DEPOSITION CALCULATOR
TECHNICAL DESCRIPTION MANUAL
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GLOSSARY

AD = the Aerodynamic Diameter of a particle, m
A_{sh} = cross sectional area of a shroud, m²
A_{gap} = cross sectional area of a gap area of a shrouded probe, m²
A_{i} = area of component inlet, m²
A_o = area of component outlet, m²
C1 = particle lift factor, s^{-0.5}
C_c = Cunningham's slip correction factor, dimensionless
C_d = drag coefficient, dimensionless
d = diameter, m
d_b = external diameter of inner probe tube in a shrouded probe, m
d_{ci} = inlet diameter of a component, m
d_{co} = outlet diameter of a component, m
d_i = inlet diameter of the inner probe in a shrouded probe, m
d_{Ni} = diameter of the nozzle inlet, m
d_o = internal diameter of the inner probe tube in a shrouded probe, m
D_{AD} = aerodynamic diameter of a subject particle, m
D_c = particle diffusion coefficient, m²/s
D_l = actual diameter of a subject particle, m
D_p = diameter of particle, m
d_{sh} = internal diameter of the shroud in a shrouded probe, m
d_{Ti} = internal diameter of the tube, m
F = correlation function, dimensionless
Fr = Froude number, dimensionless
g = Gravitational acceleration, 9.807 m/s²
k = Boltzmann's constant, 1.3807E-23 N·m/K
k_{ref} = rate of flow shear, s^{-1}
L = length, m
L_N = nozzle length, m
L_{pr} = length of inner probe in a shrouded probe, m
L_{nw} = normalized length, dimensionless, = L_{pr}/d_i
LPM = Liters per Minute
M = mass, kg
MW = Molecular weight of air, 28.962 kg/kmol
P = pressure, Pa
Q_s = sample rate, LPM
R = gas constant = R_o/MW, J/kg·K
R_b = Radius of curvature of the bend, m
Re = Reynolds number, dimensionless
Re_p = particle settling Reynolds number, dimensionless
\( R_N \) = velocity ratio for a nozzle, dimensionless

\( R_{pr} \) = velocity ratio at inner probe entrance plane, dimensionless

\( R_s \) = velocity ratio at shroud entrance plane, dimensionless

\( R_u \) = Universal gas constant, \(8314.471 \text{ J/kmol·K}\)

\( R_z \) = Factor in nozzle wall loss estimation, dimensionless

\( S \) = Sutherland constant, \(110.56 \text{ K}\)

\( Sc \) = Schmidt number, dimensionless

\( Sh \) = Sherwood number, dimensionless

\( Stk \) = Stokes number, dimensionless

\( Stk_c \) = Stokes number for a Contraction, dimensionless

\( Stk_e \) = Stokes number for an Expansion, dimensionless

\( Stk_N \) = stokes number for the nozzle, dimensionless

\( Stk_p \) = stokes number for a particle, dimensionless

\( Stk_{pr} \) = stokes number at the entrance to the inner probe, dimensionless

\( Stk_{sec} \) = stokes number in the shroud core region, dimensionless

\( Stk_{sh} \) = stokes number in the shroud, dimensionless

\( T \) = temperature, K

\( t' \) = dimensionless residence time, dimensionless

\( T_o \) = reference temperature for Sutherland equation, \(273.11 \text{ K}\)

\( u \) = numerical factor = \(0.4987445\)

\( V \) = volume, \(\text{m}^3\)

\( V_+ \) = dimensionless particle deposition velocity, dimensionless

\( V_t \) = particle deposition velocity, \(\text{m/s}\)

\( W_L \) = wall loss ratio for a probe or nozzle, dimensionless

\( Z \) = sedimentation parameter, dimensionless

\( \eta_{asp} \) = overall aspiration ratio of a shrouded probe, dimensionless

\( \eta_{asp,pr} \) = aspiration ratio of the inner probe, dimensionless

\( \eta_{asp,sh} \) = aspiration ratio of shroud, dimensionless

\( \eta_B \) = transport efficiency for a bend, dimensionless

\( \eta_{Be} \) = turbulent flow transport efficiency for a bend, dimensionless

\( \eta_{asp,N} \) = overall aspiration ratio of a nozzle, dimensionless

\( \eta_N \) = transmission or transport efficiency for a nozzle, dimensionless

\( \eta_{sp} \) = transmission or transport efficiency for a shrouded probe, dimensionless

\( \eta_{Td} \) = thermal diffusion transport efficiency for a tube, dimensionless

\( \eta_{Tgl} \) = laminar flow gravity settling transport efficiency for a tube, dimensionless

\( \eta_{Tgt} \) = turbulent flow gravity settling transport efficiency for a tube, dimensionless

\( \eta_{Te} \) = turbulent eddy transport efficiency for a tube, dimensionless

\( \eta_{Tube} \) = tube total transport efficiency, dimensionless

\( \eta_c \) = transport efficiency for a contraction, dimensionless

\( \eta_E \) = transport efficiency for an expansion, dimensionless
\( \eta_s \) = transport efficiency for a splitter, dimensionless
\( \Theta \) = component half-angle, degrees
\( \theta \) = inclination of the tube from the horizontal plane, radians
\( \lambda \) = mean free path of air in transport system, m
\( \mu \) = viscosity of air in transport system, N-s/m\(^2\), or kg/m\( s \)
\( \mu_o \) = reference viscosity for Sutherland equation, N-s/m\(^2\)
\( \xi \) = particle diffusion time, dimensionless
\( \rho \) = density of air in transport system, kg/m\(^3\)
\( \rho_i \) = density of a subject particle, kg/m\(^3\)
\( \rho_p \) = density of the particle, kg/m\(^3\)
\( \tau_+ \) = dimensionless relaxation time, dimensionless
\( \tau_N \) = aerosol particle deflection time period, s
\( u \) = velocity, m/s
\( u_{ci} \) = velocity at the inlet a component, m/s
\( u_{co} \) = velocity at the outlet a component, m/s
\( u_{ni} \) = velocity at the inlet of the nozzle, m/s
\( u_o \) = velocity of the undisturbed free stream, m/s
\( u_{pr} \) = mean velocity in the inner probe, m/s
\( u_{sh} \) = mean velocity in the shroud, m/s
\( u_{sc} \) = velocity in the core region of the shroud, m/s
\( u_{ts} \) = particle terminal velocity, m/s
\( \varphi \) = bend angle, radians
\( \kappa \) = bend curvature ratio, dimensionless
\( \phi \) = bifurcation angle, degrees

**Unit Abbreviations**

Deg. = Degree
J = Joule
kg = kilogram
kmol = kilomole
kPa = kilopascal
m = meter
mm = millimeter
\( \mu m \) = micrometer or micron
N = Newton
Pa = Pascal
s = second
\( ^\circ C \) = degrees Celsius
K = degrees Kelvin
THEORY AND DISCUSSION

1 Introduction

Deposition is software for evaluating penetration of aerosol through aerosol sampling systems. The Deposition Calculator version 1.0 represents a complete rebuild of the software using an object-oriented design.

Deposition Calculator was written using Embarcadero RAD Studio XE5. The software provides models for a number of components that are generally used in the transport system of a stack or duct sampling system. Each component model is based on peer-reviewed literature. This document provides the penetration or deposition model equations and references used in the calculation engine for the Deposition Calculator software. It does not include the source code, coding of forms, or coding of navigation methods used in the software.

2 Program Basics

An aerosol transport system is a collection of flow components such as tubes, bends, and probes that allows for the extraction and conveyance of an aerosol sample from one location to another. The term sample line is often used interchangeably with the term transport system. Deposition Calculator software allows the user to analyze a model of a transport system or sample line to determine the fraction of particles of a given size that are conveyed from the system inlet to the outlet, otherwise known as the sampling efficiency or particle penetration. Typically, some fraction of particles will be lost to the walls of the system due to mechanisms such as gravitational sedimentation, diffusion, or inertial impaction. In Deposition Calculator, a transport system is represented by a linked list of components that represent the mechanical elements of the physical transport system. Only transport components that have published efficiency models are represented in Deposition Calculator. Actual transport systems may contain features or exhibit deposition mechanisms (e.g. electrostatic deposition) that are not modeled by Deposition Calculator. Failure to accurately model the physical system may lead to a prediction of transport efficiency that does not match that of the physical system.
3 General Equations and Standard Conditions

Deposition Calculator uses 25 °C and 101.325 kPa as the standard conditions for a transport system. Particle sizes used in Deposition Calculator are based on the Aerodynamic Diameter (AD) concept (Ref 2, p 24), where the particles are assumed to be spherical in shape and have a density of 1000 kg/m³. Conversion of other particle densities to the AD can be performed by the user with the following equation, which is not included in the Deposition Calculator code.

\[
D_{AD} = D_i \left( \frac{\rho_i}{1000 \text{ kg/m}^3} \right)^{0.5}
\]

Where:
- \(D_{AD}\) = aerodynamic diameter of a subject particle, m
- \(D_i\) = actual diameter of a subject particle, m
- \(\rho_i\) = density of a subject particle, kg/m³

For example: A facility uses 3 µm plutonium dioxide particles with a density of 11.5 g/cm³, what is the aerodynamic diameter that should be used in Deposition Calculator.

\[
D_{AD} = D_i \left( \frac{\rho_i}{1000 \text{ kg/m}^3} \right)^{0.5} = (3 \mu m)(1E-06 \text{ m/\mu m}) \left[ \frac{(11.5 \text{ g/cm}^3) \left(1000 \text{ kg/m}^3\right)^{0.5}}{1000 \text{ kg/m}^3} \right] = 1.02E-06 \text{ m} = 10.2 \mu m.
\]

This indicates that a 3 µm particle with a density of 11.5 g/cm³ settles at the same velocity as a 10.2 µm particle with a density of 1 g/cm³.
The properties of air, along with the other constants used in Deposition Calculator are presented in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Universal Gas Constant</td>
<td>$R_u$</td>
<td>8314.471 J/kmol·K</td>
<td>21</td>
</tr>
<tr>
<td>Molecular Weight of Air</td>
<td>MW</td>
<td>28.962 kg/kmol</td>
<td>1</td>
</tr>
<tr>
<td>Boltzmann’s Constant</td>
<td>k</td>
<td>1.3807E-23 N·m/K</td>
<td>1</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>g</td>
<td>9.807 m/s²</td>
<td>2, p. 833</td>
</tr>
<tr>
<td>Particle Density</td>
<td>$\rho_p$</td>
<td>1000 kg/m³</td>
<td>2, p 24</td>
</tr>
</tbody>
</table>

In order to determine the total particle penetration through a transport system, calculations assume superposition of components; i.e. particle losses in any component are independent of the components upstream or downstream. In addition, for components in which particle losses due to different mechanisms are computed using mechanism-specific correlations, total penetration for the component is determined from the product of the mechanisms (superposition of mechanisms). If there are $N$ components in a system and $\eta_n$ is the penetration of aerosol in the $n^{th}$ component, the total penetration ($\eta_{tot}$) for a system transporting monodispersed particles can be assumed to be the product of the penetration of each independent node:

$$\eta_{tot} = \eta_1 \eta_2 \eta_3 \ldots \eta_n = \prod_{i=1}^{n} \eta_i$$  \hspace{1cm} Eq. 1

The density of air at the actual transport system temperature and pressure can be estimated from the Ideal Gas Law as follows:

$$\rho = \frac{M}{V} = \frac{P}{RT}$$  \hspace{1cm} Eq. 2

Where:
- $\rho$ = density of air in transport system, kg/m³
- $M$ = mass, kg
- $V$ = volume, m³
- $P$ = pressure, Pa
- $T$ = temperature, K
- $R$ = gas constant = $R_u$/MW, J/kg·K
- $MW$ = molecular weight of air, kg/kmol
The viscosity of air at the actual transport system temperature is found using the Sutherland approximation (Ref 4) as

\[
\mu = \mu_o \left( \frac{T}{T_o} \right)^{1.5} \left( \frac{T_o + S}{T + S} \right)
\]

Eq. 3

Where:
- \( \mu \) = viscosity of air in transport system, N-s/m\(^2\), or kg/m·s
- \( \mu_o \) = reference viscosity for Sutherland equation, 1.716E-05 N-s/m\(^2\), or kg/m·s
- \( T \) = temperature, K
- \( T_o \) = reference temperature for Sutherland equation, 273.11 K
- \( S \) = Sutherland constant, 110.56 K

The mean free path of air at the actual transport system temperature and pressure is found using the method developed by Jennings (Ref 1).

\[
\lambda = \frac{\pi}{8} \left( \frac{\mu}{\rho u} \right) \left( \frac{1}{\sqrt{\rho P}} \right)
\]

Eq. 4

Where:
- \( \lambda \) = mean free path of air in transport system, m
- \( \mu \) = viscosity of air in transport system, N-s/m\(^2\), or kg/m·s, [Eq. 3]
- \( \rho \) = density of air in transport system, kg/m\(^3\), [Eq. 2]
- \( P \) = pressure, Pa
- \( u \) = numerical factor = 0.4987445

The general equation for the Reynolds number (Ref 2, p 16) is:

\[
Re = \frac{\rho v L}{\mu}
\]

Eq. 5

Where:
- \( Re \) = Reynolds number, dimensionless
- \( \mu \) = viscosity of air in transport system, N-s/m\(^2\), or kg/m·s, [Eq. 3]
- \( \rho \) = density of air in transport system, kg/m\(^3\), [Eq. 2]
- \( L \) = characteristic length, m
- \( v \) = velocity, m/s

In the Deposition Calculator code, the characteristic length can be the diameter of a tube, the diameter of a particle, the diameter of a shroud or the diameter of a nozzle.
The Cunningham’s Slip Correction (Ref 5) is determined in Deposition Calculator as:

\[ C_c = 1 + \frac{\lambda}{D_p} \left[ 2.34 + 1.05 \exp \left( -0.39 \frac{D_p}{\lambda} \right) \right] \quad \text{Eq. 6} \]

Where:
- \( C_c \) = Cunningham's slip correction factor, dimensionless
- \( \lambda \) = mean free path of air in transport system, m, [Eq. 4]
- \( D_p \) = diameter of particle, m

The stokes number (Ref 2, p 25) is of the form

\[ Stk = \frac{C_c \rho_p D_p^2 v}{9 \mu d} \quad \text{Eq. 7} \]

Where:
- \( Stk \) = Stokes number, dimensionless
- \( C_c \) = Cunningham's slip correction factor, dimensionless
- \( \rho_p \) = density of the particle, kg/m\(^3\)
- \( D_p \) = diameter of particle, m
- \( v \) = velocity, m/s
- \( \mu \) = viscosity of air in transport system, N-s/m\(^2\), or kg/m-s, [Eq. 3]
- \( d \) = diameter, m
4 Particle Penetration through a Shrouded Probe

Hongrui Gong (Ref 3) and others developed a predictive model that allows the estimation of the particle penetration and the aspiration ratio of a shrouded probe at any sample rate and free stream velocity.

A generic shrouded probe is presented as Figure 1 and the associated dimensions used in Deposition Calculator are presented in Table 2. The internal diameter of the inner probe at the exit \( d_o \) in some cases is an approximation.

![Generic shrouded probe](image)

**Figure 1: Generic shrouded probe**

<table>
<thead>
<tr>
<th>Probe Name</th>
<th>( d_{sh} ) (m)</th>
<th>( d_b ) (m)</th>
<th>( d_i ) (m)</th>
<th>( d_o ) (m)</th>
<th>( L_{pr} ) (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RF2-111</td>
<td>0.0538</td>
<td>0.0437</td>
<td>0.0183</td>
<td>0.0381</td>
<td>0.1293</td>
</tr>
<tr>
<td>RF2-112</td>
<td>0.0538</td>
<td>0.0475</td>
<td>0.0311</td>
<td>0.0381</td>
<td>0.1293</td>
</tr>
<tr>
<td>RF2-113</td>
<td>0.0642</td>
<td>0.0559</td>
<td>0.0447</td>
<td>0.0381</td>
<td>0.2444</td>
</tr>
<tr>
<td>CMR4CFM-HI</td>
<td>0.0780</td>
<td>0.0680</td>
<td>0.0220</td>
<td>0.0381</td>
<td>0.2385</td>
</tr>
<tr>
<td>CMR4CFM-MI</td>
<td>0.0780</td>
<td>0.0664</td>
<td>0.0262</td>
<td>0.0381</td>
<td>0.2385</td>
</tr>
<tr>
<td>WIPP6CFM</td>
<td>0.1020</td>
<td>0.0860</td>
<td>0.0300</td>
<td>0.0510</td>
<td>0.3630</td>
</tr>
</tbody>
</table>

The aspiration ratio is found as follows:

\[
\eta_{asp} = F \eta_{asp,sh} \eta_{asp,pr} \quad \text{Eq. 8}
\]

Where:

- \( \eta_{asp} \) = overall aspiration ratio, dimensionless
- \( \eta_{asp,sh} \) = aspiration ratio of shroud, dimensionless
- \( \eta_{asp,pr} \) = aspiration ratio of the inner probe, dimensionless
- \( F \) = correlation function, dimensionless, [Eq. 13]
The aspiration ratio of the shroud and inner probe are found as

$$\eta_{asp,x} = 1 + \alpha_x (R_x - 1)$$  \hspace{1cm} \text{Eq. 9}$$

and

$$\alpha_x = \frac{1.05 Stk_x}{1 + 1.05 Stk_x}$$  \hspace{1cm} \text{Eq. 10}$$

and

$$R_x = \frac{v_o}{v_x}$$  \hspace{1cm} \text{Eq. 11}$$

Where:
- $v_o$ = velocity of the undisturbed free stream, m/s
- $v_x$ = velocity at location “x”, m/s
- $x$ = represents either the shroud, the inner probe or the shroud core region.

In their seminal paper describing the operation and performance of a shrouded probe, McFarland et. al. (Ref 20) observed that the velocity in the shroud-body gap was approximately equal to the free stream velocity. This is the result that would be predicted by an assumption of inviscid flow through the shroud gap for the case in which the sample flow rate is sufficiently low to allow near stagnation conditions to be achieved inside the shroud. The Deposition Calculator model allows the velocity reduction ratio to be determined from the probe geometry and free stream velocity, and allow the predictive model of Gong et. al. (Ref 3) to be applied to the commercial probe designs. In this model the important parameters are the actual volumetric sampling rate ($Q_s$), the cross-section area of the shroud inlet ($A_{sh}$), the cross-section area of the gap between the inner probe body and the shroud ($A_{gap}$), and the free stream velocity ($v_o$). From these design parameters we can determine the velocity at the shroud inlet ($v_{sh}$) and velocity reduction ratio ($v_o/v_{sh}$).

Three regions of probe operation are identified depending upon sample flow rate and gap area relative to the free stream velocity: full sub-isokinetic in which the free stream velocity is sufficient to maximize the gap velocity, partial sub-isokinetic operation in which the free stream velocity remains higher than shroud velocity, but is insufficient to maximize the gap velocity, and super-isokinetic in which there is no velocity reduction at the shroud inlet and the sample flow rate controls the aspiration at the inlet. Although the latter two modes fall outside of the recommended operation of a shrouded probe, they may occur in both actual sampling situations when free stream velocity varies over a broad range.
The typical mode of operation for the shrouded probe is one in which the probe is sufficiently sub-isokinetic to achieve maximum velocity of the by-pass flow through the probe-shroud gap. In this case:

\[
\frac{v_o A_{gap} + Q_s}{A_{sh}} > v_o
\]

then

\[
v_{sh} = \frac{v_o A_{gap} + Q_s}{A_{sh}}
\]

In the case where the free stream velocity is so low that the shroud samples super-isokinetic relative to the free stream:

\[
\frac{Q_s}{A_{sh}} > v_o
\]

then

\[
v_{sh} = \frac{Q_s}{A_{sh}}
\]

The last condition to consider is the intermediate case in which the shroud is sub-isokinetic relative to the free stream, but the stagnation pressure in the shroud is insufficient to maximize the gap velocity. For this case the shroud velocity will be the free stream velocity:

\[
v_{sh} = v_o
\]

Referring to Figure 1 for shrouded probe nomenclature, when calculating the aspiration ratio for the shroud (\( \eta_{asp} \)), the Stokes number is calculated with the diameter of the shroud (d_{sh}) and velocity of the undisturbed free stream (\( v_o \)). However, when calculating the aspiration ratio for the inner probe (\( \eta_{asp,pr} \)) the Stokes number is calculated with the inlet diameter of the inner nozzle (d_{i}) and the velocity in the core region (\( v_{sc} \)) of the shroud. The velocity in the core region of the probe is given by

\[
u_{sc} = v_{sh} \left[ 1 + 1.45 \left( 1 - \frac{1 + \ln R_{sh}}{R_{sh}} \right) \right] \quad \text{Eq. 12}
\]

Where:

- \( R_{sh} \) = velocity ratio = \( v_o/v_{sh} \), dimensionless
- \( v_{sh} \) = mean velocity in the shroud, m/s
The velocity ratio \( R_x \) in Eq. 9 for the aspiration ratio of the shroud is

\[
R_{sh} = \text{velocity ratio} = \frac{\nu_o}{\nu_{sh}}, \text{dimensionless, and}
\]

for the aspiration ratio of the inner probe

\[
R_{pr} = \text{velocity ratio} = \frac{\nu_{sc}}{\nu_{pr}}, \text{dimensionless}.
\]

Where:

\[
\nu_{pr} = \text{mean velocity in the inner probe, m/s}
\]

The correlation function is found as

\[
F = 1 - (R_{sh} - 1) \frac{0.861 Stk_{sh}}{[2.34 + 0.939 (R_{sh} - 1)]Stk_{sh} + 1} \tag{Eq. 13}
\]

Where:

\[
Stk_{sh} = \text{stokes number in the shroud, dimensionless [Eq. 7]}
\]

In the case of \( Stk_{sh} \), \( d = \text{diameter of the shroud (d_{sh}) and } \nu = \nu_o \).

Wall loss in a shrouded probe are found as

\[
W_L = 0.496 \left(1 + \frac{L_w}{Fr}\right)^{0.194} Stk_{pr}^{0.613} \left(\frac{\nu_{sh}}{\nu_{pr}}\right)^{1.191} \tag{Eq. 14}
\]

Where:

\[
W_L = \text{wall loss ratio, dimensionless}
\]

\[
L_w = \text{normalized length, dimensionless, } = \frac{L_{pr}}{d_i}
\]

\[
L_{pr} = \text{length of inner probe in a shrouded probe, m}
\]

\[
d_i = \text{inlet diameter of the inner probe in a shrouded probe, m}
\]

\[
Fr = \text{Froude number, dimensionless}
\]

\[
Stk_{pr} = \text{stokes number in the inner probe, dimensionless [Eq. 7]}
\]

\[
\nu_{sh} = \text{mean velocity in the shroud, m/s}
\]

\[
\nu_{pr} = \text{mean velocity in the inner probe, m/s}
\]
The Froude number is given as

\[ F_r = \frac{v_{pr}^2}{g d_i} \]  \hspace{1cm} Eq. 15

The transmission ratio or transport efficiency is found as:

\[ \eta_{sp} = \eta_{asp} (1 - W_L) \]  \hspace{1cm} Eq. 16

Where:

- \( W_L \) = wall loss ratio, dimensionless, [Eq. 14]
- \( \eta_{asp} \) = overall aspiration ratio, dimensionless, [Eq. 8]
5 Particle Penetration through a Nozzle

An empirical relationship for the aspiration ratio of a thin walled nozzle, as developed by Vincent (Ref 7), is used in Depositions Calculator. This model does assume that the sample nozzle has parallel walls that do not taper. Assuming the probe is placed parallel with, or facing into the free stream velocity component the aspiration ratio is found as follows.

\[ \eta_{\text{asp},N} = 1 + (R_N - 1) \frac{1.05 \text{Stk}_N}{1 + 1.05 \text{Stk}_N} \]  \hspace{1cm} \text{Eq. 17}

and

\[ R_N = \frac{v_o}{v_{Ni}} \]  \hspace{1cm} \text{Eq. 18}

and

\[ \text{Stk}_N = \frac{C_c \rho_p D_p^2 v_o}{9 \mu d_{Ni}} \]  \hspace{1cm} \text{Eq. 19}

where

\[ R_N = \text{velocity ratio for a nozzle, dimensionless} \]
\[ \text{Stk}_N = \text{stokes number for the nozzle, dimensionless} \]
\[ v_o = \text{velocity of the undisturbed free stream, m/s} \]
\[ v_{Ni} = \text{velocity at the inlet of the nozzle, m/s} \]
\[ d_{Ni} = \text{diameter of the nozzle inlet, m} \]

Empirical relationships for wall losses in a nozzle are present by Fan, Et. al. (Ref 8) and are used by Deposition Calculator. The Wall loss is found as Eq. 20. Note that Fan developed the wall loss equation to calculate a percent wall loss. Deposition Calculator determines wall loss as a decimal value. The difference in the two equations is in the first term. Fan used a value of 176.9, however a value of 1.769 is used by Deposition Calculator.

\[ W_L = 1.769 \left( 1 + \frac{L_N}{(d_{Ni}/2)^2} \frac{(d_{Ni}/2)}{Fr} \right)^{-9.190} R_z^{0.559} Re^{-0.216} \]  \hspace{1cm} \text{Eq. 20}
Where
\[ L_N = \text{nozzle length, m} \]
\[ d_{Ni} = \text{inlet diameter of the nozzle, m} \]

The remaining values are given below in equation form.

\[ Fr = \frac{2 u_{Ni}^2}{g d_{Ni}} \quad \text{Eq. 21} \]
\[ R_z = \frac{2 \text{Stk}_p}{\sqrt{(\tau_N u_{Ni}) / d_{Ni}/2}} \quad \text{Eq. 22} \]
\[ Re = \frac{\rho u_{Ni} d_{Ni}}{\mu} \quad \text{Eq. 23} \]
\[ \text{Stk}_p = \frac{C_c \rho_p D_p^2 u_{Ni}}{9 \mu d_{Ni}} \quad \text{Eq. 24} \]
\[ \tau_N = \frac{1}{(C1) \sqrt{k_{ref}}} \quad \text{Eq. 25} \]

and

\[ C1 = 3.08 \sqrt{(\rho \mu)} \left( D_p \rho_p \right) \quad \text{Eq. 26} \]

and

\[ k_{ref} = \frac{4 u_{Ni}}{d_{Ni}/2} \quad \text{Eq. 27} \]
The transmission ratio or transport efficiency is found as

\[ \eta_N = \eta_{asp,N} (1 - W_L) \]  \hspace{1cm} Eq. 28

Where:
- \( W_L \) = wall loss ratio, dimensionless, [Eq. 20]
- \( \eta_{asp,N} \) = overall aspiration ratio, dimensionless, [Eq. 17]
6 Particle Penetration through a Tube

Deposition Calculator models particle deposition in a tube resulting from gravitational settling, diffusional deposition and turbulent inertial deposition. In addition, different models are used for turbulent and laminar flow conditions. To address the different flow conditions, Deposition Calculator uses the following logic.

- Laminar flow model used when \( Re < 2100 \)
- Turbulent eddy flow model used when \( Re > 4000 \)
- For conditions where \( 2100 > Re < 4000 \) the minimum penetration value from both laminar and turbulent model calculations is selected.

The total penetration or transport efficiency in a tube \( (\eta_{\text{Tube}}) \) is the product of the transport efficiency for each deposition mechanism. The empirical relationship is the same as that presented in Eq. 1.

6.1 Gravitation Settling Model

The laminar gravitation-settling model is based on Heyder and Gebhart (Ref 9). The transport efficiency due to gravitation settling in laminar flow is found as

\[
\eta_{\text{gl}} = 1 - \left( \frac{2}{\pi} \right) \left[ 2K \sqrt{1 - K^{2/3}} - K^{1/3} \sqrt{1 - K^{2/3}} + \arcsin(K^{1/3}) \right] \quad \text{Eq. 29}
\]

and

\[
K = \frac{3}{4} t'
\]

\[
t' = \frac{L \, u_{ts}}{v \, d_{rl}} \cos \theta \quad \text{Eq. 31}
\]

The particle Reynolds number is found as

\[
Re_p = \frac{\rho \, u_{ts} \, D_p}{\mu} \quad \text{Eq. 32}
\]

When the particle Reynolds Number < 1.0 the particle terminal velocity is found as (Ref 2)

\[
u_{ts} = \frac{\rho_p \, D_p^2 \, g \, C_c}{18 \mu} \quad \text{Eq. 33}\]
For particle Reynolds Number \( \geq 1.0 \) particle terminal velocity is found as

\[
u_{ts} = \sqrt{\frac{4 \rho_p D_p^2 g}{3 C_d \rho}} \quad \text{Eq. 34}
\]

and

\[
C_d = \frac{24}{R_p} \left[ 1 + 0.15 R_p^{0.687} \right] \quad \text{Eq. 35}
\]

Note: The particle Reynolds Number cannot be greater than 1000 when using these equations.

For the case when the flow is turbulent, Schwendiman (Ref 10) developed the model used in Deposition Calculator. The transport efficiency due to gravitation settling in turbulent flow is found as

\[
\eta_{Tgt} = \exp(-Z) \quad \text{Eq. 36}
\]

and

\[
Z = \frac{4 t'}{\pi} \quad \text{Eq. 37}
\]

A glossary for this section is provided below:

- \( t' \) = dimensionless residence time, dimensionless
- \( Z \) = sedimentation parameter, dimensionless
- \( \nu_{ts} \) = particle terminal velocity, m/s
- \( L \) = length of tube, m
- \( \nu \) = sample velocity, m/s
- \( d_{ti} \) = internal diameter of the tube, m
- \( \theta \) = inclination of the tube from the horizontal plane, radians
- \( \rho \) = density of air in transport system, kg/m\(^3\)
- \( \rho_p \) = density of the particle, kg/m\(^3\)
- \( D_p \) = diameter of particle, m
- \( C_c \) = Cunningham's slip correction factor, dimensionless
C_d  =  drag coefficient, dimensionless

\( g \)  =  Gravitational acceleration, 9.81 m/s²

Re_p  =  particle settling Reynolds number, dimensionless

6.2 Turbulent Eddy Model

The turbulent eddy model only applies to turbulent flow. The model used in Deposition Calculator is based on work done by Liu (Ref 11), Lee (Ref 12), and Kulkarni (Ref 2).

The turbulent eddy transport efficiency is found as:

\[
\eta_{\tau呵呵} = \exp\left(\frac{-\pi d_{\tau i}L V_t}{Q}\right)
\]

Where:

\[ V_t \]  =  particle deposition velocity, m/s
\[ Q \]  =  volumetric flow rate, m³/s
\[ L \]  =  length of tube, m
\[ d_{\tau i} \]  =  internal diameter of the tube, m

In the case of laminar flow, the turbulent eddy transport efficiency (\( \eta_{\tau呵呵} \)) is set to 1.0 in Deposition Calculator.

The calculation of the particle deposition velocity must consider the value of the dimensionless relaxation time, \( \tau_+ \), which is found as

\[
\tau_+ = 0.0395 \left(Stk_p\right)^{Re^{3/4}}
\]

and

\[
Stk_p = \frac{C_c \rho_p D_p^2 v}{9 \mu d_{\tau i}}
\]

\[
Re = \frac{\rho v d_{\tau i}}{\mu}
\]

The dimensionless deposition velocity is then found as follows

When \( \tau_+ < 0.3 \) then \( V_+ = 0.0 \)
When $\tau_+ > 12.9$ then $V_+ = 0.1$

Otherwise

$$V_+ = 0.0006 (\tau_+^2)+2E-08 \ Re \quad Eq. 42$$

The particle deposition velocity is

$$V_t = \frac{V_+ v}{5.03} Re^{-1/8} \quad Eq. 43$$

A glossary for this section is provided below:

- $V_t$ = particle deposition velocity, m/s
- $V_+$ = dimensionless particle deposition velocity, dimensionless
- $L$ = length of tube, m
- $\nu$ = sample velocity, m/s
- $d_{in}$ = internal diameter of the tube, m
- $\rho$ = density of air in transport system, kg/m$^3$
- $\rho_p$ = density of the particle, kg/m$^3$
- $D_p$ = diameter of particle, m
- $C_c$ = Cunningham's slip correction factor, dimensionless
- $\tau_+$ = dimensionless relaxation time, dimensionless

6.3 Thermal Diffusion Model

The empirical relationships for both the laminar and the turbulent diffusion models in Deposition Calculator are presented by Kulkarni (Ref 2). The original work is based on Holman (Ref 14) and Friedlander (Ref 13)

In both turbulent and laminar flow the particle transport efficiency due to thermal diffusion is represented by

$$\eta_{T_d} = \exp(-\xi Sh) \quad Eq. 44$$

Where:

- $\xi$ = particle diffusion time, dimensionless
- $Sh$ = Sherwood number, dimensionless
The diffusion time is found as

$$\xi = \frac{\pi D_c L}{Q}$$

Eq. 45

and

$$D_c = \frac{k T C_c}{3 \pi \mu D_p}$$

Eq. 46

Where

- $D_c$ = diffusion coefficient, m²/s
- $L$ = tube length, m
- $Q$ = volumetric flow in tube, m³/s
- $k$ = Boltzmann constant, 1.3807E-23 N·m/K
- $T$ = temperature of air in transport system, K
- $\mu$ = viscosity of air in transport system, N·s/m²
- $D_p$ = particle diameter, m

For a Re < 4000 (laminar flow)

$$Sh = 3.66 + \frac{0.2672}{(\xi + 0.10079 \xi^{1/3})}$$

Eq. 47

and for Re > 2100 (turbulent flow)

$$Sh = 0.0118 Re^{7/8} Sc^{1/3}$$

Eq. 48

Where:

- $Sc$ = Schmidt number, dimensionless

The Schmidt number is given as

$$Sc = \frac{\mu}{\rho D_c}$$

Eq. 49
7  *Particle Penetration through a Bend*

Deposition Calculator uses two different models to calculate the transport efficiency based on the data presented below as Figure 1. The development of both models was based on testing in either the laminar or turbulent flow regimes, but none of the test data was in the transition flow region. The Pui model for \( \text{Re} = 1000 \) (Blue line in Figure 2) represents most of the data with the exception of \( \text{Re} = 100 \) for which it provides conservative data. However, the turbulent model of Pui (Pink line in Figure 2) does follow the turbulent data points for Stokes number greater than 0.1. To address the different flow conditions, Deposition Calculator uses the following logic.

- Pui turbulent model used for \( \text{Re} > 4000 \) and Stokes number > 0.1
- Pui \( \text{Re}=1000 \) model used for all other conditions.

![Figure 2: Bend transport efficiency data and various curve fits](image)

Using the data of Pui (Ref 16) and others, Kulkarni (Ref 2) presents the following database correlation for the deposition of particles in bend under turbulent flow conditions; the Pui turbulent model.
\[ \eta_{Bt} = \exp(-2.823 \, Stk \, \varphi) \]  

Eq. 50

Where:

\begin{align*}
Stk & = \text{Stokes number, dimensionless} \\
\varphi & = \text{bend angle, radians}
\end{align*}

In all cases, the models assume a smooth bend with a bend curvature ratio \((\kappa) \geq 4\). The bend curvature ratio is

\[ \kappa = \frac{R_b}{(d_{Ti}/2)} \]  

Eq. 51

Where:

\begin{align*}
R_b & = \text{Radius of curvature of the bend, m}
\end{align*}

The Pui Re=1000 model, presented by Kulkarni (Ref 2), is a fit to the data of Pui. However, the model also provides a good fit for most other data. The model is presented here as

\[ \eta_B = \left[ 1 + \left( \frac{Stk}{0.171} \right)^{0.452} \right]^{\frac{2\varphi}{\pi}} \]  

Eq. 52
8  Particle Penetration through a Contraction

A model for predicting depositional losses in contractions where the entrance and exit tubes are both circular was developed by Muyshondt (Ref 17). The empirical relationship used by Deposition Calculator for particle transport efficiency in a contraction component is presented below. The relationship is used for both turbulent or laminar flow conditions.

\[ \eta_c = 1 - \frac{1}{1 + \left[ \frac{Stk_c \left( 1 - \left( \frac{A_o}{A_i} \right) \right)}{3.14 \exp(-0.0185 \Theta)} \right]^{1.24}} \]

Eq. 53

Where:

\[ A_i = \text{area of the component inlet, m}^2 \]
\[ A_o = \text{area of the component outlet, m}^2 \]
\[ \Theta = \text{component half-angle, degrees} \]

The Stokes number for a contraction component is found as

\[ Stk_c = \frac{\rho_p D_p^2 v_i C_c}{9 \mu d_{co}} \]

Eq. 54

Where:

\[ v_i = \text{velocity at the inlet a component, m/s} \]
9 Particle Penetration through an Expansion

A model for predicting depositional losses in expansions where the entrance and exit tubes are both circular was developed presented by Muyshondt (Ref 18). The empirical relationship used by Deposition Calculator for particle transport efficiency in an expansion component is presented below. The relationship is used for both turbulent or laminar flow conditions.

\[ \eta_E = 1-1.1358 R_{ex}^2 \exp[-0.5 (b_1^2 + b_2^2)] \]  
\[ \text{Eq. 55} \]

and

\[ R_{ex} = 1 - \frac{A_i}{A_o} \]  
\[ \text{Eq. 56} \]

\[ b_1 = \ln \left( \frac{\text{Stk}_e R_{ex}}{0.5518} \right) \frac{1}{1.9661} \]  
\[ \text{Eq. 57} \]

\[ b_2 = \ln \left( \frac{\Theta}{12.519} \right) \frac{1}{2.7825} \]  
\[ \text{Eq. 58} \]

The Stokes number for an expansion component is found as

\[ \text{Stk}_e = \frac{\rho_p D_p^2 v_o C_c}{9 \mu d_{ci}} \]  
\[ \text{Eq. 59} \]

Where:
- \( A_i \) = area of the component inlet, m\(^2\)
- \( A_o \) = area of the component outlet, m\(^2\)
- \( \Theta \) = component half-angle, degrees
- \( v_o \) = velocity at the outlet a component, m/s
- \( d_{ci} \) = diameter at the component inlet or in this case the expansion inlet, m
10  Particle Penetration through a Splitter

Gupta (Ref 19) developed empirical relationships for several splitter designs. There is no taper on the inlet and outlet tubes of the model used by Deposition Calculator. The empirical relationship for estimating transport efficiency is presented below. The relationship is used for both turbulent or laminar flow conditions.

\[
\ln(\eta_s) = a + \frac{b}{1 + \left(\frac{Stk}{c}\right)^d} + \frac{e}{1 + \left(\frac{\phi}{f}\right)^g} + \frac{h}{\left[1 + \left(\frac{Stk}{c}\right)^d\right]\left[1 + \left(\frac{\phi}{f}\right)^g\right]} \quad \text{Eq. 60}
\]

Where:
- \(\phi\) = bifurcation angle, degrees
- \(Stk\) = Stokes number where \(d =\) inlet diameter, dimensionless
- \(a = -2.635\)
- \(b = 2.623\)
- \(c = 0.4573\)
- \(d = 1.680\)
- \(e = 2.291\)
- \(f = 56.45\)
- \(g = 3.870\)
- \(h = -2.288\)
REFERENCES

6. S Chandra, *Shrouded Probes for Aerosol Sampling in Ducts and Stacks*, Dissertation, Texas A&M University, College Station, TX, 1996
10. LC Schwendiman, GE Stegen, and JA Glissmeyer, Report BNWL-SA-5138, Battelle Pacific Northwest Laboratory, Richland, WA, 1975
18. A. Muyshondt, *Aerosol Deposition in Transport Lines*, Dissertation, Texas A&M University, College Station, TX, 1995

APPENDIX - A

Hand Calculations
A-1  General Equations

The general equations can be checked with the Deposition Calculator Fluid Tab on the main screen. The results, based on the following input values, are presented in Table A 1, along with the results from hand calculations using the indicated equation.

**Input:**
Temperature (°C) = 25
Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density of Air (kg/m³), ρ</td>
<td>Eq. 2</td>
<td>1.1839</td>
<td>1.1839</td>
</tr>
<tr>
<td>Dynamic Viscosity (kg/m·s), μ</td>
<td>Eq. 3</td>
<td>1.837E-05</td>
<td>1.837E-05</td>
</tr>
<tr>
<td>Mean Free Path (µm), λ</td>
<td>Eq. 4</td>
<td>0.0667</td>
<td>0.0667</td>
</tr>
</tbody>
</table>
A-2 Shrouded Probe

In order to check the intermediate results for the aspiration ratio and transmission efficiency, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 2, along with the results from hand calculations using the indicated equation.

**Input:**
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Free Stream Velocity (m/s) = 7
- Inclination from Horizontal (Deg) = 0
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 25
- Pressure (kPa) = 101.325
- Probe Type = RF2-111

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cunningham slip correction (unitless), Cc</td>
<td>Eq. 6</td>
<td>1.0156</td>
<td>1.0156</td>
</tr>
<tr>
<td>Mean velocity in shroud (m/s), ( \nu_{sh} )</td>
<td>-----</td>
<td>2.799</td>
<td>2.799</td>
</tr>
<tr>
<td>Ratio free stream velocity to mean velocity in the shroud (unitless), ( R_{sh} )</td>
<td>Eq. 11</td>
<td>2.500</td>
<td>2.500</td>
</tr>
<tr>
<td>Stokes number in shroud (unitless), ( Stk_{sh} )</td>
<td>Eq. 7</td>
<td>0.0799</td>
<td>0.0799</td>
</tr>
<tr>
<td>( \alpha_{s} ) (unitless)</td>
<td>Eq. 10</td>
<td>0.0774</td>
<td>0.0774</td>
</tr>
<tr>
<td>Aspiration ratio of shroud (unitless), ( \eta_{asp,sp} )</td>
<td>Eq. 9</td>
<td>1.116</td>
<td>1.116</td>
</tr>
<tr>
<td>Core region of shroud velocity (m/s), ( \nu_{sc} )</td>
<td>Eq. 12</td>
<td>3.747</td>
<td>3.747</td>
</tr>
<tr>
<td>Mean velocity in inner probe (m/s), ( \nu_{pr} )</td>
<td>-----</td>
<td>3.6119</td>
<td>3.6119</td>
</tr>
<tr>
<td>Ratio free stream velocity to mean velocity in the shroud (unitless), ( R_{pr} )</td>
<td>Eq. 11</td>
<td>1.0376</td>
<td>1.0376</td>
</tr>
<tr>
<td>Stokes number in shroud core (unitless), ( Stk_{sc} )</td>
<td>Eq. 7</td>
<td>0.1258</td>
<td>0.1258</td>
</tr>
<tr>
<td>( \alpha_{pr} ) (unitless)</td>
<td>Eq. 10</td>
<td>0.1167</td>
<td>0.1167</td>
</tr>
<tr>
<td>Aspiration ratio of inner probe (unitless), ( \eta_{asp,pr} )</td>
<td>Eq. 9</td>
<td>1.004</td>
<td>1.004</td>
</tr>
<tr>
<td>Correlation function (unitless), ( F )</td>
<td>Eq. 13</td>
<td>0.9206</td>
<td>0.9206</td>
</tr>
<tr>
<td>Overall probe aspiration ratio (unitless), ( \eta_{asp} )</td>
<td>Eq. 8</td>
<td>1.032</td>
<td>1.032</td>
</tr>
<tr>
<td>Stokes number at the entrance to the inner probe (unitless), ( Stk_{pr} )</td>
<td>Eq. 7</td>
<td>0.1212</td>
<td>0.1212</td>
</tr>
<tr>
<td>Parameter</td>
<td>Equation</td>
<td>Value 1</td>
<td>Value 2</td>
</tr>
<tr>
<td>-----------------------------------</td>
<td>----------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>Normalized length (unitless), $L_w$</td>
<td>Eq. 14</td>
<td>7.066</td>
<td>7.066</td>
</tr>
<tr>
<td>Froude number (unitless), $Fr$</td>
<td>Eq. 15</td>
<td>72.690</td>
<td>72.690</td>
</tr>
<tr>
<td>Wall loss (unitless), $W_L$</td>
<td>Eq. 14</td>
<td>0.1023</td>
<td>0.1023</td>
</tr>
<tr>
<td>Probe transport efficiency (unitless), $\eta_{sp}$</td>
<td>Eq. 16</td>
<td>0.9265</td>
<td>0.9265</td>
</tr>
</tbody>
</table>
A-3 Nozzle

In order to check the intermediate results for the aspiration ratio and transmission efficiency, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 3, along with the results from hand calculations using the indicated equation.

**Input:**
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Inlet diameter (mm) = 13
- Nozzle length (mm) = 50
- Free Stream Velocity (m/s) = 7
- Inclination from Horizontal (Deg) = 0
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 25
- Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cunningham slip correction (unitless), $C_c$</td>
<td>Eq. 6</td>
<td>1.0156</td>
<td>1.0156</td>
</tr>
<tr>
<td>Mean velocity in nozzle (m/s), $v_{Ni}$</td>
<td>-----</td>
<td>7.1573</td>
<td>7.1573</td>
</tr>
<tr>
<td>Ratio free stream velocity to mean velocity in the nozzle (unitless), $R_N$</td>
<td>Eq. 18</td>
<td>0.9780</td>
<td>0.9780</td>
</tr>
<tr>
<td>Stokes number at nozzle entrance (unitless), $Stk_N$</td>
<td>Eq. 19</td>
<td>0.3307</td>
<td>0.3307</td>
</tr>
<tr>
<td>Aspiration ratio of the nozzle (unitless), $\eta_{asp,N}$</td>
<td>Eq. 17</td>
<td>0.9943</td>
<td>0.9943</td>
</tr>
<tr>
<td>Froude number (unitless), $Fr$</td>
<td>Eq. 21</td>
<td>803.36</td>
<td>803.36</td>
</tr>
<tr>
<td>Factor in Wall loss equation (unitless), $R_z$</td>
<td>Eq. 22</td>
<td>0.1990</td>
<td>0.1990</td>
</tr>
<tr>
<td>Reynolds number in nozzle, $Re$</td>
<td>Eq. 23</td>
<td>5995.0</td>
<td>5995.0</td>
</tr>
<tr>
<td>Stokes number for particle in nozzle (unitless), $Stk_p$</td>
<td>Eq. 24</td>
<td>0.3381</td>
<td>0.3381</td>
</tr>
<tr>
<td>Aerosol particle deflection time period (s), $\tau_N$</td>
<td>Eq. 25</td>
<td>0.0105</td>
<td>0.0105</td>
</tr>
<tr>
<td>Particle lift factor ($s^{-0.5}$), $C_1$</td>
<td>Eq. 26</td>
<td>1.4365</td>
<td>1.4365</td>
</tr>
<tr>
<td>Rate of flow shear ($s^{-1}$), $k_{ref}$</td>
<td>Eq. 27</td>
<td>4404.5</td>
<td>4404.5</td>
</tr>
<tr>
<td>Wall loss (unitless), $W_L$</td>
<td>Eq. 20</td>
<td>0.1004</td>
<td>0.1004</td>
</tr>
<tr>
<td>Probe transport efficiency (unitless), $\eta_N$</td>
<td>Eq. 28</td>
<td>0.8945</td>
<td>0.8945</td>
</tr>
</tbody>
</table>
A-4 Tubes

Deposition Calculator uses several models to determine transport efficiency in a tube. As discussed in Section 6, different models may be used for turbulent and laminar flow conditions. To address the different flow conditions, Deposition Calculator uses the following logic.

- Laminar flow model used when \( Re < 4000 \)
- Turbulent eddy flow model used when \( Re > 2100 \)
- For conditions where \( 2100 > Re < 4000 \) the minimum penetration value from both laminar and turbulent model calculations is selected.

Three separate cases are evaluated in the hand calculation to test each flow condition.

Note that Deposition Calculator performs an iterative solution for the particle Reynolds number and the particle terminal velocity in the Gravitation Settling model, when the particle Reynolds number is greater than 1. A similar iterative solution has been used in the hand calculations. The approach is to estimate an initial terminal velocity with Eq. 33, then estimate the particle Reynolds number with the terminal velocity determined with Eq. 33. The drag coefficient is then estimated using the particle Reynolds number. A new terminal velocity is determined using Eq. 33. The two terminal velocities are compared and must agree within a difference of 0.0001 otherwise a new particle Reynolds number with the last terminal velocity is determined, followed by a new drag coefficient and a new terminal velocity. This process is repeated unit the difference between the new and the old terminal velocities is <0.0001.

A-4.1 Case 1: Turbulent flow

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 4, along with the results from hand calculations using the indicated equation.

Input:

<table>
<thead>
<tr>
<th>Input</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Size (µm)</td>
<td>10</td>
</tr>
<tr>
<td>Particle Density (kg/m³)</td>
<td>1000</td>
</tr>
<tr>
<td>Tube Internal diameter (mm)</td>
<td>25.4</td>
</tr>
<tr>
<td>Tube length (m)</td>
<td>1.0</td>
</tr>
<tr>
<td>Inclination from Horizontal (Deg.)</td>
<td>0</td>
</tr>
<tr>
<td>Sample Flow Rate (LPM)</td>
<td>100</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>25</td>
</tr>
<tr>
<td>Pressure (kPa)</td>
<td>101.325</td>
</tr>
</tbody>
</table>
### Table A.4: Tube Case 1 Equation Comparison

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number (unitless), Re</td>
<td>Eq. 5</td>
<td>5383.0</td>
<td>5383.0</td>
</tr>
<tr>
<td>Particle Reynolds number (unitless), Re_p</td>
<td>Eq. 32</td>
<td>0.00194</td>
<td>0.00194</td>
</tr>
<tr>
<td>Terminal Velocity (m/s), (u_{ts})</td>
<td>Eq. 33 or Eq. 34</td>
<td>0.00301</td>
<td>0.00301</td>
</tr>
<tr>
<td>Dimensionless residence time (unitless), (t')</td>
<td>Eq. 31</td>
<td>0.0361</td>
<td>0.0361</td>
</tr>
<tr>
<td>Sedimentation parameter (unitless), (Z)</td>
<td>Eq. 37</td>
<td>0.0459</td>
<td>0.0459</td>
</tr>
<tr>
<td>Transport Efficiency, Gravitational Settling in turbulent flow (unitless), (\eta_{Tgl})</td>
<td>Eq. 36</td>
<td>0.9551</td>
<td>0.9551</td>
</tr>
<tr>
<td>Particle Stokes number (unitless), (St_k)</td>
<td>Eq. 40</td>
<td>0.0795</td>
<td>0.0795</td>
</tr>
<tr>
<td>Dimensionless relaxation time (unitless), (\tau_+)</td>
<td>Eq. 39</td>
<td>1.9742</td>
<td>1.9742</td>
</tr>
<tr>
<td>Dimensionless particle deposition velocity (unitless), (V_+)</td>
<td>Eq. 42</td>
<td>0.002446</td>
<td>0.002446</td>
</tr>
<tr>
<td>Particle deposition velocity (m/s), (V_t)</td>
<td>Eq. 43</td>
<td>0.0005466</td>
<td>0.0005466</td>
</tr>
<tr>
<td>Transport Efficiency, Turbulent Eddy (unitless), (\eta_{Te})</td>
<td>Eq. 38</td>
<td>0.9742</td>
<td>0.9742</td>
</tr>
<tr>
<td>Particle diffusion coefficient (m²/s), (D_c)</td>
<td>Eq. 46</td>
<td>2.414E-12</td>
<td>2.414E-12</td>
</tr>
<tr>
<td>Particle diffusion time (unitless), (\xi)</td>
<td>Eq. 45</td>
<td>4.551E-09</td>
<td>4.551E-09</td>
</tr>
<tr>
<td>Sherwood number in turbulent flow (unitless), (Sh)</td>
<td>Eq. 48</td>
<td>4035.4</td>
<td>4035.4</td>
</tr>
<tr>
<td>Schmidt number (unitless), (Sc)</td>
<td>Eq. 49</td>
<td>6429107</td>
<td>6429107</td>
</tr>
<tr>
<td>Transport Efficiency, Thermal Diffusion (unitless), (\eta_{Td})</td>
<td>Eq. 44</td>
<td>0.99998</td>
<td>0.99998</td>
</tr>
<tr>
<td>Tube Transport Efficiency (unitless), (\eta_{Tube})</td>
<td>Eq. 1</td>
<td>0.9304</td>
<td>0.9304</td>
</tr>
</tbody>
</table>

#### A-4.2 Case 2: Laminar flow

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A.5, along with the results from hand calculations using the indicated equation.

**Input:**
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
Tube Internal diameter (mm)  = 38.1
Tube length (m) = 1.0
Inclination from Horizontal (Deg.) = 0
Sample Flow Rate (LPM) = 57
Temperature (°C) = 25
Pressure (kPa) = 101.325

Table A 5: Tube Case 2 Equation Comparison

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number (unitless), Re</td>
<td>Eq. 5</td>
<td>2045.4</td>
<td>2045.4</td>
</tr>
<tr>
<td>Particle Reynolds number (unitless), Reₚ</td>
<td>Eq. 32</td>
<td>0.00194</td>
<td>0.00194</td>
</tr>
<tr>
<td>Terminal Velocity (m/s), ᵥₜₛ</td>
<td>Eq. 33 or Eq. 34</td>
<td>0.00301</td>
<td>0.00301</td>
</tr>
<tr>
<td>Dimensionless residence time (unitless), t’</td>
<td>Eq. 31</td>
<td>0.0949</td>
<td>0.0949</td>
</tr>
<tr>
<td>Sedimentation parameter (unitless), K</td>
<td>Eq. 30</td>
<td>0.07116</td>
<td>0.07114</td>
</tr>
<tr>
<td>Transport Efficiency, Gravitational Settling in laminar flow (unitless), ηₗₚ</td>
<td>Eq. 29</td>
<td>0.8856</td>
<td>0.8856</td>
</tr>
<tr>
<td>Transport Efficiency, Turbulent Eddy (unitless), ηₑₑ</td>
<td>Eq. 38</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>Particle diffusion coefficient (m²/s), Dₑ</td>
<td>Eq. 46</td>
<td>2.414E-12</td>
<td>2.414E-12</td>
</tr>
<tr>
<td>Particle diffusion time (unitless), ₓ</td>
<td>Eq. 45</td>
<td>7.984E-09</td>
<td>7.984E-09</td>
</tr>
<tr>
<td>Sherwood number in laminar flow (unitless), Sh</td>
<td>Eq. 47</td>
<td>1330.0</td>
<td>1330.0</td>
</tr>
<tr>
<td>Schmidt number (unitless), Sc</td>
<td>Eq. 49</td>
<td>6429107</td>
<td>6429107</td>
</tr>
<tr>
<td>Transport Efficiency, Thermal Diffusion (unitless), ηₜₜ</td>
<td>Eq. 44</td>
<td>0.99999</td>
<td>0.99999</td>
</tr>
<tr>
<td>Tube Transport Efficiency (unitless), ηₐₜₜ</td>
<td>Eq. 1</td>
<td>0.8856</td>
<td>0.8856</td>
</tr>
</tbody>
</table>

A-4.3 Case 3: Transitional flow

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 6, along with the results from hand calculations using the indicated equation.
Input:
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Tube Internal diameter (mm) = 25.4
- Tube length (m) = 1.0
- Inclination from Horizontal (Deg.) = 0
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 20
- Pressure (kPa) = 99

Table A 6: Tube Case 3 Equation Comparison

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number (unitless), Re</td>
<td>Eq. 5</td>
<td>3088.9</td>
<td>3088.9</td>
</tr>
<tr>
<td>Particle Reynolds number (unitless), Reₚ</td>
<td>Eq. 32</td>
<td>0.00198</td>
<td>0.00198</td>
</tr>
<tr>
<td>Terminal Velocity (m/s), uₜₛ</td>
<td>Eq. 33 or Eq. 34</td>
<td>0.00305</td>
<td>0.00305</td>
</tr>
<tr>
<td>Dimensionless residence time (unitless), t'</td>
<td>Eq. 31</td>
<td>0.0641</td>
<td>0.0641</td>
</tr>
<tr>
<td>Sedimentation parameter (unitless), Z</td>
<td>Eq. 37</td>
<td>0.0816</td>
<td>0.0816</td>
</tr>
<tr>
<td>Sedimentation parameter (unitless), K</td>
<td>Eq. 30</td>
<td>0.04807</td>
<td>0.04805</td>
</tr>
<tr>
<td>Transport Efficiency, Gravitational Settling in turbulent flow (unitless), ηᵣₑₜₓ</td>
<td>Eq. 36</td>
<td>0.92164</td>
<td>0.92166</td>
</tr>
<tr>
<td>Transport Efficiency, Gravitational Settling in laminar flow (unitless), ηᵣₑₜₗ</td>
<td>Eq. 29</td>
<td>0.92171</td>
<td>0.92173</td>
</tr>
<tr>
<td>Selected Transport Efficiency for Gravitation Settling (unitless)</td>
<td>-----</td>
<td>0.92164</td>
<td>0.92166</td>
</tr>
<tr>
<td>Particle Stokes number (unitless), Stkₚ</td>
<td>Eq. 40</td>
<td>0.0459</td>
<td>0.0459</td>
</tr>
<tr>
<td>Dimensionless relaxation time (unitless), τ₊</td>
<td>Eq. 39</td>
<td>0.7517</td>
<td>0.7517</td>
</tr>
<tr>
<td>Dimensionless particle deposition velocity (unitless), V₊</td>
<td>Eq. 42</td>
<td>0.0004008</td>
<td>0.0004008</td>
</tr>
<tr>
<td>Particle deposition velocity (m/s), Vᵣ</td>
<td>Eq. 43</td>
<td>5.471E-05</td>
<td>5.471E-05</td>
</tr>
<tr>
<td>Transport Efficiency, Turbulent Eddy (unitless), ηᵣₑₜₑ</td>
<td>Eq. 38</td>
<td>0.9954</td>
<td>0.9954</td>
</tr>
<tr>
<td>Particle diffusion coefficient (m²/s), Dₑ</td>
<td>Eq. 46</td>
<td>2.405E-12</td>
<td>2.405E-12</td>
</tr>
<tr>
<td>Particle diffusion time (unitless), δ</td>
<td>Eq. 45</td>
<td>7.953E-09</td>
<td>7.953E-09</td>
</tr>
<tr>
<td>Parameter</td>
<td>Equation</td>
<td>Turbulent Flow</td>
<td></td>
</tr>
<tr>
<td>--------------------------------------------------------------------------</td>
<td>----------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>Sherwood number (unitless) in turbulent flow, ( Sh )</td>
<td>Eq. 48</td>
<td>2479.8</td>
<td></td>
</tr>
<tr>
<td>Sherwood number (unitless) in laminar flow, ( Sh )</td>
<td>Eq. 47</td>
<td>1331.7</td>
<td></td>
</tr>
<tr>
<td>Schmidt number (unitless), ( Sc )</td>
<td>Eq. 49</td>
<td>6410288</td>
<td></td>
</tr>
<tr>
<td>Transport Efficiency, Thermal Diffusion in turbulent flow (unitless)</td>
<td>Eq. 44</td>
<td>0.999998</td>
<td></td>
</tr>
<tr>
<td>Transport Efficiency, Thermal Diffusion in laminar flow (unitless)</td>
<td>Eq. 44</td>
<td>0.999999</td>
<td></td>
</tr>
<tr>
<td>Selected Transport Efficiency, Thermal Diffusion (unitless), ( \eta_{Td} )</td>
<td>----</td>
<td>0.99998</td>
<td></td>
</tr>
<tr>
<td>Tube Transport Efficiency (unitless), ( \eta_{Tube} )</td>
<td>Eq. 1</td>
<td>0.9174</td>
<td></td>
</tr>
</tbody>
</table>
A-5  Bend Model

Deposition Calculator uses two models to determine transport efficiency in a bend. As discussed in Section 7, one model is used for turbulent flow when the Stokes number is greater than 0.1 and for another for any other flow condition. To address the different flow conditions, Deposition Calculator uses the following logic.

- Pui turbulent model used for Re > 4000 and Stokes number > 0.1
- Pui Re=1000 model used for all other conditions.

Three separate cases are evaluated in the hand calculation to test each flow condition.

A-5.1  Case 1: Turbulent flow and Stokes Number is Less than 0.1

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 7, along with the results from hand calculations using the indicated equation.

Input:
Particle Size (µm) = 10
Particle Density (kg/m³) = 1000
Tube Internal diameter (mm) = 25.4
Bend Angle (Deg.) = 90
Bend Radius (m) = 0.1
Inclination from Horizontal (Deg.) = 0
Sample Flow Rate (LPM) = 100
Temperature (°C) = 25
Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number (unitless), Re</td>
<td>Eq. 5</td>
<td>5383</td>
<td>5383</td>
</tr>
<tr>
<td>Stokes number of particle (unitless), Stk</td>
<td>Eq. 7</td>
<td>0.0795</td>
<td>0.0795</td>
</tr>
<tr>
<td>Bend curvature ratio (κ)</td>
<td>Eq. 51</td>
<td>7.874</td>
<td>7.847</td>
</tr>
<tr>
<td>Bend Transport Efficiency in turbulent flow with Stokes less than 0.1 (unitless), η_B</td>
<td>Eq. 52</td>
<td>0.8673</td>
<td>0.8673</td>
</tr>
</tbody>
</table>
**A-5.2 Case 2: Laminar flow**

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 8, along with the results from hand calculations using the indicated equation.

**Input:**
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Tube Internal diameter (mm) = 38.1
- Bend Angle (Deg.) = 45
- Bend Radius (m) = 0.1
- Inclination from Horizontal (Deg.) = 0
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 25
- Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number (unitless), Re</td>
<td>Eq. 5</td>
<td>2045</td>
<td>2045</td>
</tr>
<tr>
<td>Stokes number of particle (unitless), Stk</td>
<td>Eq. 7</td>
<td>0.0134</td>
<td>0.0134</td>
</tr>
<tr>
<td>Bend curvature ratio (κ)</td>
<td>Eq. 51</td>
<td>5.249</td>
<td>5.249</td>
</tr>
<tr>
<td>Bend Transport Efficiency in laminar flow (unitless), $\eta_B$</td>
<td>Eq. 52</td>
<td>0.9985</td>
<td>0.9985</td>
</tr>
</tbody>
</table>

**A-5.3 Case 3: Turbulent flow and Stokes Number is Greater than 0.1**

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 9, along with the results from hand calculations using the indicated equation.

**Input:**
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Tube Internal diameter (mm) = 25.4
Bend Angle (Deg.) = 90
Bend Radius (m) = 0.11
Inclination from Horizontal (Deg.) = 0
Sample Flow Rate (LPM) = 150
Temperature (°C) = 25
Pressure (kPa) = 101.325

Table A 9: Bend Case 3 Equation Comparison

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number (unitless), Re</td>
<td>Eq. 5</td>
<td>8074</td>
<td>8074</td>
</tr>
<tr>
<td>Stokes number of particle (unitless), Stk</td>
<td>Eq. 7</td>
<td>0.1193</td>
<td>0.1193</td>
</tr>
<tr>
<td>Bend curvature ratio (κ)</td>
<td>Eq. 51</td>
<td>8.661</td>
<td>8.661</td>
</tr>
<tr>
<td>Bend Transport Efficiency in turbulent flow with Stokes number greater than 0.1 (unitless), η_{Bt}</td>
<td>Eq. 50</td>
<td>0.5892</td>
<td>0.5892</td>
</tr>
</tbody>
</table>
A-6 Contraction Model

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 10, along with the results from hand calculations using the indicated equation.

Input:
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Inlet Internal Diameter (mm) = 25.4
- Outlet Internal Diameter (mm) = 12.7
- Contraction Half Angle (Deg) = 45
- Inclination from Horizontal (Deg) = 0
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 25
- Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Table A 10: Contraction Model Equation Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>Stokes number in contraction (unitless), Stk_c</td>
</tr>
<tr>
<td>Contraction transport efficiency (unitless), η_c</td>
</tr>
</tbody>
</table>
A-7 Expansion Model

In order to check the intermediate results, a label object was added to the main screen. Each result was then directed to the new label object. The results, based on the following input values, are presented in Table A 11, along with the results from hand calculations using the indicated equation.

Input:
- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Inlet Internal Diameter (mm) = 25.4
- Outlet Internal Diameter (mm) = 50.8
- Expansion Half Angle (Deg) = 45
- Inclination from Horizontal (Deg) = 0
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 25
- Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stokes number (unitless), Stk_e</td>
<td>Eq. 59</td>
<td>0.01133</td>
<td>0.01133</td>
</tr>
<tr>
<td>( R_{ex} ) parameter (unitless)</td>
<td>Eq. 56</td>
<td>0.75</td>
<td>0.75</td>
</tr>
<tr>
<td>( b_1 ) parameter (unitless)</td>
<td>Eq. 57</td>
<td>-2.1225</td>
<td>-2.1225</td>
</tr>
<tr>
<td>( b_2 ) parameter (unitless)</td>
<td>Eq. 58</td>
<td>0.4598</td>
<td>0.4598</td>
</tr>
<tr>
<td>Expansion transport efficiency (unitless), ( \eta_E )</td>
<td>Eq. 55</td>
<td>0.9396</td>
<td>0.9396</td>
</tr>
</tbody>
</table>
A-8  Splitter Model

In the case of a splitter, Deposition Calculator presents the results on the Splitter menu. The results, based on the following input values, are presented in Table A 12, along with the results from hand calculations using the indicated equation.

**Input:**

- Particle Size (µm) = 10
- Particle Density (kg/m³) = 1000
- Inlet Internal Diameter (mm) = 25.4
- Bifurcation Angle (Deg) = 45
- Sample Flow Rate (LPM) = 57
- Temperature (°C) = 25
- Pressure (kPa) = 101.325

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation Number</th>
<th>Hand Calculation</th>
<th>Deposition Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stokes number (unitless), Stk</td>
<td>Eq. 7</td>
<td>0.0453</td>
<td>0.0453</td>
</tr>
<tr>
<td>Splitter transport efficiency (unitless), ηs</td>
<td>Eq. 60</td>
<td>0.97025</td>
<td>0.97025</td>
</tr>
</tbody>
</table>