

2 Bridging Science and Application in Aerosol Measurement: Accessing Available Tools

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INTRODUCTION

An aerosol is an assembly of liquid or solid particles suspended in a gaseous medium, for example, air, long enough to be observed and measured. The need to measure aerosols has increased dramatically in recent years. This need has arisen in various disciplines. Although much information is available in the published literature, the scientists and practitioners making aerosol measurements in one application may have little or no awareness of the knowledge and experience gained in other applications.

For instance, environmental engineers and industrial hygienists make aerosol measurements in order to ensure that the public and the industrial work force are not exposed to hazardous aerosols at undesirable concentration levels. Faced by increasingly complex and demanding regulations, the aerosol measurements are becoming more costly in equipment and in time to perform, and they may require more than elementary knowledge to perform and interpret. The results are critical as expensive control measures may have to be put in place as a result of such measurements.

In contrast, the scientists and engineers concerned with industrial materials are developing an ever-increasing number of manufacturing processes in which the material passes through an aerosol phase that needs to be monitored and controlled. For instance, powders and pigments may be produced by passing the feed materials into a flame, plasma, laser, or flow furnace where they evaporate. Upon cooling, a very high concentration of very small particles is formed. With time, the aerosols may agglomerate to a lower concentration of larger particles. At any time, the trajectories of these particles may be directed by external forces, for example, diffusion or an applied electric field, to deposit the particles in a prede-

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terminated manner, thus forming products such as ceramics or optical fibers. While producing desirable materials in this manner, the aerosol may have to be measured not only to ensure an optimum amount of uniform product but also to avoid exposure of humans to processing materials that may be quite hazardous.

As a consequence, the novice and the experienced scientist or practitioner alike may have to become familiar with new principles, aerosol measurement techniques and applications. This book attempts to address all of these aspects by dealing with aerosol measurement in three parts. Part I is devoted to the basic concepts of aerosol mechanics (i.e., the behavior of particles suspended in air under the influence of various forces and conditions). This section ends with a chapter combining the concepts of aerosol mechanics with real world situations where measurements must take into account the aerosol-laden environment as well as which properties of the aerosol can be measured with the tools available. Part II expands the latter by devoting a chapter to each principle instrumental technique or group of techniques. Part III begins with a description of nonspherical properties and then discusses a wide range of applications. Each application requires a specific set of aerosol properties to be measured, thus dictating the type of measurement technique or group of associated techniques that can be used.

The book attempts to give the fundamental principles in sufficient detail so that scientists and practitioners may use them in deciding which aerosol properties to measure and how to interpret the results. The technique and application chapters attempt to guide them in performing the actual measurements. As such, the book bridges science and application in aerosol measurement.

There are a number of tools available to aid in understanding and measuring aerosols. The scientific literature provides a wealth of information to aid in selecting instrumentation and understanding aerosol behavior. Supplementary references are cited at the end of each chapter. A summary list of books and journals is given below (adapted from the Education Committee of the American Association for Aerosol Research, 1990, *A Bibliography of Aerosol Science and Technology, Aerosol Science and Technology*, 14:1–4). Perhaps a more complete list of currently available books on a host of aerosol and related topics can be found on the Internet at www.amazon.com or other bookseller sites by entering the appropriate search criteria. A new resource for the aerosol community is being developed at www.aerosolonline.com. This site is supported by the International Aerosol Assembly and lists data available on members, instrument manufacturers, and other useful aerosol-related information.

ASSOCIATED FIELDS

Many aerosol studies grew historically from applications in the health- and environment-related areas. Quite often, publications featuring aerosol measurements are presented in the chemistry, physics, biology, optics, or engineering disciplines. Other areas involving overlapping particle sizes and similar particle dynamics arose in industrial applications and have retained their own societies and journals. Two such areas closely related to aerosol studies are the studies of powders and sprays. Sprays have been especially important in combustion technology, while both sprays and powders have been important techniques in material manufacturing. A relatively new area of research and development emphasis is in the small particle region of the aerosol range, approaching the molecular size range. This area has been given various names, including *nanotechnology*, referring to the approximate range of 1 to 100 nm usually addressed. Some of the journals and references in these fields are included in the References.

COMPUTER TECHNOLOGY

Computer technology has advanced significantly in recent years, closely following Moore's law of doubling in complexity or power every 18 to 24 months. This has opened up calcula-

tion opportunities in a number of areas that were previously very difficult or expensive. Easy-to-use programs are now available in a number of areas to aid in various aspects of aerosol research and applications. The Internet is now a rich source of information about aerosol instruments and measurement techniques, researchers, companies, and so forth. There are a variety of information sources with software reviews, lists of programs, and software companies. Two such sources are *Research and Development* magazine (www.rdmag.com) and *Scientific Computing and Instrumentation* magazine (www.scamag.com).

LANGUAGES

Traditional programming languages such as Basic, FORTRAN, Pascal, and C have generally become more powerful and integrated into the general computer environment. Higher level languages more suited to the scientific environment have been developed. The programs mentioned here are only provided as examples of the available computational tools and do not comprise a comprehensive list by any means. Many programs have multiple capabilities and include the functions for equation solving, statistical analysis, curve fitting, and graphing. Mathematica (*WOL*),* and MathCad (*MAS*) are examples of higher level programs (having their own “language”) in which the user can enter equations directly and provide rapid calculation and graphing of complex sets of equations. Perhaps the most ubiquitous calculation tool currently in use is the spreadsheet. Originally developed as a business tool, current spreadsheet programs such as Excel (*MIC*) and Quattro Pro (*CRL*) have extensive libraries of functions that allow a user to perform complex calculations in a short period of time. Most of these programs can be linked to one another via special programming or other commercially available software. A collection of spreadsheets was prepared to allow the user to play “what if?” games with the formulas in this book to provide better understanding of concepts and to predict behavior of various aerosol systems. These spreadsheets are described below.

Aerosol behavior is largely dependent on air movement and properties. Air motion, turbulence, particle trajectories, and heat transfer in various systems can be calculated with computational fluid dynamics (CFD) programs such as Fluent and FIDAP (*FLT*). These calculations generally require a great deal of computing power, but simple problems can be solved on current personal computers. However, these are complex programs that require not only a background in fluid dynamics theory but also training in their use.

The chapter in the previous edition of this book on data acquisition was dropped because of the difficulty of addressing such a complex topic in the limited space available. The use of video recording was described as a powerful adjunct to aerosol measurements. This has been applied with great success in the industrial hygiene area, allowing correlation of recorded activities with aerosol and other measurements. The measurements can be recorded with data acquisition software. There are many data acquisition systems available, from stand-alone portable devices that can be integrated with hand-held instruments to more complex systems requiring computer support and extensive programming. This area has become much more amenable to the infrequent user, with powerful visually oriented languages such as Labview (*NAT*) and LabTech Notebook (*ADT*). These allow relative ease of integration of complex control and data acquisition functions with real-time computer screen visualization and control. Some training in these programs is helpful, but simple problems can generally be solved with the manuals available.

Many aerosol instruments come with automated data logging built in or can be readily interfaced with a computer to allow data viewing and analysis. Often, the manufacturers of these instruments also provide a means of interface with conventional programs, such as spreadsheets, so that a new language or operating system does not have to be learned for each instrument.

*See Appendix I for full manufacturer addresses referenced by the italicized three-letter codes.

Analysis of particle shape is often a useful adjunct to other types of particle measurement. Particle shape gives clues regarding the history of a particle and can be important for particle dynamics (see Chapter 23). Image analysis is a technique that can be used to quickly accumulate statistics on many particles. Image analysis can easily be integrated with a light microscope, although contrast and refraction effects limit the size of particle that can be accurately imaged, especially after collection on a filter. Electron microscopy generally allows better imaging for interface to image analysis systems. There are many commercial image analysis systems. An image analysis program developed by the National Institutes of Health (NIH Image) is freely available, and there is a list server where questions and discussion can be posted. Information and downloading instructions are available at rsb.info.nih.gov/nih-image/.

Light scattering from particles is commonly used as a detection or particle analysis technique. The prediction of light scattering from individual particles is discussed in Chapter 15 and can be accomplished with computer codes that implement the equations mentioned. Sources on the Internet for some of these codes have been compiled and listed at the web sites www.eee.metu.edu.tr/~ngencer/codes.htm and diogenes.iwt.uni-bremen.de/~wriedt/Mie_Type_Codes/body_mie_type_codes.html.

Data analysis and presentation have also been made easier, with many programs available for statistical analysis, curve fitting, and graphing. A program designed specifically for aerosol distributions is DistFit (*TSI*). Neural networks have also been used to analyze data. This technique uses a network of simulated neurons that “learn” relationships from a training set and can then be applied to new situations. However, to provide accurate results, the applications require that the relationship space is well-represented by the training set. This technique sometimes has an advantage in finding relationships in data more accurately than traditional statistical analysis. Once a network is trained, it can often provide more rapid analysis of new data than other types of analysis. A disadvantage is that a closed-form function describing the solution is not readily available, as the solution is stored in the neural network.

AEROSOL CALCULATOR

The Aerosol Calculator (Baron 1999) is a collection of spreadsheets (Excel, *MIC*) that is available from several sources (www.tsi.com, www.bgiusa.com) and is keyed to the equations in this book as well as in the texts by Hinds (1982, 1999). The spreadsheets are updated as new additions and corrections are made. Some additional calculations are provided along with reference to the source literature. The principal spreadsheet (AeroCalc) contains a series of modules, each calculating a specific equation or set of equations. The modules can be copied into a new spreadsheet and, by creating arrays and linking appropriate modules, complex systems can be modeled and investigated. It is recommended that the calculations be performed on a copy of the spreadsheet, to prevent corruption of the original file by errors. The individual spreadsheets in the Aerosol Calculator collection are listed in Table 2-1. The following discussion assumes some familiarity with spreadsheet operation.

Each module in AeroCalc is self-contained and consists of a set of input parameters with indicated units followed by the calculated output parameter(s). Two separate sheets are provided, one in SI units and the other in cgs units, bridging the units used in the first (Willeke and Baron, 1993) and second editions of this book and by Hinds (1982, 1999). The calculations have been performed using relatively common functions in an attempt to make it easier for the user to understand and modify. No macros were used. However, some calculations require the iteration function to be turned on. These calculations will not work in spreadsheet programs that do not support the iteration function.

TABLE 2-1. Spreadsheet Programs Used to Perform Various Aerosol-Related Calculations^a

AeroCalc.xls	Calculations keyed to specific equations in this text and several other references
sizedis.xls	Calculation of lognormal distributions with discrete size distribution intervals. Surface area and volume distributions are calculated assuming spherical particles. A simulation of random number count errors is included, as well as calculation of respirable, thoracic, inhalable, and PM10 dust fractions. See Chapters 25, 27, and 29 for definitions of these terms
size2d.xls	Calculation of a two-dimensional size distribution, e.g., for fibers with length and diameter. See Chapter 23
2Drect.xls	Calculation of Laplacian function in two-dimensional rectangular coordinate system. It can be used for electric fields or for potential flow in any two-dimensional field. For calculating potential flow, see the example in White, F. M., 1986, <i>Fluid Mechanics</i> , 2nd Ed., pp. 497-500. Each spreadsheet cell represents an x-y coordinate in the electric or flow field. The problem is defined by the boundary values, and the cells inside the boundary are filled with replicated calculation cells. Each internal cell performs an identical calculation based on nearest neighbor values. The array size that can be solved is limited by the memory and calculation speed of the computer. The array is solved by iteration, and the number of iterations increases with the number of cells in the array
2Daxial.xls	Similar to 2Drect.xls except that it is used for cylindrically symmetrical two-dimensional problems
Probit.xls	Calculation and plotting of probits for a size distribution measurement. This is useful for graphical presentation of size distribution data on a log probability plot. See Chapter 22

^aInstructions and references for each module are in the corresponding spreadsheets.

The application of the equations provided in various references allows the user to better understand the limitations and usefulness of these equations through the use of the spreadsheet programs. Not only can the reader of the book perform calculations without having to do extensive programming, unit conversion, and error checking, but the software allows graphing of the results as a function of the variables, such as particle size, temperature, and flow rate, for better understanding of the text description. Some of the calculations are empirical and have limits based on the data set from which they were derived. Frequently, these limits have been indicated in AeroCalc, but the user must be aware of other limitations described in the text and in the original references.

The calculations possible with this program become much more meaningful and powerful if the user understands the equations and the assumptions behind the equations; errors can result if the user enters improper values or misinterprets the results. Thus, the program does not substitute for that understanding, though it certainly allows the user to “play” with the parameters in the equations for a better understanding of aerosol behavior. Some example applications of the AeroCalc program are indicated below.

AeroCalc

The general format of the AeroCalc spreadsheet is indicated in Figure 2-1. The modules are separated with a line of asterisks, and the input and calculated parameters are separated with a line of dashes. Column A contains the description of the module at the top, followed by descriptions of the input and calculated parameters. Column B contains the input and calculated parameters, while column C contains the units. Although not shown in this example, column C contains comments about specific parameters indicating value limits

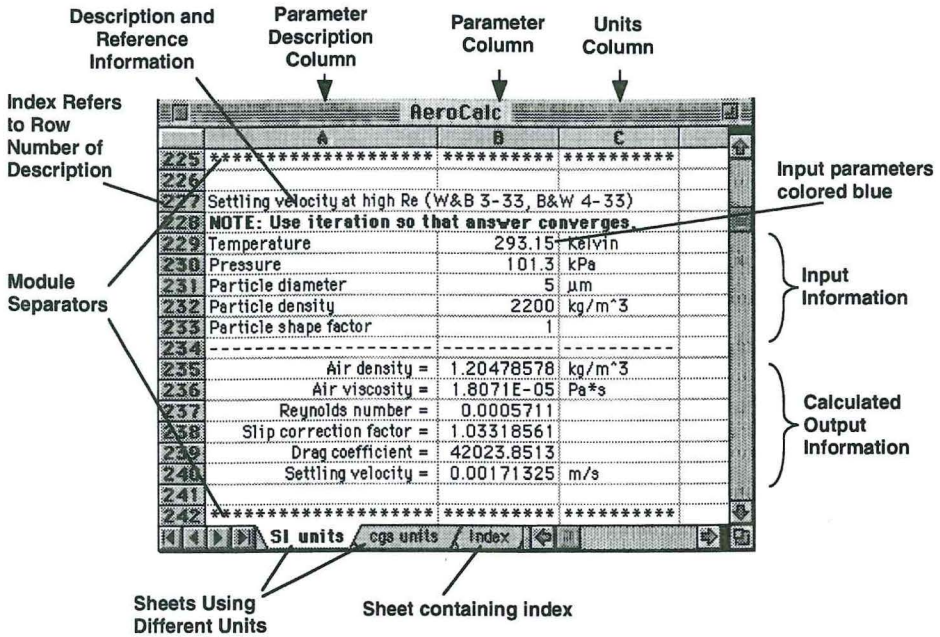


Fig. 2-1. Example module in AeroCalc spreadsheet indicating several typical features. Bold row 228 indicates that the iteration function (under menu Tools:Options:Calculation) must be turned on for the results to be calculated correctly. If iteration is not turned on, an error message regarding circular references appears on startup of the program. This message can be ignored if the modules being used do not require iteration.

or other warnings. Occasionally there is a table of useful values in columns C, D, and E. There is an index of all the calculations in columns I and J between rows 2 and approximately 105. There is also a table of conversion factors in columns I and J between rows 117 and 205.

In the example in Figure 2-1, iteration of the calculation is required to reach the correct answer. In the Excel menu bar, under Tools, Options, Calculation, there is an option to select Iteration with a maximum number of iterations and the degree of precision (maximum change). If this is not turned on, Excel will report on startup that “circular references” exist. This will not affect other calculations, and the warning can be turned off. Most of the calculations will reach a solution with fewer than 100 iterations at a maximum change of 0.0001, but some, as indicated in the module header, may take more.

In the example, the calculation of settling velocity depends on the drag coefficient when the velocity is outside the Stokes regime (Reynolds number, $Re < 0.1$ in Stokes regime). However, the drag coefficient depends on the final velocity, so iteration of the calculation is required to reach the correct solution. Any of the input parameters can be changed to observe the effect on the calculated values. This can provide useful information. However, it is easy to expand the usefulness by creating an array of calculations that are identical except for one changing parameter.

Figure 2-2 displays the calculation in Figure 2-1 with several additional columns inserted between columns B and C. Column B is then replicated to the right to fill the inserted columns. To observe the change in the calculated values of settling velocity as a function of particle diameter, each subsequent column can be changed by an increment. In Figure 2-2,

AeroCalc							
A	B	C	D	E	F	G	H
227	Settling velocity at high Re (W&B 3-33, B&W 4-33)						
228	NOTE: Use iteration so that answer converges.						
229	Temperature	293.15	293.15	293.15	293.15	293.15	Kelvin
230	Pressure	101.3	101.3	101.3	101.3	101.3	kPa
231	Particle diameter	5	10	20	40	80	μm
232	Particle density	2200	2200	2200	2200	2200	kg/m ³
233	Particle shape factor	1	1	1	1	1	1
234	-----						
235	Air density =	1.20479	1.20479	1.20479	1.20479	1.20479	kg/m ³
236	Air viscosity =	1.8E-05	1.8E-05	1.8E-05	1.8E-05	1.8E-05	Pa*s
237	Reynolds number =	0.00057	0.0045	0.03567	0.27715	1.92823	10.3567
238	Slip correction factor =	1.03319	1.01659	1.0083	1.00415	1.00207	1.00104
239	Drag coefficient =	42023.9	5338.72	672.831	88.7937	14.6451	4.05698
240	Settling velocity =	0.00171	0.00674	0.02675	0.10393	0.36153	0.97091 m/s

Fig. 2-2. Particle diameter is changed, starting in column C, by multiplying the value in the previous column by a factor of two. The settling velocity can be plotted as a function of particle diameter.

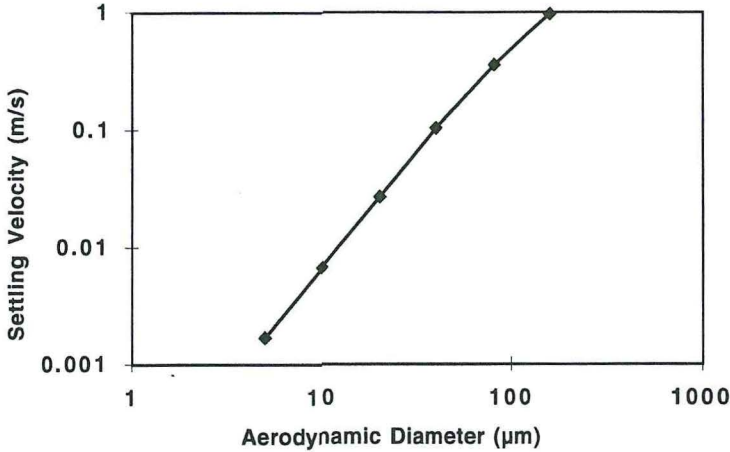


Fig. 2-3. Plot of particle setting velocity as a function of particle diameter on a long-log scale using the Excel chart capability.

[Col C, Row 231] is set = 2 × [Col B, Row 231]. This equation is replicated to the rest of Row 231. It is also convenient to set the other input parameter column data to equal the corresponding values in the column B. That way, only the values in column B need to be changed, and the entire array recalculates appropriately.

The values calculated in Figure 2-2 can immediately be plotted as indicated in Figure 2-3. Noncontiguous rows can be selected for plotting by replicating the rows elsewhere on the spreadsheet. Alternatively, they can be selected directly by holding down the keyboard control key (command key on the Macintosh) while selecting the second row. In this example, we have changed particle diameter in a geometric rather than a linear progression, and it is convenient to display the results on a log-log scale. The nonlinearity of the resulting curve is an indication of the change in the drag coefficient outside the Stokes regime. The number of columns can be increased, using smaller increments in particle diameter, and the data replotted to obtain a smoother curve.

It is often desirable to determine the input parameter that gives a target output value. This can be done by trial and error, replacing the input parameter with various values, until the target value is reached with acceptable precision. Alternatively, Excel has a feature called the "Solver" under the Tools menu that allows automatic calculation of the appropriate input value to give a selected target value. The Solver may not always work properly with modules that use iteration for their solution.

Several modules can be linked together to perform more complex calculations. For instance, a common situation in aerosol measurement is the desire to ensure that the sampling system conveying particles to a measurement instrument has minimal, or at least known, losses. There are AeroCalc modules that calculate the losses in various inlets, tubing, and bends under laminar and turbulent conditions. By assuming that each of these components act independently (not always a good assumption; see Chapter 8), we can estimate the overall loss in the inlet system. For instance, if we have an inlet, followed by a bend, a length of tubing, a second bend, and another section of tubing, the overall efficiency of aerosol reaching the sensor relative to the air concentration is, to first approximation, the product of each individual efficiency η

$$E = \eta_{inlet}\eta_{tube1}\eta_{bend1}\eta_{tube2}\eta_{bend2}\eta_{tube2} \quad (2-1)$$

By linking spreadsheet modules that calculate each η and the overall efficiency, it is possible to optimize the overall efficiency by varying the flow rate and the lengths, diameters, and orientation of each component.

The calculations in the modules can also be linked to the size distribution spreadsheets indicated in Table 2-1. One example of such a calculation is given in Chen and Baron (1996) where the calculated fiber deposition efficiency in a tubular inlet was compared successfully with experimental deposition measurements. Another example is given in Baron (1996) where the aerodynamic diameters of fibers likely to deposit in the thoracic region of the respiratory system, represented by an aerodynamic selection system, were compared with current microscope measurement procedures.

The Aerosol Calculator provides a convenient set of tools that allow rapid calculation of a wide range of parameters in aerosol mechanics. It can be used to increase understanding of aerosol behavior, indicating the most important mechanisms operating in a given situation.

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