and fixed carbon in the mixture are 30% and 70%, respectively. About 300,000 cells were used to resolve the flow field. The initial velocity of particles is the same as the velocity of the carrier fluid and charge and particle size distributions are random. Furthermore, with each particle-wall collision, particles lose part of their charge randomly.
Table 1. Input parameters used for reference case.

<table>
<thead>
<tr>
<th>Co-flow Velocity $u_c$</th>
<th>Main Flow Velocity $u_f$</th>
<th>Fixed Carbon Density $\rho_c$</th>
<th>Ash Density $\rho_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.125 m/s</td>
<td>2.5 m/s</td>
<td>1917 kg/m$^3$</td>
<td>976 kg/m$^3$</td>
</tr>
<tr>
<td>Fluid Density $\rho_f$</td>
<td>Fluid Viscosity $\mu_f$</td>
<td>Particle Mass Flow Rate</td>
<td>Electric Field Strength</td>
</tr>
<tr>
<td>1.2 kg/m$^3$</td>
<td>1.79×10$^{-5}$ Pa.s</td>
<td>2.2×10$^{-4}$ kg/s</td>
<td>460 kV/m</td>
</tr>
</tbody>
</table>

Table 2. Injection characteristics used for the reference case.

<table>
<thead>
<tr>
<th>Injections Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
</tr>
<tr>
<td>Carbon</td>
</tr>
<tr>
<td>Ash</td>
</tr>
</tbody>
</table>

Table 3. Nondimensional numbers used for the reference simulation.

<table>
<thead>
<tr>
<th>$\Pi_1$</th>
<th>$\Pi_2$</th>
<th>$\Pi_3$</th>
<th>$\Pi_4$</th>
<th>$\Pi_5$</th>
<th>$\Pi_6$</th>
<th>$\Pi_7$</th>
<th>$\Pi_8$</th>
<th>$\Pi_9$</th>
<th>$\Pi_{10}$</th>
<th>$\Pi_{11}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>125</td>
<td>3800</td>
<td>1600</td>
<td>0.14</td>
<td>4.5</td>
<td>20</td>
<td>2</td>
<td>815</td>
<td>1.25</td>
<td>2.5</td>
<td>9.6</td>
</tr>
</tbody>
</table>

The first simulation is called “the reference simulation”. Here, 50,000 particle streams are introduced at the injection surface. The left frame of Figure 6 shows contours of electric potential between the two electrodes in a vertical plane normal to the electrodes, where it is seen that electric potential changes linearly. The middle frame shows velocity vectors in a mid-plane parallel with the electrodes. As is evident, the velocity field is nearly uniform, with the core velocity slightly lower than velocities at the sides. The relatively uniform velocity at the core is typical of mean turbulent velocity profiles; however, the reason that the velocity is lower in the core than at the sides is due to the fact that the co-flow velocity was higher than that of the carrier fluid velocity in these simulations. The right frame of Figure 6 shows trajectories of some particles in the computational domain. Here, to aid with visualization, only trajectories of 260 particles out of a total of 50,000 particles are plotted. Particles are initially color-coded (blue, red, and green) representing strongly charged negative, positive, and nearly uncharged particles. As is evident, strongly charged particles collide with the electrode of opposite polarity immediately after injection, while nearly uncharged particles move downward without colliding with the walls. However, all particles are eventually represented by the green color because of charge decay. The number of particle collisions with and bounce backs from walls depends on an assigned random charge decay factor.
To explore the effect of co-flow in separator performance and its role in the stability of the confined jet (carrier fluid), two additional simulations were done with co-flow eliminated. In the first simulation, all the nondimensional numbers remain the same except for $\Pi_9$, which is now zero. In the second simulation, the velocity of the carrier fluid was also increased. The left frame of Figure 7 shows velocity vectors for the first case. In contrast to the velocity vectors of the reference simulation, which were nearly uniform throughout the domain, in this simulation the velocity field consists of a core that is not blunt and two vortices that are formed around the core because of sudden expansion of the jet. These vortices are initially small, but they grow until they reach the channel outlet. At this time, a back flow is formed, which can destabilize the main jet. Even if the jet remains stable, this flow pattern is not desirable because particles will be trapped inside these vortices, which is detrimental to the grade recovery curve. The carrier airflow that brings the coal particle into the separation chamber is susceptible to generating self-sustained oscillations. This is a known fact, which is generally true for flows in cavity-type geometries. Oscillations are caused by the creation of backflow at the channel exit, which leads to a feedback effect (Maurel et al., 1996). The right frame of Figure 7 shows a side-view of particle trajectories, where it is seen that they strongly correlate with the flow pattern. It will be shown in the next section that separation efficiency for this case is lower than that of the reference frame.

Figure 8 shows contours of the magnitude of the fluid velocity field for the second simulation in two perpendicular vertical planes, where the carrier fluid becomes unstable and tilting of the main jet toward electrodes and other walls and lack of symmetry in the flow field are clearly seen. Obviously, this asymmetry will adversely affect separation efficiency.
E. Parametric Study

In what follows, results of a parametric study of the problem using the geometrical setup shown in Figure 3 are presented.
1) Effect of Stokes Number $\Pi_1 = \frac{St}{(\rho_c u_i d_{\text{max}}^2)/(\mu_i D_h)}$

The Stokes number is the ratio of particle response time to convective time of the flow field. In other words, if the Stokes number is low, particle inertia is small (i.e., very fine particles) and particles will adjust rather instantaneously with changes in the flow field. On the other hand, if the Stokes number is large, particles will not be influenced much by changes in fluid velocity. For this project, the Stokes number of the reference case was 125 and two simulations were performed at Stokes numbers of 500 and 25. Figure 9 compares separation efficiency for these cases with that of the reference case. As is evident, the separation efficiency decreases as the Stokes number increases. This is because as the Stokes number becomes larger, the particle size increases, and therefore, the particle charge to mass ratio will decrease. This emphasizes further that triboelectrostatic separation is more effective in manipulating fine particles.

![Figure 9. Effect of $\Pi_1$.](image)

2) Effect of Reynolds number $\Pi_2 = \frac{Re}{(\rho_c u_i D_h)/(\mu_f)}$

The Reynolds number represents the ratio of inertia forces to viscous forces. The Reynolds number for the reference simulation was 3800 based on the hydraulic diameter of the central opening. Thus, the flow is perceived to be inertia dominated. To explore the effect of this parameter, two simulations at Reynolds numbers of 38,000, and 380,000 were performed. The left frame of Figure 10 compares grade recovery for these cases with that of the reference case, where it is seen that increasing the Reynolds number leads to an increase in grade recovery. This is because for this set of parameters, when carrier fluid velocity is increased, it carries particles for a longer distance along the channel before the electric field diverts them toward one of the electrodes. Accordingly, particles have a shorter time to remix when they lose their charge and bounce back from the wall. Comparing trajectories of particles for $Re = 380,000$ (Figure 10, right frame) with those of the reference case (Figure 6, right frame) clearly supports this argument.
Figure 10. Effect of $\Pi_2$ (Reynolds number). Trajectories shown on the right are for $\Pi_2 = 380,000$.

3) Effect of carbon/fluid density ratio $\Pi_3 = \rho_c / \rho_f$

Densities of carbon and ash in coal are well-documented in the literature and do not vary too much from sample to sample. Nevertheless, it was beneficial to explore the effect of this parameter on grade recovery. Here, $\Pi_3$ was 1600 for the reference case and two cases were examined with $\Pi_3 = 800$ and 3200. Figure 11 provides simulation results showing that grade recovery is essentially unaffected by changing of this parameter. Inspection of selected trajectories did not show a pronounced difference between the three cases; however, based on another set of simulations conducted during the course of this project, it was found that a decrease in the density difference of particles would generally lead to a decrease in separation efficiency. That is because the efficiency of electro-separation is higher when positively and negatively charged particles respond differently to electric forces. However, when the density of particles becomes the same, their response becomes nearly the same. This is seen in the $\Pi_3 = 800$ case where density of ash and fixed carbon are equal and in the $\Pi_3 = 3200$ case, where there is some improvement in grade recovery.

4) Effect of ratio of particle to carrier fluid mass flow rate $\Pi_4 = \dot{m}_p / \rho_f u_f D_h^2$

A number of simulations were performed to explore the effect of this parameter. However, as it turned out, variation of this parameter did not affect the grade recovery curve noticeably. This is mainly due to the low volume fraction of particles in conjunction with the fact that the methodology does not account for particle/particle interactions.
5) Effect of electric force over the buoyancy $\Pi_5 = \frac{Eq_{\text{max}}}{(\rho_c - \rho_r)gd_{\text{max}}}$

This parameter represents the ratio of electric force to buoyancy. The reference parameter was $\Pi_5 = 4.5$, and two simulations were performed at 0.1 and 40. Figure 12 shows results of this simulation, where it is seen that a ten-fold increase in this parameter does not affect the grade recovery curve, while a forty-five-fold decrease leads to improvement of the grade recovery curve. Inspection of trajectories showed that in the range of $\Pi_5 \leq 4.5-40$, the electric force is much more dominant than the buoyant force. As such, variations of this parameter within this range did not affect points of collision of particles with electrodes. However, when this parameter was decreased to 0.1, the gravitational force became more dominant and shifted collision points dramatically downward. As a result, particles had less time to remix after rebounding from walls, and therefore, there was improvement in grade recovery.
6) Effect of electric force over the fluid drag $\Pi_6 = \frac{E}{\mu_i u_i d_{\text{min}}}$

This parameter represents the ratio of electric force to fluid drag. For the reference case $\Pi_6 = 20$, and two simulations were performed at 4 and 40 with Figure 13 showing results. Interestingly, the behavior of the grade recovery curve with this parameter is not monotonic; i.e., both with an increase and a decrease in this parameter, the grade recovery improves. The justification for this behavior comes from the fact that due to the random charge distribution, some particles will be strongly charged while others will be weakly charged. Weakly charged particles generally move in the middle and do not divert toward electrodes, while strongly charged particles will be readily attracted toward the electrode of opposite polarity. When this parameter is increased from 20 to 40, the electric field will be more dominant than fluid drag forces. As a result, particles with lower charge will be more influenced by the electric field, which tends to improve the separation efficiency. On the other hand, decreasing this parameter from 20 to 4, eliminates the unwanted remixing of highly charged particles. It appears that the interplay between these opposing effects determines grade recovery. For the case shown here, the positive impact of the increase in the electric field on weakly charged particles are more than its negative impact on highly charged particles. A similar argument can be used to justify the increase in grade recovery because of a decrease in $\Pi_6$.

![Figure 13. Effect of $\Pi_6$.](image)

7) Effect of maximum to minimum charge ratio $\Pi_7 = \frac{q_{\text{max}}}{q_{\text{min}}}$

The particle charge distribution is determined from the particle size distribution using a linear relation given by Equation 22. For the reference case $\Pi_7 = 2$, and two simulations were performed at $\Pi_7 = 1$ and 6.25. Here, the ratio of these charges was changed by increasing the minimum charge. Thus, the average particle charge for $\Pi_7 = 1$ is greater than that of the reference case, while the opposite is true about $\Pi_7 = 6.25$. Figure 14 shows grade recovery curves, where it is seen that separation efficiency decreases for both cases. This apparently contradicting result (i.e., nonmonotonic behavior of the
separation efficiency with respect to $\Pi_7$) is similar to what was seen in the case of $\Pi_6$ and can be explained using a similar argument. There is an optimum average charge distribution, where the effect of the electric field on particles is just enough to separate them without dramatic rebounding and their remixing. Below this optimum charge distribution, separation efficiency drops down because the electric field does not separate particles as effectively, while above the optimum charge distribution, the electric field is excessive, leading to rebounding and remixing of particles.

![Figure 14. Effect of $\Pi_7$.](image)

8) Effect of ratio of co-flow over carrier flow velocity $\Pi_9 = u_c/u_f$

As previously discussed, adding a co-flow in general improves separation efficiency because it eliminates unwanted side vortices around the carrier fluid (the main jet). Furthermore, the co-flow can be used to control particles more efficiently. For the reference simulation, $\Pi_9 = 1.25$, and two cases were simulated; one with $\Pi_9 = 0$ (zero co-flow) and one at 0.4. Figure 14 shows grade recovery curves, where it is seen that lowering the co-flow adversely affects grade recovery.

![Figure 15. Effect of $\Pi_9$ (co-flow).](image)
9) Effect of Geometry

The angle of reflection of charged particles after their collision with walls strongly influences the grade recovery curve. Particles lose part of their charge and bounce back with a reflection angle that is the same as the angle of incidence. Depending on the particle velocity, it is possible that particles move toward the electrode of the same charge. One way to reduce the adverse effect of particle/wall collision is to increase the separation distance between electrodes gradually to decrease the angle of reflection. This can be seen from Figure 16, which shows the angles of incidence and reflection for a straight (blue line) and an inclined (red line) channel. To explore this idea, several simulations were performed using an expanded channel as shown in Figure 17. Figure 18 compares separation efficiencies for these two channels, where it is seen that the divergent channel leads to improved separation efficiencies in all cases.

![Figure 16. Comparison of incidence/reflection angles in divergent (red) and straight (blue) channels. Here, $\theta'_1 = \theta'_2$ is related to the straight channel while $\theta_1 = \theta_2$ is related to the inclined channel.](image)

![Figure 17. Setup used to study geometric design.](image)
Conclusions

1. Governing nondimensional parameters of triboelectrostatic separation of coal were identified. Nondimensionalization was useful to represent results universally and to capture the interplay of various parameters in an unambiguous way.

2. A computational methodology was developed to simulate the triboelectrostatic separation process. Results provide a detailed description of electro-separation phenomena, such as flow patterns, particle trajectories, and electric fields, which are typically hard to discern by performing experiments. Computational results were generally in line with available experimental data and intuition. It was shown that the interplay between particle residence time, particle/wall collision point and angle, and charge to mass ratio is the single most important parameter determining separation efficiency. Thus, effects of various controlling parameters such as electric field strength, particle charge, and carrier fluid velocity will ultimately boil down to how these parameters affect this interplay.

3. It was shown that co-flow is necessary to stabilize the flow by eliminating side vortices that can trap particles. The co-flow was also useful in preventing asymmetry even in stable jets, and therefore, to increase separation efficiency.

4. The effect of channel geometry was explored and it was shown that a slightly divergent channel provides better separation efficiency by reducing the angle of incidence/reflection, and therefore, preventing particles from being thrown toward the electrode of the same charge following collision with a wall.

Recommendation

1. Results from this study show the need for understanding the charging process during tribocharging and particle/particle charge transfer in the separation chamber to mimic reality more closely.
REFERENCES


DISCLAIMER STATEMENT

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