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PARTICLE SIZE DEFINITIONS FOR PARTICULATE DATA ANALYSIS

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PARTICLE SIZE DEFINITIONS FOR PARTICULATE DATA ANALYSIS

by

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PREFACE

The work was performed in the Environmental and Materials Sciences Division of Midwest Research Institute (MRI). Dr. J. B. Galeski, Senior Chemical Engineer, Environmental Systems Section, served as the project leader, and Mr. M. P. Schrag, Head, Environmental Systems Section, was the project manager.

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SUMMARY

This report presents the results of a measurement survey to identify all equations required to represent particle size data according to each of three particle diameter definitions--Stokes, classical aerodynamic, and aerodynamic impaction (or Lovelace diameter). Although the particle diameter definitions themselves are relatively simple, inconsistencies were found among various investigations in the use of particle size definitions, particularly in nomenclature. It is not always clear from the descriptions of various authors which definition is intended. The present study presents a consistent set of definitions and equations for use in interpreting particle size and impactor data such as that found in the Fine Particle Emissions Information System (FPEIS) data base. The equations may also be useful to readers of fine particle sampling reports who may wish to convert the data from one definition to a more convenient one.

INTRODUCTION

Particulate sampling data are expressed in the literature in various ways; this tendency being reflective, in part, of a broad spectrum of environmental impacts. Physiological, meteorological, and other impacts generally are influenced differently by particle size and geometry. The impacts are determined in many cases by analytical approximations which yield alternative characteristic particle size definitions. Examples include Stokes' or settling diameter, classical aerodynamic diameter, aerodynamic impaction diameter and numerous other definitions, described by Raabe (1). For fine particulates, assuming spherical particles, alternative definitions may yield differences of 30% or more in the reported diameter. Furthermore, relationships between alternative size definitions are not always well understood.

The objective of this study is to identify the equations required to represent particle size data according to three diameter definitions--Stokes', classical aerodynamic, and aerodynamic impaction. The primary purpose of this study is to facilitate understanding and use of data contained in the FPEIS--a computerized data base currently being developed by IERL-RTP to contain all currently available fine particle source test measurements and control device(s) parameters, test details, particulate physical, biological, and chemical properties, and particle size distribution data. By providing a uniform compilation of fine particle information and data, the FPEIS can serve the needs and interests of a broad spectrum of users. These users include plant officials, control device manufacturers, measurement equipment/method developers, government officials responsible for the development of fine particulate control strategies, and other researchers.

The purpose of this document is to supplement existing FPEIS guideline documents (2,3,4). Definitions of each particle size basis, mathematical formulae, and techniques for interconversion of particle data are presented in the following sections.

PARTICLE SIZE DEFINITIONS

Particle size definitions considered here include:

(1) Stokes', or settling diameter;
(2) Classical aerodynamic diameter; and
(3) Aerodynamic impaction diameter (the latter also referred to alternatively as the "Lovelace diameter" or "aerodynamic resistance diameter" (1)).

It is recognized that a number of alternative diameter definitions exist which are not presented here. The reader is referred to references presented throughout this discussion for additional information on size and measurement techniques pertinent to specific technology areas.

STOKES' DIAMETER (1,5)

The aerodynamic separation of spherical particles is described by their terminal settling speeds in any fluid and expressed as:

$$V_s = \frac{g \rho C(D_s) D_s^2}{18 \eta}, \quad Re \leq 0.5 \tag{1}$$

Where V_s = terminal velocity of a particle in free fall, m/sec

g = gravitational constant (9.80665 m/sec^2)

ρ = particle density, kg/m^3

D_s = Stokes' diameter, m

η = fluid viscosity, kg/m-sec

Re = Reynold's number, dimensionless

$C(D_s)$ = slip correction factor for spherical particles of diameter D_s, dimensionless.

As indicated, Eq. (1) is valid for values of the Reynold's number less than 0.5 (Stokes' regime) (1).

The slip correction factor $C(D_s)$ (sometimes called the Cunningham correction) is an empirical factor which corrects Stokes' law for discontinuities when the mean free path (λ) of the fluid medium is comparable to the particle diameter. An approximation for the slip correction factor $C(D_s)$ for spherical particles is given by:

$$C(D_s) \simeq 1 + 2A \left(\frac{\lambda}{D_s}\right) \tag{2}$$

with

$$A = \alpha + \beta e^{-(\gamma D_s/2\lambda)} \tag{3}$$

The terms α, β, and γ are empirical constants; currently accepted values of these constants are presented in Table 1.

TABLE 1. CONSTANTS FOR USE IN CALCULATING SLIP CORRECTION FACTOR

	α	β	γ
Fuchs (6)	1.246	0.42	0.87
Reif (7)	1.26	0.45	1.08
Cushing et al. (8)	1.23	0.41	0.88

Numerical constants presented in Table 1 are based on experimental data and reflect some variation probably resulting from differences in experimental technique. The resultant variation in the slip correction factor is relatively small (about 2 to 3% for particle diameters in the range 10^{-3} to 10^{-2} μm, decreasing to about 0.1% at $D_s = 0.1$ μm) (1). Constants reported by Reif (9) were based on experimental investigations by Langmuir, those of Fuchs (6) were based on Millikan's classic oil drop experiments, while the constants used by Cushing, et al. (10), are averages based on data for a number of different types of particulate. Recent theoretical studies have shown that "constants" used in calculating the slip correction according to Eqs. (2) and (3) are actually slightly variable, depending on the fluid medium and the particle surface properties (11). Values of the slip correction factor are presented in Figure 1 for various values of temperature, pressure, and Stokes' diameter. The slip correction factor increases with temperature and decreases with pressure, and this factor becomes increasingly significant for very fine particles at low pressures. For coarser particles and/or for higher pressures the Cunningham factor approaches unity and its variation with temperature and pressure is insignificant.

For a given fluid, the mean free path (λ) is a function of temperature (which determines the mobility of gas particles), pressure (which determines molecular concentration), and gas composition (9). Compositional dependence may be expressed in terms of molecular diffusivity, thermal conductivity or viscosity, the gas viscosity being most commonly used. An approximation for the mean free path which is considered acceptable for particle size calculations is presented in Eq. (4) (10).

$$\lambda = \lambda_o \ (\eta/\eta_o) \ (T/T_o)^{1/2} \ (P_o/P) \qquad (4)$$

where η is the gas viscosity at stated conditions, kg/m-sec

η_o is the gas viscosity at reference conditions, kg/m-sec

T is the absolute temperature, °K

T_o is the reference temperature, 296.16° K (23.0°C)

P is the absolute pressure, kPa

P_o is the reference pressure, 101.3 kPa (1.0 atm)

λ_o is the mean free path at reference standard conditions, μm

λ is the mean free path at stated conditions, μm

The accepted mean free path of air at reference conditions of 23°C, 1 atmosphere is 0.0653 μm (1).

The viscosity of gas mixtures (η) used in Eqs. (1) and (4) may be estimated from single component viscosity data using a procedure developed by Cushing, Lacy, McCain and Smith (8).

$$\eta = \sum_{i=1}^{n} \frac{\eta_i}{\left[1 + 1/x_i \sum_{\substack{j=1 \\ j\neq i}}^{n} x_j \Phi_{ij}\right]} \qquad (5)$$

where Φ_{ij} is defined by the equation:

$$\Phi_{ij} = \frac{\left[1 + (\eta_i/\eta_j)^{1/2} \ (M_j/M_i)^{1/4}\right]^2}{(4/\sqrt{2})\left[1 + (M_i/M_j)\right]^{1/2}} \qquad (6)$$

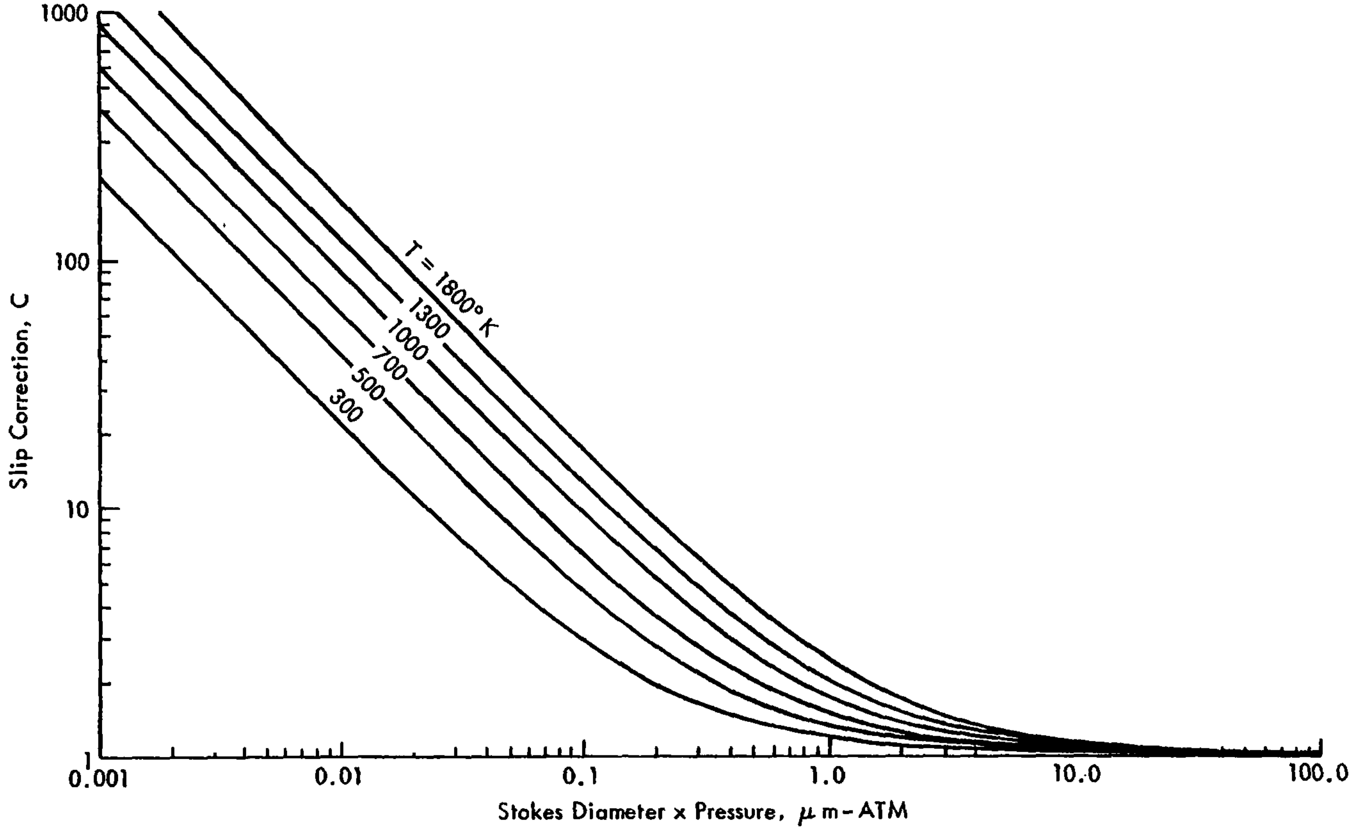

Figure 1. Variation of Cunningham Correction Factor in Air with Temperature and Pressure (10)

and η_i = viscosity of component i, kg/m-sec

x_i = mole fraction of component i

M_i = molecular weight of component i

The viscosity of gases increases approximately as the 0.6 power of the absolute temperature, and is also very weakly dependent on pressure. For air at pressures less than 20 atm and at temperatures greater than 300°K, dependence of viscosity on pressure is negligible. The temperature dependence of single component viscosities for use in Eqs. (5) and (6) can be found in standard references, for example CRC "Handbook of Chemistry and Physics" (12), or equivalent sources.

Experimentation has shown that, for purely viscous flow at low Reynold's numbers, the fluid resistance is described by Stokes' Law, even for particles of nonspherical shape, if a numerical coefficient is introduced to account for the particle shape (6). This correction is commonly referred to as the "dynamic shape factor." For particle shapes which approximate regular polyhedra, the shape exerts less than a 10% influence on apparent (measured) diameter, but for aggregates (6), and for rod-like geometries such as asbestos, the particle shape may exert an influence of 30% or more on the measured diameter (6,13). Such geometries occur in rather limited instances and are not considered in detail in this report. Where such geometries occur, and a shape factor is used to describe the fluid resistance, the term "sedimentation diameter" should be used rather than Stokes' diameter.

CLASSICAL AERODYNAMIC DIAMETER

The classical aerodynamic diameter is defined as the diameter of a unit density sphere with the same settling velocity as the particle in question. This definition is mathematically equivalent to that recommended by the Task Group on Lung Dynamics for use in studies of aerosol deposition in respiratory compartments (14). The classical aerodynamic diameter differs from the Stokes' diameter only by virtue of differences in density, assumed equal to unity, and the slip correction factor, which, by convention is calculated for the aerodynamic equivalent diameter. From Eq. (1),

$$D_{Ae} = \sqrt{\frac{18\eta V_s}{gC(D_{Ae})}} \qquad (7)$$

where D_{Ae} = "classical" aerodynamic equivalent diameter, meters

[η, V_s, g, C as previously defined (Eq. (1).]

AERODYNAMIC IMPACTION DIAMETER

The aerodynamic impaction diameter (also referred to as the aerodynamic resistance diameter or the Lovelace aerodynamic diameter) is used by Calver (15), Mercer (16), and other investigators working with impactors.* The aerodynamic impaction diameter is defined as the product of the Stokes' diameter times the square root of the product: particle density times slip correction factor (5,15).

$$D_{Ai} = D_s \sqrt{C(D_s)\,\rho} \tag{8}$$

The significance of the aerodynamic impaction diameter is that the quantity represented by Eq. (8) provides a unique measure of the performance of impactors and other inertial classifiers (including sedimentation and elutriation separators). The basis of this diameter definition is that it is not possible, using inertial classifiers, to distinguish between two particles having the same aerodynamic impaction diameter. From Eq. (8), it follows that two particles having the same aerodynamic impaction diameter may have different Stokes' diameters, provided that the product $D_s[C(D_s)\rho]^{1/2}$ remains constant. If particles having varying densities are present, the aerodynamic impaction diameter should yield a more uniform measure of stage performance than alternative size definitions, according to the theory of Ranz and Wong (17). Note that this definition is dimensionally different from the preceeding definitions, since the density factor is included in the diameter definition.

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* However, this definition is not used in the major portion of impactor test data reported in the literature.

PARTICLE SIZE CONVERSIONS

Equations required for interconversion among the three alternative diameter definitions are presented in Table 2. The relationship between classical aerodynamic and Stokes' diameters is illustrated graphically in Figure 2 for assumed spherical particles of density 2.4 g/cm^3. The relationship between aerodynamic impaction (Lovelace) diameter and Stokes' diameter is illustrated graphically in Figure 3 for assumed spherical particles having densities ranging from 1.0 to 3.0 g/cm^3. Note that the second aerodynamic diameter definition (aerodynamic impaction or Lovelace diameter) is dimensionally different from either previous definition since a density factor is present. As is evident from Figures 2 and 3, the relationship between classical aerodynamic equivalent and Stokes' diameter is qualitatively similar to that for the aerodynamic impaction, or Lovelace diameter, and Stokes' diameter. For spherical particles, the aerodynamic diameter conventions considered here are numerically nearly identical for particles greater than about 1 μm; at 1.0 μm, and ambient conditions, the aerodynamic impaction or Lovelace diameter is greater than the classically defined aerodynamic diameter by only about 10% (1). However, at 0.5 μm, the discrepancy under ambient sampling conditions approaches 15% (1), and increases at smaller particle sizes.

In several cases, conversions between alternative diameter definitions involve inherent computational difficulties, since it is not always possible to express one diameter definition as an explicit function of another (see Table 2). In such cases, either approximations or trial and error exact solutions are required. An approximation given by Raabe (1) which can be used to obtain explicit solutions for equations in Table 2 is to represent the slip correction factor by the following approximate expression:

$$C(D_s) \cong 1 + 2.52 \left(\frac{\lambda}{D_s}\right), \quad D_s \geq 0.5\ \mu m \qquad (9)$$

Eq. (9) is reportedly valid for Stokes' particle diameters greater than about 0.5 μm (1). An alternative simplification suggested here is to approximate the slip correction factor for particles less than D_s = 0.5 μm by the following approximate relationship:

$$C(D_s) \cong 1 - \beta\gamma + 2(\alpha + \beta) \frac{\lambda}{D_s}, \quad D_s < 0.5\ \mu m \qquad (10)$$

TABLE 2. EQUATIONS USED FOR PARTICLE SIZE CONVERSIONS--CLASSICAL AERODYNAMIC, STOKES' DIAMETER, AND AERODYNAMIC IMPACTION (LOVELACE) DIAMETER

Diameter definition (given)	Conversion equation[a/] Stokes' diameter (D_s)	Classical aerodynamic equivalent diameter (D_{Ae})	Aerodynamic impaction (Lovelace diameter (D_{Ai})
Stokes' diameter (D_s)	1.0	$D_{Ae} = D_s \left[\frac{\rho C(D_s)}{C(D_{Ae})} \right]^{1/2}$	$D_{Ai} = D_s [C(D_s)\rho]^{1/2}$
Classical aerodynamic diameter (D_{Ae})	$D_s = D_{Ae} \left[\frac{C(D_{Ae})}{\rho C(D_s)} \right]^{1/2}$	1.0	$D_{Ai} = D_{Ae} [C(D_{Ae})]^{1/2}$
Aerodynamic impaction (Lovelace) diameter (D_{Ai})	$D_s = D_{Ai} \left[\frac{1}{C(D_s)\rho} \right]^{1/2}$	$D_{Ae} = D_{Ai} \left[\frac{1}{C(D_{Ae})} \right]^{1/2}$	1.0

* Notation: D_s = Stokes' diameter, μm
D_{Ae} = Classical aerodynamic equivalent diameter, μm
D_{Ai} = Aerodynamic impaction (Lovelace) diameter, $\mu m\text{-}g^{1/2}\text{-}cm^{-3/2}$
ρ = Particle density, g/cm^3
$C(D_s)$, $C(D_{Ae})$, $C(D_{Ai})$ = Slip correction factors (Dimensionless)--see Eqs. (2) and (3).

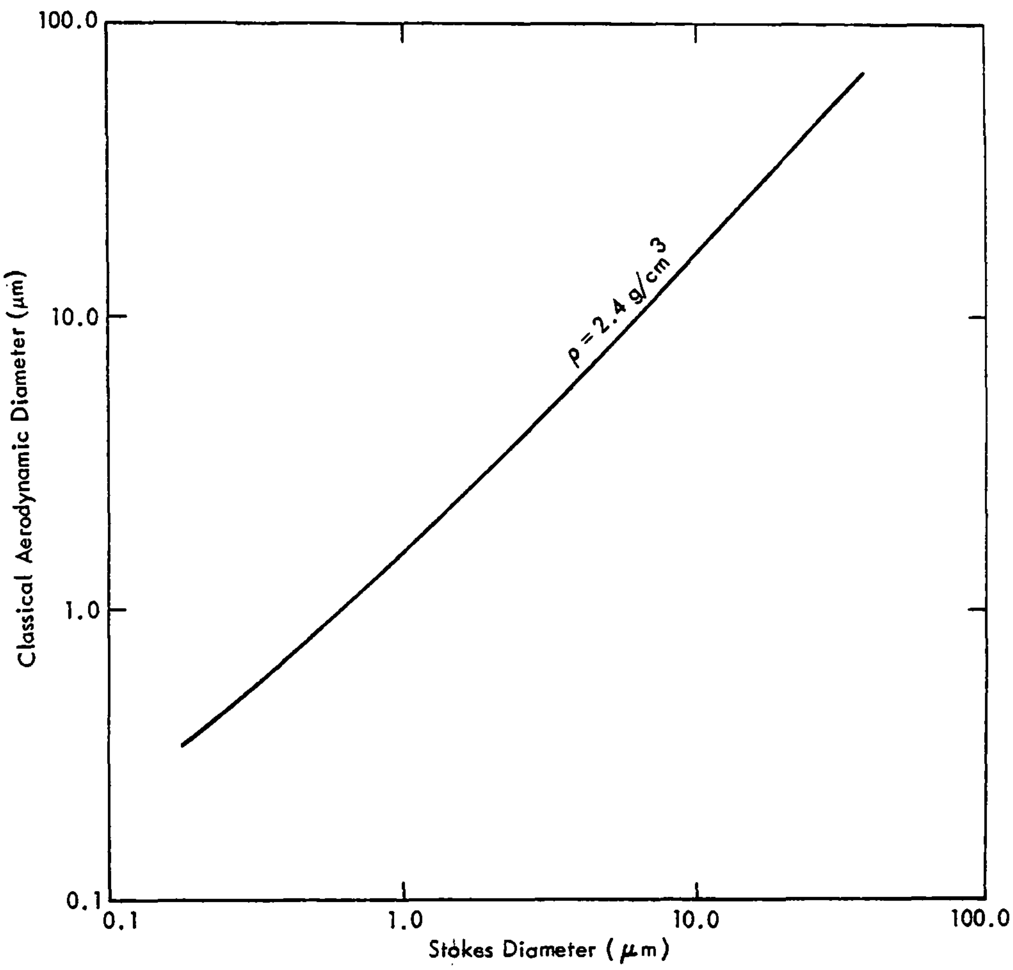

Figure 2. Relationship Between Stokes' Diameter and Classical Aerodynamic Diameter for a Spherical Particle, $\rho = 2.4$ g/cm^3 (8)

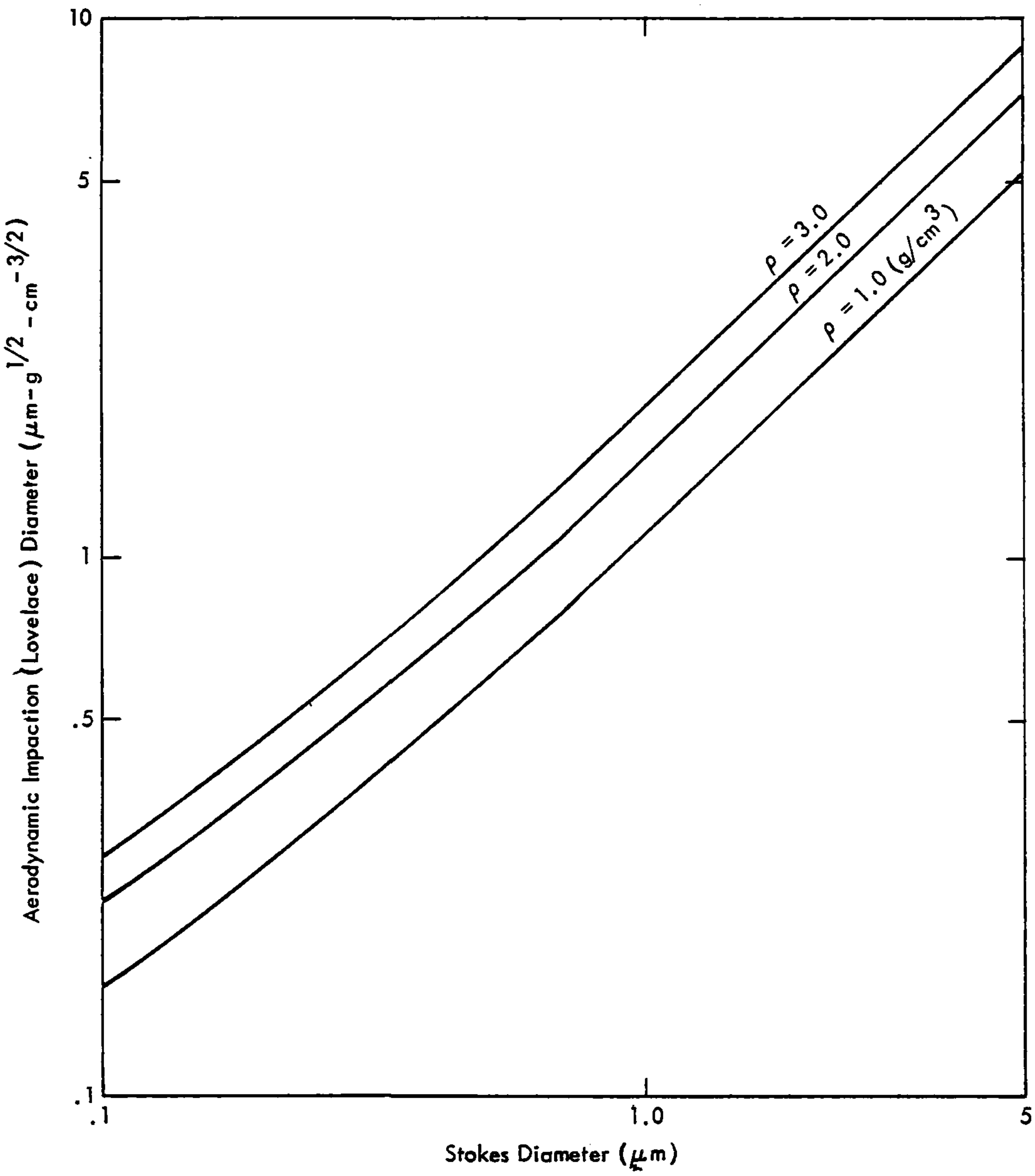

Figure 3. Relationship Between Stokes' Diameter and Aerodynamic Impaction Diameter for Spherical Particles, $\rho = 1.0$ - $3.0\ g/cm^3$ (13)

Eq. (10) is derived from a truncated McLaurin series approximation to Eqs. (2) and (3), and is extremely accurate for particles less than about 0.1 μm. Eqs. (9) and (10) have the same functional form so that a direct (approximate) solution of equations in Table 2 can be accomplished using different parameters for particles less than or greater than 0.5 μm, Stokes' diameter.

The preceding discussion has outlined methodology for conversion of alternative particle diameter definitions from reduced data; the next section will outline methodology and equations for data reduction from impactor test data according to alternative particle diameter definitions.

CASCADE IMPACTOR PARTICLE SIZE DATA REDUCTIONS

Separation of spherical particles in impactors can be approximated by the following equation (1):

$$L = \frac{V_o \rho C(D_s) D_s^2}{18\eta} \tag{11}$$

where L is the stopping distance(6), meters

V_o is the axial component of particle velocity, m/sec

ρ, $C(D_s)$, D_s, η as previously defined (Eq. 1).

According to the treatment of Ranz and Wong (17), the preceding equation is written in dimensionless form and V_o is taken as the impactor stage exit velocity.

$$\psi = \frac{L}{d_i} = \frac{V_o \rho C(D_s) D_s^2}{18\eta d_i} \tag{12}$$

where d_i is the jet diameter, meters.

The impactor sizing equation, as developed by Cushing, et al. (8), includes minor modifications of Eq. (12) to permit analysis of multiple jets per stage, to include different calibration constants for each stage, and to compensate for pressure losses through the impactor. Rearranging Eq. (12), and making appropriate substitutions,

$$D_s = k_d\, k_i \left(\frac{\eta d_i^3\ P_i\ X_i}{\rho C(D_s) P_o Q}\right)^{1/2} \tag{13}$$

where k_d is a dimensional constant

k_i is the calibration constant for the ith stage (dimensionless)

χ_i is the number of jets at stage i

P_o is the pressure at the impactor orifice, kPa

P_i is the pressure at the exit of stage i, kPa

Q is the volumetric flow rate at the impactor orifice, m^3/sec

η, d_i, ρ, $C(D_s)$ as previously defined (Eqs. (1) and (12).

In order to determine the particle size distribution from impactor data, the usual assumption made is that each stage can be characterized by a "cut-off diameter"--the diameter at which particle collection efficiency for the stage is 50%. It is further assumed that collection efficiency is zero for particles having diameters less than the cut-off diameter. Thus, the fundamental impactor performance variable for a given test is the cut-off diameter, also called the "cut-point." Either the Stokes', classical aerodynamic equivalent, or aerodynamic impaction (Lovelace) diameter definitions may be used (as well as other definitions (1)). Further details regarding impactor size reduction techniques are available in Reference 8. Equations relating the cut-off diameter to test data are presented in Table 3 for alternative size definitions.

From Table 3, use of either the Stokes' definition or the classical aerodynamic equivalent diameter definition would require approximate or iterative solutions for each stage cut-off diameter. According to the aerodynamic impaction (Lovelace) diameter convention, the slip correction factor is not used in calculating the cut-off diameters.

TABLE 3. EQUATIONS USED FOR CALCULATING IMPACTOR CUT-OFF DIAMETER (D_{50}) FOR ALTERNATIVE DIAMETER DEFINITIONS

Diameter convention	Cut-off diameter (D_{50})[a]
Stokes' (D_s)	$k_d\ k_i \left[\frac{\eta d_i^3\ P_i \chi_i}{\rho P_o C(D_s) Q}\right]^{1/2}$
Classical aerodynamic equivalent (D_{Ae})	$k_d\ k_i \left[\frac{\eta d_i^3\ P_i \chi_i}{P_o C(D_{Ae}) Q}\right]^{1/2}$
Aerodynamic impaction (Lovelace) diameter (D_{Ai})[b]	$k_d\ k_i \left[\frac{\eta d_i^3\ P_i \chi_i}{P_o Q}\right]^{1/2}$

a/ Notation: D_{50} = cut-off diameter, μm
k_d = dimensional constant
$= 10^3 \left[\frac{18\pi}{4}\right]^{1/2}$ for dimensions specified below
k_i = impactor calibration constant for ith stage, dimensionless
η = gas viscosity, kg/m-sec
d_i = impactor jet diameter, cm
P_i = pressure at stage jet exit, kPa
P_o = pressure at orifice, kPa
χ_i = number of jets per stage
Q = volumetric flow at orifice, m^3/sec
$C(D_s)$, $C(D_{Ae})$ = slip correction factors (dimensionless)
i = stage index (dimensionless)

b/ According to the aerodynamic impaction diameter definition, D_{50} is dimensionally (μm) $(g/cm^3)^{1/2}$ (15).

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16. ABSTRACT
The report gives results of a survey to identify all equations required to represent particle size data according to each of three particle diameter definitions: Stokes, classical aerodynamic, and aerodynamic impaction (or Lovelace diameter). Although the particle diameter definitions themselves are relatively simple, inconsistencies were found among various investigations in the use of particle size definitions, particularly in nomenclature. It is not always clear from the descriptions of various authors which definition is intended. The present study presents a consistent set of definitions and equations for use in interpreting particle size and impactor data such as that found in EPA's Fine Particle Emissions Information System (FPEIS) data base. The equations may also be useful to readers of fine particle sampling reports who may wish to convert the data from one definition to a more convenient one.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution	Impact	Air Pollution Control	13B
Dust	Impactors	Stationary Sources	11G
Analyzing	Stokes Law (Fluid Mechanics)	Particulate	14B
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