Simulation in the field of gas filtration and separation

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VOLUME I

CONTENT VOLUME I

CONTENT VOLUME II

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Tuesday, March 22, 2011

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SORTING OF DIFFERENT MATERIALS

WASHING AND EXTRACTION

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L2 - Centrifugal Sedimentation Technology I Chairman: Sebastian Stahl	**13:15-14:30 h**
G1 - Measurement Techniques Chairman: Wilhelm Höflinger	**13:15-14:30 h**
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G7 - Surface Filtration **15:00-16:15 h**
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L13 - Cake Filtration Technology **16:45-18:00 h**
Chairman: Gernot Krammer

L14 - Electrostatic & Electrokinetic Effects in Separation Processes **16:45-18:00 h**
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G8 - Mist and Droplet Separation **16:45-18:00 h**
Chairman: Siegfried Ripperger

S6 - Simulation in the field of gas filtration and separation **16:45-18:00 h**
Presenter: Paolo Tronville

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L16 - Rotary Cake Filtration Technology **8:30-9:45 h**
Chairman: Harald Anlauf

M5 - New Membranes **8:30-9:45 h**
Chairman: Thomas Peters

G9 - Poster Session II **8:30-9:45 h**
Chairman: Hans-Joachim Schmid

L17 - Depth Filtration – Modelling and Simulation II **11:00-12:15 h**
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L18 - Regenerable and Non-Regenerable Filters for Cleaning of low concentrated Liquids I Chairman: Sebastian Stahl **11:00-12:15 h**

M6 - Special Applications **11:00-12:15 h**
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G10 - HEPA/ULPA Filters **11:00-12:15 h**
Chairman: Arunangshu Mukhopadhyay

L19 - Depth Filtration – Modelling and Simulation II **13:15-14:30 h**
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L20 - Regenerable and Non-Regenerable Filters for Cleaning of low concentrated Liquids II Chairman: Siegfried Ripperger **13:15-14:30 h**

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L22 - Removal of Particles and Scales from Surfaces **15:00-16:15 h**
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G13 - Industrial Gas/Air Cleaning I **15:00-16:15 h**
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L23 - Separation Enhancement by Flocculation **16:45-18:00 h**
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L24 - Removal of Pollutants from Water by Catalytic, Biological and Encymatic Treatment Chairman: Harald Anlauf **16:45-18:00 h**

G15 - Industrial Gas/Air Cleaning II **16:45-18:00 h**
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G16 - Special Filter Media II **16:45-18:00 h**
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SIMULATION IN THE FIELD OF GAS FILTRATION AND SEPARATION

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ABSTRACT

The paper surveys the history and present status of simulation of equipment to capture aerosols and gaseous air contaminants. Simulation of both industrial and effluent separation devices and fibrous filters are reviewed. Problems involved in simulating actual operating conditions, unusual atmospheres, turbulence and nano-scale filter structures are discussed, along with the computational limits of current CFD schemes. Suggestions are made for further refinement of simulation models to obtain better agreement between simulations and experimental data.

KEYWORDS

Air Filters, CFD, Fibrous Filters, Filtration Performance, Gas Cyclone, Modelling, Simulation, Venturi Scrubber

1. Introduction

Detailed calculation of the performance of gas phase separation equipment involves solutions of sets of differential equations which describe flow through the separation devices. The strength of computational fluid dynamics (CFD) in solving such equations has created a mindset which equates CFD with simulation. However, in gas filtration and separation technology, we find useful simulations which do not use CFD.

In the broadest sense, simulation includes all laboratory tests, where the tested device may be only part of an actual device, or a small-scale model of it. Tests try to mimic field conditions, but often use conditions far from those in actual applications.

A second type of simulation occurs when analyzing data from experiments. Before any mathematical description of a gas cleaning device can be made, some model for the performance of the device must be assumed. Indeed, one can devise mathematical models without any experimentation, or use them to guide experiments. The extent to which the mathematical model reflects the actual geometry of the device simulated, and the physics of its behavior, can determine how accurate its predictive equations will be.

Often the search for descriptive equations requires gross simplifications of the actual shapes and operating conditions to allow mathematical analysis. These results may be useful for selection of equipment or improving its design. But in many cases, the geometry of a device is too complicated for classic mathematical analysis. In CFD we have a means to overcome this barrier. It breaks our models into thousands of little pieces that can be digested by computer codes, and produces performance descriptions whose accuracy can a least be quantified. If CFD analysis gives performance predictions close enough to measured data, the model used for the verified CFD calculation can be extended to predict performance at other conditions, and for equipment optimization. If CFD fails, we revise the model, and try again.

We have some guidance in the simulation process, or at least warnings of troubles ahead, attributed to some great thinkers:
“A scientific theory should be as simple as possible, but no simpler” (A. Einstein);
“All models are wrong, but some are useful” (Statistician George Box);
“Correlation does not imply causation” (Somebody long before Aristotle).
With these understandings of the nature of simulations, let us examine how they have assisted the development of filtration and separation technology.

2. Venturi scrubbers

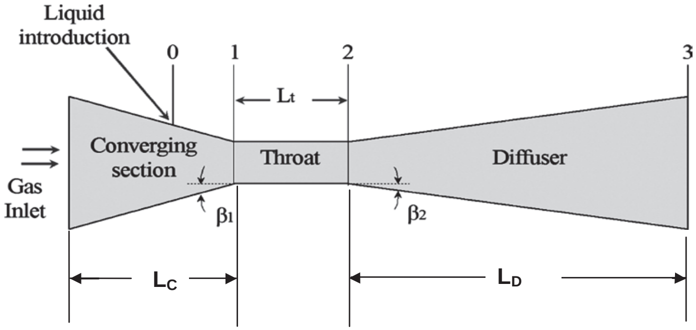


Figure 1 - Venturi Scrubber Schematic [adapted from Economopoulou (2007)]

Figure 1 shows a longitudinal section of a venturi. Although the geometry of the venturi is simple, analysis of its performance is not. At least the following parameters must be considered in to determine the pressure drop and efficiency of the venturi:

Gas flow volume	Liquid injection position	Particle concentration,
Liquid-flow rate	Gas and liquid properties	density, morphology
Venturi geometry	Droplet characteristics	and diameter

The venturi must be followed by a cyclone to capture the droplets bearing particles captured in the venturi. The efficiency and pressure drop of this cyclone are parameters in the overall system performance. The simulation of the cyclone portion of such a system is considered in the next section.
The equations listed below show the level of complexity involved in various analyses. Subscripts *G* and *L* refer to gas and liquid; subscripts *p* and *d* to particle and droplet.

2.1 Venturi Pressure Drop

There are many reports of test results on venturi scrubbers with wide ranges of the above parameters. Some of these test sets were used to develop predictive performance equations incorporating the physical phenomena considered pertinent by the authors. Examples of equations predicting venturi pressure drop are contained in Calvert (1970 and later), Boll (1973), Hesketh (1974), Yung (1977), and Leith et al. (1985). In spite of these years of study, the prediction of pressure drop by these analytical methods is poor. Figure 2 gives the agreement between the pressure drop predictions of Leith and measurements for a wide range of venturi sizes and operating conditions. At 0.59 kPa, the agreement ranges from -28% to +80%. If the velocity pattern, which determines pressure drops in a gas cleaning device, is based on an unreliable model, then modeling particle capture using that model is futile.

Clearly, something is needed beyond correlations of empirical data, even if the correlations are guided by what seem to be reasonable physical concepts. CFD might be that something.

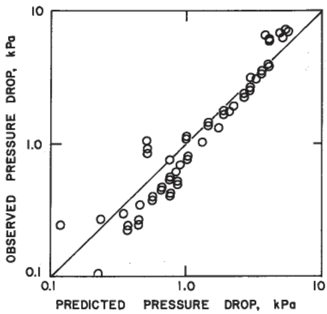


Figure 2 - Comparison, measured values of pressure drop to analytical predictions [from Leith et al. (1985)]

2.2 *Venturi Particle Efficiency and Penetration*

The analysis of particle capture is far more complicated, and the accuracy of prediction less reliable. In this discussion, we will list expressions for penetration, which measures the fraction of pollutant that passes a separator. [Penetration = (1-Efficiency), both fractions].

An example of the limited use of predictive equations is shown in Hesketh (1973):

$$\text{Penetration} = C_o / C_i = \frac{95200}{v_t^{2.86} \rho_G^{1.43} A_t^{0.19} R_{LG}^{1.12}} \qquad (1)$$

Unfortunately, this expression contains nothing related to dust properties, so is merely a correlation built on the data set Hesketh used.

A later example is from Costa et al. (2005), a correlation including both inertial and diffusion collection on water droplets in a venturi:

$$\text{Penetration} = \exp\left[-51.9\left(\frac{Q_L(1-F_f)\rho_L D_d}{A_t \mu_G}\right)^{0.19}\left(\psi^{0.169} + 2813 Pe^{-0.581}\right)\right] \qquad (2)$$

Where

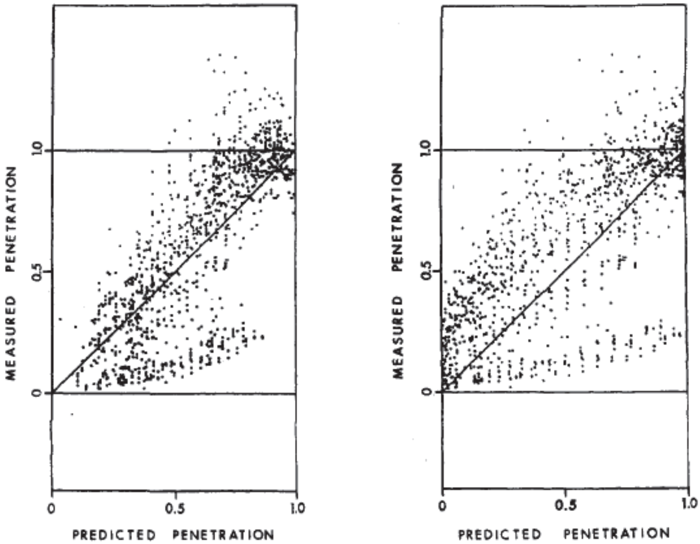
$$\psi = \frac{\rho_p d_p^2 v_G C}{18 \mu_G D_d} \text{ (inertial parameter)} \qquad (3)$$

$$Pe = \frac{3\pi v_G D_d \mu_G d_p}{K_B T C} \qquad (4)$$

These expressions gave remarkably good fits to experimental data when only a single variable was considered (e.g. particle diameter), but penetration by Equation 2 including all variables gave predictions of penetrations of 1% to 7% for measured values in the range of 0.1% to 9%. Penetration is, admittedly, a demanding criterion for judging predictive equations.

Yung et al. (1977) and Boll (1973) both modified an earlier analysis by Calvert, eliminating some of the assumptions, which also eliminated some empirical constants. To display Yung's efficiency equation set takes almost a whole page; Boll's expression is in differential form, and must be solved by numerical methods.

Rudnick et al (1986) applied the expressions developed by Yung and Boll to efficiency test data on three venturis. Plots of predicted vs. measured penetration results are shown in Figure 3 which shows that these regression equations for penetration, hence efficiency, essentially predict nothing, in spite of their complexity.



Results using Yung (1978) Results using Boll (1973)

Figure 3 - Comparison of venturi penetrations predicted by Yung and Boll equations to measured data [from Rudnick et al. (1986)]

2.3 Venturi CFD Simulations

CFD analyses of various aspects of venturi performance include studies by: Anathanarayanan and Viswanathan (1999); Ravi et al. (2003); Ahmadvand and Talaie (2009); Pak and Chang (2006).

Analysis of particle capture by venturis must include, in addition to the above list of items needed for pressure drop calculation, particle wettability. A great deal of attention has been given to the particle size distribution of the droplets created in the venturi throat, and to their spreading across the throat area. Each of the authors of these CFD studies assures us that the agreement between measurement and CFD simulation was excellent. It would be interesting to have the kind of comparison made by Rudnick et al. on a wide array of venturi scrubber designs. The labor involved would, however, be immense.

What we do know is that every CFD analysis needs to include verification studies. The ideal CFD solution to its sets of differential equations would use infinitesimal steps of time and space coordinates. We must do with finite steps, but there are techniques for extrapolating the results to “zero” scale of the computational mesh used. A reliable CFD analysis requires at least three runs using successively smaller mesh scales in order to perform the extrapolation to zero scale. The paper of Herman et al. (2006) illustrates this process. The internet site of the US space agency NASA offers an extensive tutorial on this and other recommended procedures for verification and validation of CFD calculations. (See www.grc.nasa.gov/www/wind/valid/homepage.html)

3. Cyclones

The first patent for a dust-collecting cyclone was apparently issued to J.M. Finch in 1885. Although his cyclone little resembles present-day designs, the germ of the cyclone concept was there. Dirty gas entered a cylinder tangentially at high velocity, and the bulk of the flow exited axially. In Finch's design, dust was expelled by centrifugal force through slots in the wall of the cylinder, a more complicated and less effective scheme than the flow reversal and bottom dust drop-out of current cyclone designs. The configuration of Figure 4 uses Finch's tangential entry, but the swirling flow reverses at the bottom of the cyclone cone, and dust drops out of the cyclone cone into a hopper. This design was widely used by the early 1900s, and is still important.

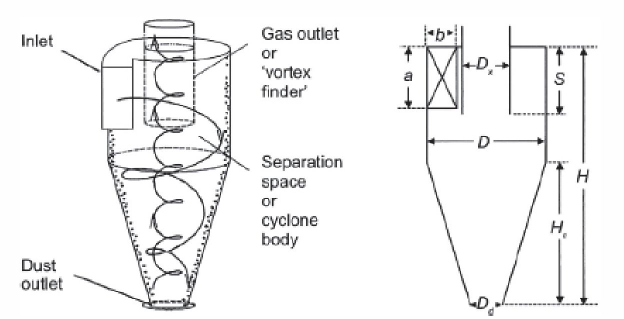


Figure 4 - Tangential-inlet cyclone and defining dimensions [from Gronald (2011)]

Efforts toward improved performance produced many modifications to the basic cyclone concept, with elements inserted into the cyclone to channel flows and counter-flows of gas and dust. The cyclonic, centrifugal concept is available in a wide array of sizes, from tiny sampling instruments to units a meter or more in diameter. In addition, there are designs which substitute a spin-generating helix in the inlet air flow for the tangential inlet. These are called axial-flow cyclones.

Mathematical analysis of what was happening inside cyclones was rather limited in the 19th century. Some pieces of the puzzle were available then. We speak of "Newtonian fluids" because the great polymath produced the first serious understanding of viscosity, in the mid-17th century. (Most analysis of the motion of small particles in cyclones is pure Newtonian mechanics, and there is a lot of use of Newton's calculus, also). Bernoulli, Euler, d'Alembert, Lagrange, and Laplace all made significant contributions to the necessary mathematics, still used in our CFD codes. Navier made his contribution to the laws governing fluid flows in 1822, and Stokes his in 1842. By 1851 Stokes had also derived the expression for the aerodynamic drag on a small particle, fundamental to the simulation of particle motion in a cyclone. Other early advances came from: Hagen and Poiseuille (laminar pipe flow, 1839); Darcy (porous-bed flow, 1856); Rayleigh (convection, 1880s).

Most of the great advances in fluid mechanics which form the basis of our present simulations took place after 1900. Reynolds published his first work shedding some light on turbulent flow a little earlier, in 1895. To name a few other contributors: Prandtl (boundary-layer theory, 1904); Buckingham (dimensional analysis, 1914); G. I. Taylor (turbulence, 1923); von Karman (turbulence, boundary layer theory, supersonic flow, 1930s); Kolmogorov (turbulence, 1940); Spalding (turbulence, CFD, 1970s).

The parameters defining cyclone operation include those in the venturi list above, including parameters related to liquids when the cyclone collects liquid particles. The cyclone geometry must of course be defined, along with any "bleed air" flow withdrawing the separated dusty portion of the flow. The more sophisticated studies include the effects of boundary layer conditions at the surface of the cyclone cone.

3.1 Empirical Correlations of Cyclone Performance

An excellent review of cyclone modeling is given by Zhao (2007). He identifies three model forms: "equilibrium orbit"; "timed flight"; and hybrids of these. He then notes that there are three approaches to obtaining expressions for cyclone pressure drop and efficiency/penetration from these models.

The first method uses detailed definition of the physical mechanisms present in the model, and mathematical description of these. The second method uses dimensionless groups, and seeks the combinations of these groups and exponents applied to them which best fit measured performance data. Finally, there is CFD.

Zhao's paper describes rigorous means to optimize predictive equation parameters using the dimensionless group method. His results appear to provide a substantial improvement over earlier attempts to correlate empirical data obtained on cyclones.

The regression equations compared in Zhao's paper are representative of the work on cyclone performance that has appeared in the literature: Barth (1956); Leith and Licht (1971); Dietz (1981); Mothes and Löffler (1988); Li and Wang (1989); Iozia and Leith (1990); Clift et al. (1991). Citations for these studies are given by Zhao.

3.2 CFD Predictions of Cyclone Performance

In most cases, cyclone flow will be turbulent, and a turbulence model with its parameters must be chosen. The Reynolds stress model for turbulence (RSM) has proved to be the most reliable. Equations calculating the level of gas "slip" at the cyclone walls and at the surface of particles must be supplied.

Boysan et al. (1982); Zhou et al. (1990); Ogawa (1997); Meier and Mori (1999); Witt et al.(1999); Zhao et al. (2004); Martignoni et al. (2007); Bernardo et al. (2006) present analyses of cyclone performance using CFD. Shalaby (2007) is essentially a tutorial on the application of CFD to cyclones, with explanations of many CFD problems. Figure 5 is an example of the velocity patterns obtained in his study. The tangential inlet flow is not shown, but the velocity differences between outer (blue) and inner (red) vortices are shown. The boundary layer on the inside the discharge pipe appears, graded from blue (low velocity) through green and yellow to red (high velocity).The color image appears in the thesis.

Comparisons between CFD predicted and measured values of cyclone performance are rare in published literature. Figure 6 is one example, from Crosby and Frye (2008). The results from Shepherd and Lapple (1940), long before CFD, are closer to measured values than Crosby and Frye's CFD results. The measurements of efficiency at 1/6 normal gravity were made on an aircraft on a parabolic flight path, which simulates zero gravity for about 30 seconds. Validating CFD can be difficult.

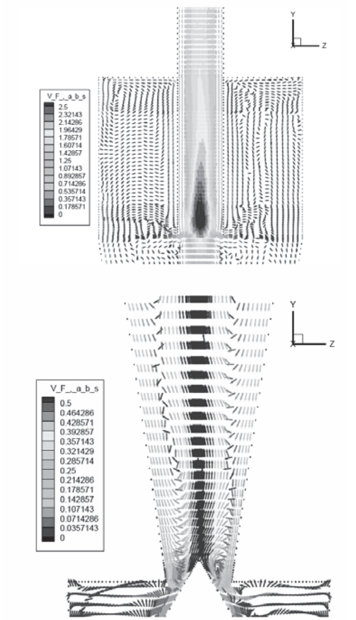


Figure 5 - CFD-generated pattern of velocity vectors for tangential-inlet cyclone [from Shalaby (2007)]

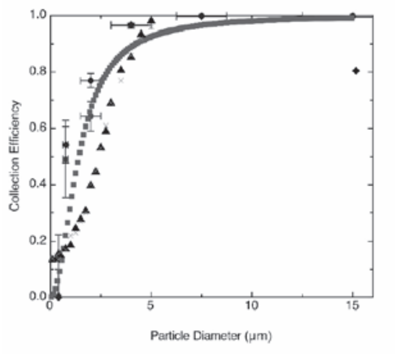


Figure 6 - Cyclone Efficiency Dependence on Particle Diameter [from Crosby and Frye (2008)]

Predicted:

■ Shepherd & Lapple (1940)

▲ Crosby & Frye (CFD, normal gravity)

x Crosby & Frye (CFD, zero gravity)

Measured:

♦ Crosby & Frye (normal gravity)

● Crosby & Frye (CFD, 1/6 normal gravity)

4. Louvers

We have found a limited number of references for simulations of this form of inertial separator. Figure 7 shows the geometry of a flat-blade louver separator.

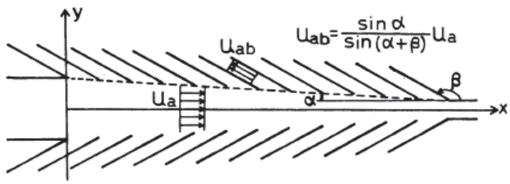


Figure 7 - Geometry Used for CFD Simulations of Louver Performance [from Hiyoshi (1988)]

Hiyoshi traced large (12 μm to 102 μm mass mean diameter) particle paths through this simulation of a louver cross-section, using CFD methods. They obtained the results shown in Figure 8. By positioning a plate splitting the central chamber in half the performance was greatly improved, apparently holding impacting particles. At high inlet velocities, without a center plate, the CFD- calculated paths sometimes showed particles bouncing back and forth between the opposite sets of louver blades. Enikeev (1995) modeled the paths of water droplets by CFD in similar structures.

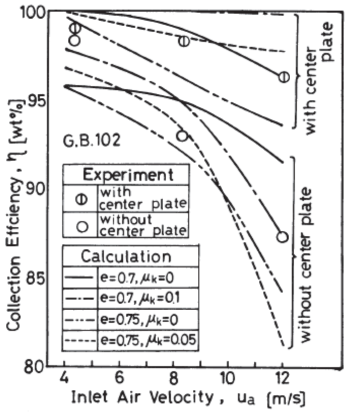


Figure 8 - CFD Simulations of Louver Efficiency [from Hiyoshi (1988)]

5. Electrostatic Precipitators

Electrostatic precipitators (ESP) have three quite different geometries: wire-tube, two-stage, and single-stage. The application of the wire-tube design is today largely limited to the capture of liquid particles, or those with other properties (such as very high electrical resistivity). These make wet operation of the units desirable. Two-stage precipitators, with a short ionizer section followed by a set of charged parallel plates, are used in ventilation systems, including residential applications. The single-stage design, with a row of discharge electrodes between parallel collector plates, is used in large-scale industrial applications, especially for capture of fly-ash from coal-fired power plants. The physical phenomena are similar in all three forms; we will discuss only the single stage form. A schematic section of this is shown in Figure 9.

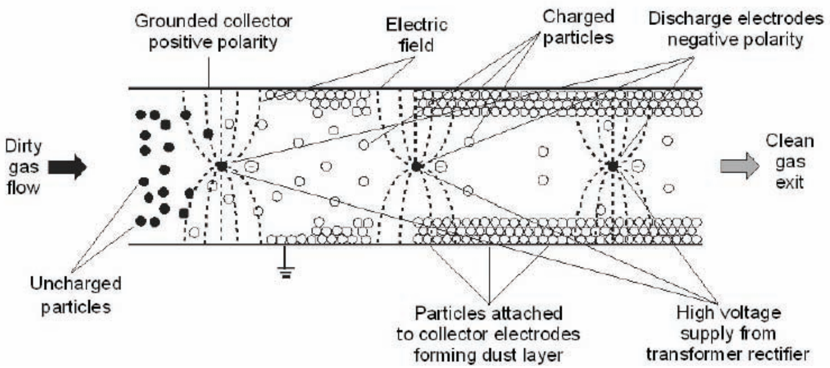


Figure 9 - Schematic Cross-Section of a Single-Stage Electrostatic Precipitator [from Parker and Plaks (2004)]

The figure is actually far simpler than reality, for the electric field lines actually fill the entire interior space. Discharge electrodes may be cylindrical wires as shown, or they may be complicated fluted or scalloped structures, or even carry rows of sharp points. The collector plates are not usually continuous as shown, but are divided into sections to allow motion when rapped. These collector plate sections are also formed into shapes which provide rigidity and spaces where collected particles are somewhat protected from being blown back into the passing gas stream.
The discharge electrodes are held at high negative voltage, either steady DC or pulsing, relative to the grounded collector plates. Excitation is typically 70 kV, which is sufficient to ionize the gas in a small diameter “corona” surrounding the discharge electrodes. Both (+) and (-) ions are present within the corona zone, but beyond it only (-) ions are found. Passing particles accumulate the (-) ion charges, and are driven toward the collector plates. These particles may adhere to the collector plates or to particles previously deposited on the plates, or they may rebound from the plates. If the particles are poor electrical conductors - if they have high resistivity - areas may form in the collected deposits which produce (+) ions. This is called “back ionization”, and causes some particles to be driven back into the passing gas flow.
A realistic model of a single-stage ESP must simulate all of the phenomena just described, plus the flow of gas in the space between the collector plates. Fortunately, the electrostatic fields and ion creation and flow are little influenced by the gas flow velocity pattern (but are dependent in predictable ways on the thermo-physical properties of the gas). Hence the ion density pattern, and the charging rate of particles, can be defined. Less fortunately, the behavior of the gas is modified by the presence of ions in an electric field. And of course, the usual problems of modeling flow that may be viscous or turbulent are present. In addition, the flow is actually 3-dimensional, with some of what is called “sneakage” of dusty gas escaping treatment at the top and bottom of the collector plates.
The development of models has progressed from the very simple one-dimensional expression of Deutsch (1922), here shown in a general form applicable to both wire-in-tube and single-stage plate precipitators:

$$Penetration = \exp\left(\frac{A_P \cdot w_P}{Q}\right) \tag{5}$$

Where
A_P = area of the collector plates; w_P = particle migration velocity near the plates;
Q = gas volumetric flow.

Through the years, the pieces of the ESP puzzle have been added to the Deutsch equation, with many laboratory and field studies providing the data to back up concepts. An understanding of ESP problems can be gained by browsing the 154-page training manual (Parker and Plaks, 2004) for the computer program ESPVI 4.0. Additional material on the concepts used in this code is available in chapters by Lawless and Altman and Lawless and Plaks in EPRI (1990a). ESPVI 4.0 includes a database defining particle properties based on field tests. The agreement between its predictions of efficiency and energy use are apparently sufficient for the US Environmental Protection Agency to approve its use in licensing electrical utilities.
Although ESPVI 4.0 is very detailed, it contains many simplifications not necessary with CFD modeling. There have been numerous applications of CFD to ESP modeling. Examples include: Soldati (2003); Talaie (2005); Lin and Tsai (2010).

6. Filters with Cleanable Surface-Loading Media

Cleanable media filters using tubular fabric bags and cartridge filters are widely applied in industrial exhaust pollution control. These devices rely for efficiency on the buildup of collected dust on the filter media surface, and intermittent removal of this dust “cake”. The most popular method of cleaning is the pulsejet, which uses pulses of compressed air to induce a reverse airflow through the filter media. This is applicable to both baghouses and cartridge type filters. For baghouses, however, cleaning can also be accomplished by flow reversing dampers, and by shaking the bags. Realistic simulation of cleanable-media performance needs to consider the parameters and processes listed below.

Media Type: Woven, nonwoven felted and laminated fabrics; pleated filter cartridges	Gas properties Gas humidity Flow volume	Particle concentration, density, morphology and diameter
distribution		
Cleaning method: shaking, collapse, pulse-jet	Pulse-jet pressure, frequency, duration	Particle adhesion and release behavior
Media area Shaker acceleration	Pulse-jet venturi design & position	Particle load on fabric or cartridge media

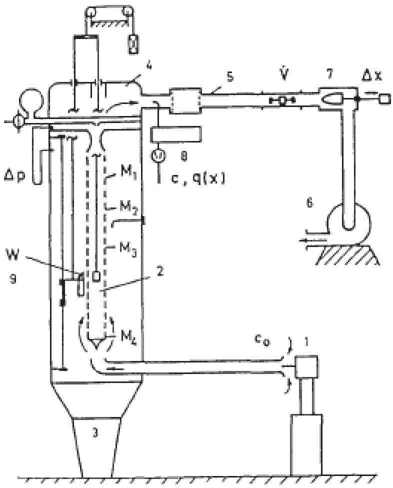


Figure 11 - Pulse-Jet Bag Filter Tester [from Schmidt and Löffler (1990)]
1: Dust Feeder; 2: Filter Bag; 3: Hopper; 4: Compressed Air Pulse System;
7: Flow Control; 8: Particle Counter; 9: Radioisotope Dust Cake Mass Scanner.

Most literature on cleanable media filters consists of reports of field experience, with almost no quantitative determination of the impact of the above factors, or use of mathematical models. Schmidt and Löffler (1990) describe a single-tube fabric collector with pulse-jet cleaning, with simultaneous measurement of the pulse waveform and fabric acceleration. The thickness of deposited dust was measured by adsorption of radioisotope emissions. They also report attempts to define the internal structure of the dust cake. Cleanable filter behavior is a topic ripe for study.

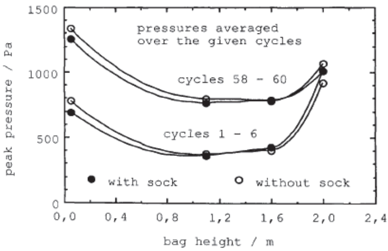


Figure 10 - Peak excess pressure inside bag during cleaning pulses, as a function of position above lower end of bag [from Schmidt and Löffler (1990)]

7. Simulation of Fibrous Air Filters

In a few forms of fibrous air filters the air flow approaches the filter medium at full duct velocity, perpendicular to the medium. In most filter designs filter medium is pleated; to increase media area and lower media velocity. In another design, filter medium is formed into pleated panels which are also arranged in larger-scale "pleats". Analysis of flow through filters with pleats must consider the flow through the filter medium per se, and also through the inlet and outlet regions upstream and downstream of the filter medium. Let us first examine the modeling of filter media.

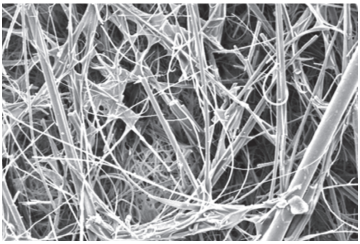


Figure 12 - SEM image of a typical air filter medium, showing a wide range of fiber diameters, random structure, and binder bridges

7.1 Classic Models for Filter Media

Figure 12 is a SEM image of a typical air filter medium. We repeat this familiar image because it shows the randomness of fibers in most media, and also the web-like binder bridges joining the fibers. Few simulations of fibrous filter media have simulated this element of fibrous media, which sometimes makes up as much as 15% of the solids volume of filter media. Binder needs to be added to simulations, just as it must be added to real media.

Early attempts modeling fibrous filtration had to use very simple, orderly models. One was by Langmuir (1942). His model represented a filter by a single fiber sitting in lonely splendor, with gas flow at uniform velocity distant from the fiber. One might say that this model meets Einstein's criterion for simplicity, and the remarkable thing is that it provided some useful information. Oseen and Lamb had solved the pattern of gas flow for this model in 1910-1911. Langmuir treated the case of viscous flow, and

included two particle-capture “mechanisms”: “direct interception” and “diffusion”. He also dealt with the problem of the effect of nearby fibers by introducing an empirical coefficient related to the fractional solids of the filter medium. He showed that for a given fiber diameter and fractional solids, there is a particle diameter which is removed with least efficiency. This particle diameter is what we refer to as the maximum penetrating particle size (MPPS). It the reason that HEPA filters are usually specified as having “> X% efficiency on 0.3 µm diameter particles”. Langmuir suggested the 0.3 µm diameter as the appropriate MPPS for the HEPA filters then in use, at their usual operating conditions.
Problems arise in modeling filter media with a range of fiber diameters. The model requires that one determines an “effective fiber diameter” experimentally, along with the empirical correction for fractional solids. Such approach tells very little about how to design a sheet of filter media.
Numerous investigators developed the theoretical behavior of various regular arrays of uniform-diameter fibers. Geometries analyzed included rectangular and staggered rows of fibers, and a few with more than one fiber diameters. Brown’s book (1993) describes these studies in great detail. Kuwabara made a major contribution in 1959 with a way around the problem of nearby fibers. His concept (expressed for a 2D section cut through the filter medium) was that each fiber was at the center of an imaginary circle, now called a “Kuwabara Cell”. The outer diameter of the cell was set so that the ratio of the fiber cross-section to the cell cross-section equals the fractional solids for the filter medium. Boundary conditions for the fiber and the outer cell were adjusted to allow analytical solutions, avoiding the need for finite-difference calculations not readily available in 1959.
The Kuwabara cell is a fine example of a model which is completely wrong, but produces some useful results. Kuwabara cells joined together to simulate a significant piece of filter media must overlap. Simulations closer to actual filter media geometries had to await the development of computational fluid dynamics.

7.2 CFD Simulations of Fibrous Filter Media

It is possible to analyze models simulating filter media performance in 3 dimensions (3D) even using something less than a supercomputer. The group at the Fraunhofer Institute, e.g. Cheng et al. (2009) and others investigating woven and nonwoven fabrics, see Wang et al. (2006), have modeled media with random fiber diameters located randomly in 3D spaces. Other studies have been satisfied with 2D sections through media. This allows random fiber diameters and full media depth to be simulated without heavy computational burdens, see Tronville and Rivers (2005), Herman et al. (2006). These studies allow evaluation of the proper boundary conditions at the surface of both the fibers and particles, which may have diameters as low as a few hundred nanometers. At those boundaries, gas may have zero velocity, or different levels of “slip”. For filter media with fiber diameters still smaller, the usual Navier-Stokes equations describing the flow may need to be replaced with the Burnett equations, or entirely different computational procedures, such as the Lattice Boltzmann method and Direct Monte Carlo Simulation (DMCS). DMCS mimics the detailed molecular motions of gases.
Predicting particle capture from physical fundamentals, whether by classic analysis or CFD, is more difficult than just predicting pressure drop caused by the air flow resistance. One must first get a reliable flow model to get reliable solutions of particle motion. Including electrostatic effects adds complexity. The buildup of particles on filter fibers has been simulated in 2D and 3D, but with inevitable simplification of

models, more so in 2D than 3D. There is always a trade-off between realistic modeling and computation time.

7.3 CFD Simulations of Complete Filters

For CFD determination of the gas velocity pattern, pressure drop and particle capture in a pleated filter, the filter medium may be replaced with a region of the same thickness and uniform, isotropic permeability K_M. The assumptions here are that the filter medium is uniform, with thickness s_M and pressure drop Δp_M proportional to velocity v_M:

$$K_M = \frac{v_M \cdot \mu \cdot s_M}{\Delta p_M} \tag{6}$$

In similar fashion, for these determinations on multi-panel filters the panels may be represented by regions of the panel thickness s_P and uniform and isotropic permeability K_P. In this case, the panel pressure drop is not linear with panel velocity v_P, but a function of v_P. Usually, a quadratic in v_P is adequate, hence panel permeability K_P is:

$$K_P = \frac{(av_P + bv_P^2) \cdot \mu \cdot s_P}{\Delta p_P} \tag{7}$$

The simplest way to determine a and b in Eq. (7) is to measure the pressure drop across a single panel for a range of velocities v_P, with flow perpendicular to the panel face. Existing CFD codes allow the insertion of this information into flow analysis where some zones in the calculation domain are identified as porous media.

8. Devices for Gaseous Contaminant Capture

Adsorption is the separation of unwanted gaseous components (pollutants) from a gas stream by trapping on the surface of a solid. Adsorption is the dissolving of such components within the body of a solid or liquid. Adsorption is greatly intensified when the surface of the solid is expanded by pores of microscopic size. Both adsorption and absorption have been studied in great detail by chemical engineers, and are described in established texts like Bird et al (2002). With some simplifying assumptions, sorption processes are often well described by analytical solutions to differential equations, so that numerical approaches are not needed.

There are, however, complexities. The speed of a sorption process is dependent on the thermo-physical properties of each gas molecular species involved, and especially on the concentrations of each in the carrier gas. If more than one contaminant species (including water vapor) is present, each may interfere with the separation of others from the carrier gas. Captured contaminant molecules may be released from the sorptive material by temperature changes, adsorption of other species, or the continued passage of unpolluted carrier gas. As contaminant molecules accumulate on or within the sorptive material, the rate of molecular transfer from the carrier gas decreases.

The literature on sorption is immense. Of special value in the separation of contaminants from breathable air is the series by Nelson et al. (1976) which applies to gas masks and building ventilation. CFD is not much needed in studies of deep granular beds. However, the flow characteristics of so-called tray adsorbers and pleated media containing adsorptive material can be treated as described above for particulate filters of multi-panel mini-pleat and pleated forms. Venturi scrubbers and baghouses are sometimes used as contactors for absorption and chemisorption.

Chemisorbers incorporate reactive chemicals on the surfaces of their carrier bodies or in scrubbing liquids. There are no universally reactive substances, so specific pollutants must be targeted, and reaction rates added to the parameter list. The literature on chemisorption is, therefore, much devoted to specified pollutants.

9. Conclusions

Empirical, analytical, and numerical means exist to simulate the performance of gas flow separation equipment, with CFD being the most recent development.
Meaningful predictions can only be made when all significant phenomena are incorporated in the models assumed for analysis. When a predictive method is developed, its accuracy should be tested on a broad array of measured data before it is used to design or optimize separation systems.
A validated database of fully defined systems and their performance results would be useful to verify the accuracy of future predictive methods.

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