Model for Penetration Probability

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Model Description

The primary objective is to develop a semi-empirical quantitative model to enable the prediction of the penetration probability of a material system as a function of the face velocity and the particle size.

For any material system forming a fibrous filter of thickness *t* in the flow direction, the penetration *P* can be written down in the general form

$$P = \exp(-\alpha t), \tag{1}$$

where α is the collection per unit of filter depth, referred to here as the 'layer efficiency', given by

$$\alpha = (4/\pi)\left(\sigma / d_f\right) E, \tag{2}$$

in which *E* if the single fiber collection efficiency embodying the essential physics of the filtration process and σ is the volume fraction of fibers (packing density or solidity). The latter is defined as the ratio of the fiber volume to the total volume. Note that $\sigma = 1 - \phi$ where ϕ is the porosity.

For the present purposes, a relative simple picture of the deposition process will be assumed in which inertia and diffusion are regarded as the primary mechanisms. The Peclet number (Pe) describes a particle's tendency to deposit via diffusion and is quantified by the following equation:

$$\text{Pe} = \frac{V_f\, d_f}{D}, \tag{3}$$

where V_f is the face velocity (cm s^{-1}) or velocity of air entering the filter, d_f is the (effective) fiber diameter (cm), and *D* is the diffusion coefficient of the particle $\left(\text{cm}^2\, s^{-1}\right)$. For a particle of diameter D_p (cm), the diffusion coefficient can be determined using the following relationship:

$$D = \frac{k_B\, T C_c}{3\, \pi \eta D_p}, \tag{4}$$

where k_B is Boltzmann's constant (erg K^{-1}), *T* is the temperature (K), η is the dynamic viscosity of air (poise or g cm^{-1} s^{-1}) and C_c is the Cunningham slip correction factor. The inertial parameter is governed by the Stokes number (Stk) which is quantified as follows:

$$\text{Stk} = \frac{\rho_p\, D_p^2\, V_f\, C_c}{18\, \eta d_f}, \tag{5}$$

where ρ_p is the particle density (g cm^{-3}). The Cunningham slip correction factor C_c is determined from the following equation:

$$C_c = 1 + 1.246\, \frac{\lambda}{r_p} + 0.42\, \frac{\lambda}{r_p} \exp\left(-0.87\, \frac{r_p}{\lambda}\right), \tag{6}$$

where λ is the mean free path of air molecules (cm) and $r_p = D_p/2$ is the particle radius. Some relevant physical constants are: k_B = 1.38 × 10^{-16} erg K^{-1}; η = 1.83 × 10^{-4} poise; and λ = 0.653 × 10^{-5} cm at atmospheric pressure.

From Eqs (1) and (2), we may write down

$$-(d_t / t) \log(P) = f(\mathrm{Stk}, \mathrm{Pe}) = kE \equiv y \ . \tag{7}$$

Then in relation to the present situation (assumptions), Eq. (7) may be expressed in the form

$$y = f_1(\mathrm{Stk}) + f_2(\mathrm{Pe}) \ . \tag{8}$$

There is no analytical form for this relationship, but one empirical option consistent with the expected pattern is

$$y = a\,\mathrm{Stk}^b + c\,\mathrm{Pe}^d \ , \tag{9}$$

where *a*, *b*, *c*, and *d* are coefficients that need to be determined from measurements of penetration probability for material system.

Implementation of Model

In this section, we provide an implementation of the model described in the previous section.

- Define some physical constants required by the penetration model for material system

```
kB = 1.38 × 10^-16 ;           (* Boltzmann's constant in erg K^-1 *)
T = 293.0 ;                   (* air temperature in K *)
λ = 0.653 × 10^-5 ;
(* mean free path of air molecules at atmospheric pressure in cm *)
η = 1.83 × 10^-4 ;             (* dynamic viscosity of air in poise (g cm^-1 s^-1) *)
ρP = 1.0                       (* density of particles in g cm^-3 *)
1.
```

- Function to compute the Cunningham slip correction factor

```
(* Cunningham slip correction *)
(* Dp is the particle diameter in cm *)
Cc[Dp_] := 1.0 + 1.246 × 2 λ/Dp + 0.42 × 2 λ/Dp Exp[-0.87 Dp/(2 λ)]
```

- Function to compute the diffusion coefficient *D* of the particle

```
(* Diffusion coefficient D in cm^2 s^-1 *)
(* Dp is the particle diameter in cm *)

DiffCoef[Dp_] := (kB T Cc[Dp]) / (3.0 Pi η Dp)
```

- Function to compute Peclet number Pe which measures the effects of Brownian diffusion

```
(* Peclet number Pe - Brownian diffusion *)
(* Vf is face velocity in cm s^-1 *)
(* df is effective fibre diameter in cm *)
(* Dp is the particle diameter in cm *)
(* DiffCoef is diffusion coefficient *)

Pe[Vf_, Dp_] := (Vf df) / DiffCoef[Dp]
```

- Function to compute Stokes number Stk which measures the effects of inertial impaction

```
(* Stokes number Stk - inertial impaction *)
(* ρp is the particle density in g cm^-3 *)
(* Dp is the particle diameter in cm *)
(* Vf is the face velocity in cm s^-1 *)
(* df is effective fibre diameter in cm *)
(* Cc is the Cunningham slip correction *)
(* DiffCoef is the diffusion coefficient in cm^2 s^-1 *)
(* η is the dynamic viscosity of air in poise (g cm^-1 s^-1) *)

Stk[Vf_, Dp_] := (ρp Dp^2 Vf Cc[Dp]) / (18.0 η df)
```

- Model for penetration probability for material system (as a function of face velocity and particle diameter)

```
model[Vf_, Dp_] := a Stk[Vf, Dp]^b + c Pe[Vf, Dp]^d
```

Application of the Model to Material Systems

In this section, we apply the model for penetration probability to four different material systems. Each of these material systems are dealt with in a separate subsection.

Combat Uniform

The first step is to provide the data that can be used to determine the coefficients *a*, *b*, *c*, and *d* for the penetration model.

Define the thickness of the material system for Combat Uniform.

```
(* Thickness of material system (t) *)
t = 0.40 * 0.1;    (* converted from mm to cm *)
```

Extraction and Visualization of Penetration Data

- First, let us import the data file containing penetration data through Combat Uniform at two different pressure drops obtained from swatch-level testing. The columns in the data file are as follows:
  - column 1 : particle diameter (μm)
  - column 2 : penetration probability (for 25 Pa pressure drop across the filter)
  - column 3 : penetration probability (for 125 Pa pressure drop across the filter)

```
data = Import["C:\\Deposition on Humans Project\\Aerosol Deposition
      Project - Persons\\Fabrics\\Combat\\peneCombat.txt", "Table"];
```

Display the penetration data for the Combat Uniform as table.

```
dataFormatted =
  {NumberForm[#[[1]], {4, 3}], NumberForm[#[[2]], {4, 2}], NumberForm[#[[3]], {4, 2}]} & /@ data;
colLabels = Style[#, Bold] & /@ {"Dp (μm)", "P(at 25 Pa)", "P (at 125 Pa)"};
Grid[Join[{colLabels}, dataFormatted],
 Dividers → {{1 → True, 2 → True, 3 → True, 4 → True}, {1 → True, 2 → True, -1 → True}},
 Alignment → Center,
 Spacings → {4.5, 0.5}]
```

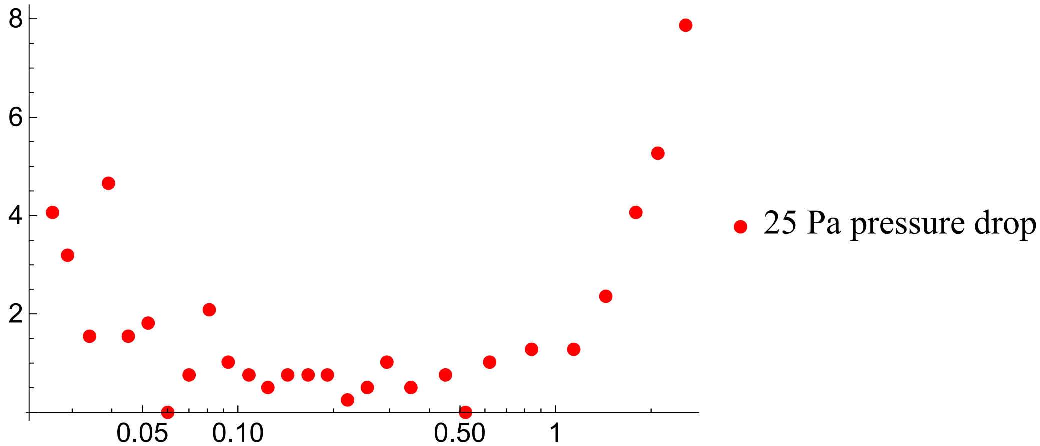
D_p (μm)	P(at 25 Pa)	P (at 125 Pa)
0.026	0.85	0.86
0.029	0.88	0.96
0.034	0.94	0.94
0.039	0.83	0.92
0.045	0.94	0.92
0.052	0.93	0.92
0.060	1.00	0.94
0.070	0.97	0.92
0.081	0.92	0.93
0.093	0.96	0.92
0.108	0.97	0.94
0.124	0.98	0.94
0.143	0.97	0.93
0.166	0.97	0.92
0.191	0.97	0.95
0.221	0.99	0.93
0.255	0.98	0.93
0.294	0.96	0.94
0.350	0.98	0.97
0.450	0.97	0.94
0.520	1.00	0.94
0.620	0.96	0.93
0.840	0.95	0.84
1.140	0.95	0.76
1.440	0.91	0.67
1.790	0.85	0.58
2.100	0.81	0.55
2.570	0.73	0.49

- Next, we transform the imported penetration data into a form that can be used for nonlinear model fitting.

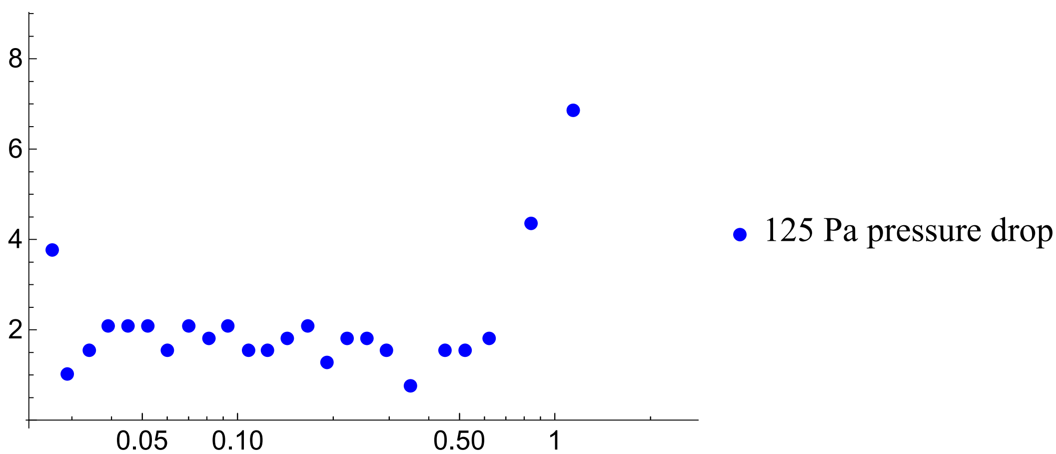
```
dimData = Dimensions[data];
vf25 = 6.65;
(* face velocity for 25 Pa pressure drop across material system in cm s^-1  *)
vf125 = 24.21;
(* face velocity for 125 Pa pressure drop across material system in cm s^-1 *)
vf25Vec = Table[vf25, dimData[[1]]];
vf125Vec = Table[vf125, dimData[[1]]];
(* Form vectors for particle diameter, penetration at 25 Pa pressure drop,
and penetration at 125 Pa pressure drop *)
{diam, pene25, pene125} = {data[[All, 1]], data[[All, 2]], data[[All, 3]]};

(* Compute the transformed penetration data *)
(* Transformed penetration probability y = -(1/t) log(P),
where P is the penetration probability *)
(* y has dimensions of cm^-1 *)
(* y for pressure drop of 25 Pa across material system *)
y25 = -Log[pene25] / t;
(* y for pressure drop of 125 Pa across material system *)
y125 = -Log[pene125] / t;

(* Construct data structure for nonlinear least squares fitting *)
(* Note that particle diameter is converted from μm to cm *)
(* Each data triple consists of face velocity (cm s^-1), particle diameter (cm),
and transformed penetration probability y = (-1/t) log(P) (cm^-1) *)
data1ToFit = Transpose[{vf25Vec,  diam * 10.^(-4), y25}];
data2ToFit = Transpose[{vf125Vec, diam * 10.^(-4), y125}];
dataToFit = Join[data1ToFit, data2ToFit];
(* Total penetration data set {{V_f, D_p, y}..} *)
```

- Visualization of transformed penetration data

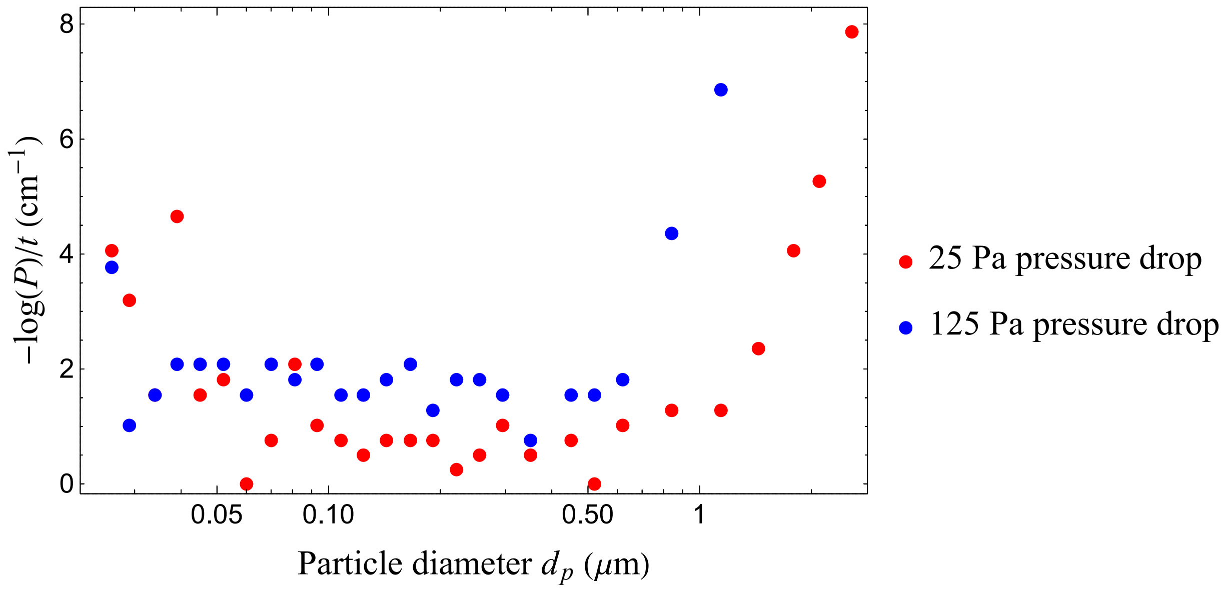
```
ploty25 = ListLogLinearPlot[{diam, y25}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
ploty125 = ListLogLinearPlot[{diam, y125}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
Show[ploty25, ploty125,
 Frame → True,
 BaseStyle -> {"TimesNewRoman", 14},
 FrameLabel → {Style["Particle diameter d_p (μm)", FontFamily → "Times New Roman", 18],
   Style["-log(P)/t (cm^-1)", FontFamily → "Times New Roman", 18]},
 ImageSize → 450]
```



Determination of Coefficients for Penetration Model for Combat Uniform

In this sub-section,we use the penetration data obtained in the last sub-section to determine the coefficients for the penetration model for the Combat Uniform using nonlinear least-squares fitting.

```
(* Nonlinear fitting of transformed penetration probability model to the data *)
(* For the fitting, it is necessary to choose a reasonable fibre diameter d_f *)

df = 1.0 × 10^-4;  (* fiber diameter in cm *)
Clear[a, b, c, d];
nlm = NonlinearModelFit[dataToFit, model[v, x], {a, b, c, d}, {v, x}];
(* Extract the best fit parameters *)
{a, b, c, d} = {a, b, c, d} /. nlm["BestFitParameters"]
(* Display table of estimated parameter statistics *)
nlm["ParameterTable"]
```

```
{0.101359, -0.519135, 0.000444615, 1.05104}
```

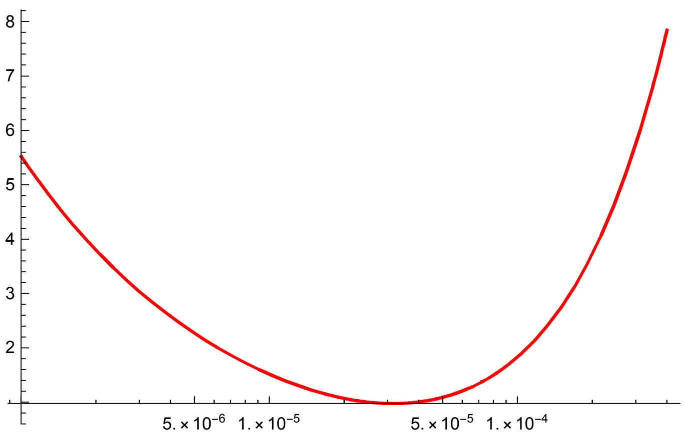
	Estimate	Standard Error	t-Statistic	P-Value
0.101359	0.101359	0.0785944	1.28965	0.20288
−0.519135	−0.519135	0.132823	−3.90848	0.000269989
0.000444615	0.000444615	0.000299962	1.48224	0.144312
1.05104	1.05104	0.0689385	15.2461	7.87264×10^{-21}

Visualization of the Fit of Model to Data

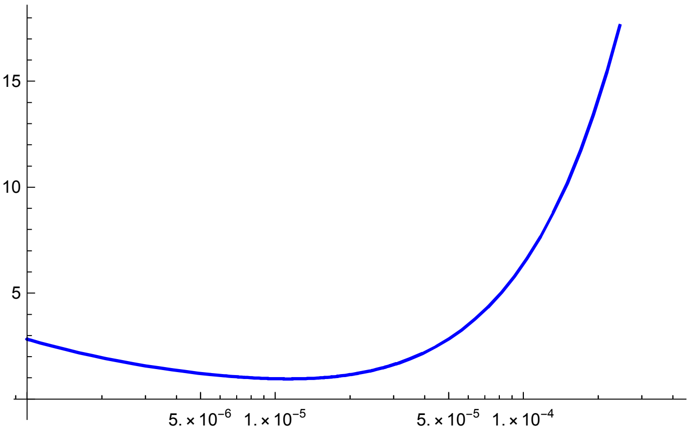
```
(* Provide plot showing the predicted transformed penetration probability and the
   measured transformed penetration probability *)
(*-----------------------------------------------------------------------------
                                                --*)
```

First visualization in terms of 2-D line plot

```
Vf = vf25;
ploty25theor =
 LogLinearPlot[model[Vf, x], {x, 1.0 × 10^(-6), 4.0 × 10^(-4)}, PlotStyle → Red]
```

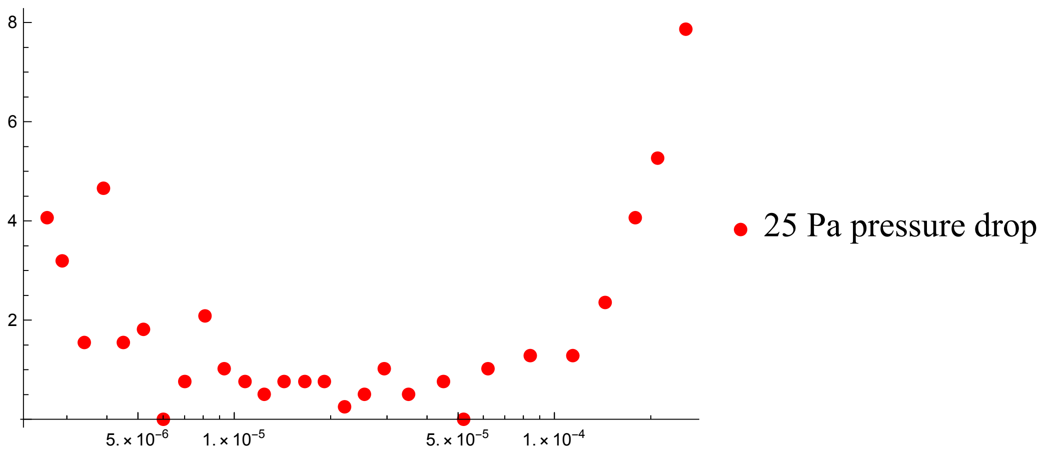


```
Vf = vf125;
ploty125theor = LogLinearPlot[model[Vf, x], {x, 1.0 × 10^-6, 4.0 × 10^-4}, PlotStyle → Blue]
```

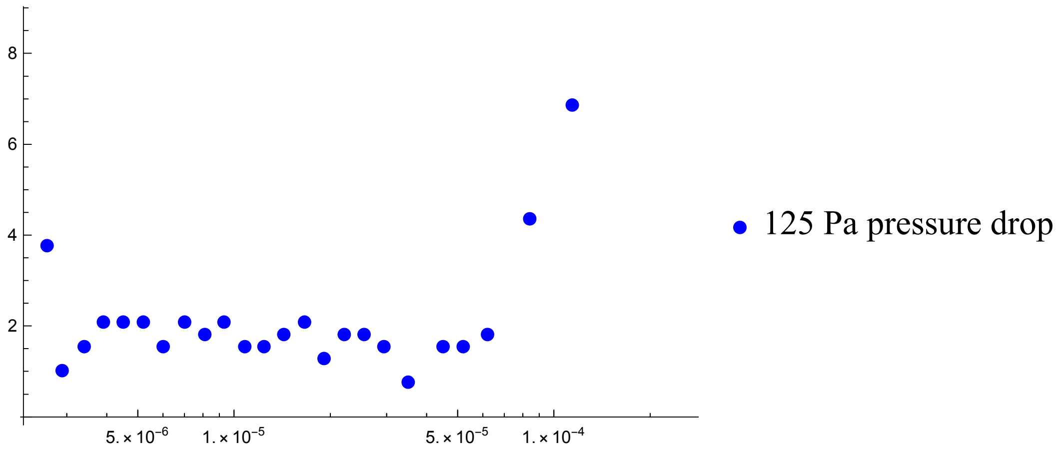



```
data1m = Transpose[{diam * 1.0 × 10^(-4), y25}];
data2m = Transpose[{diam * 1.0 × 10^-4, y125}];
```

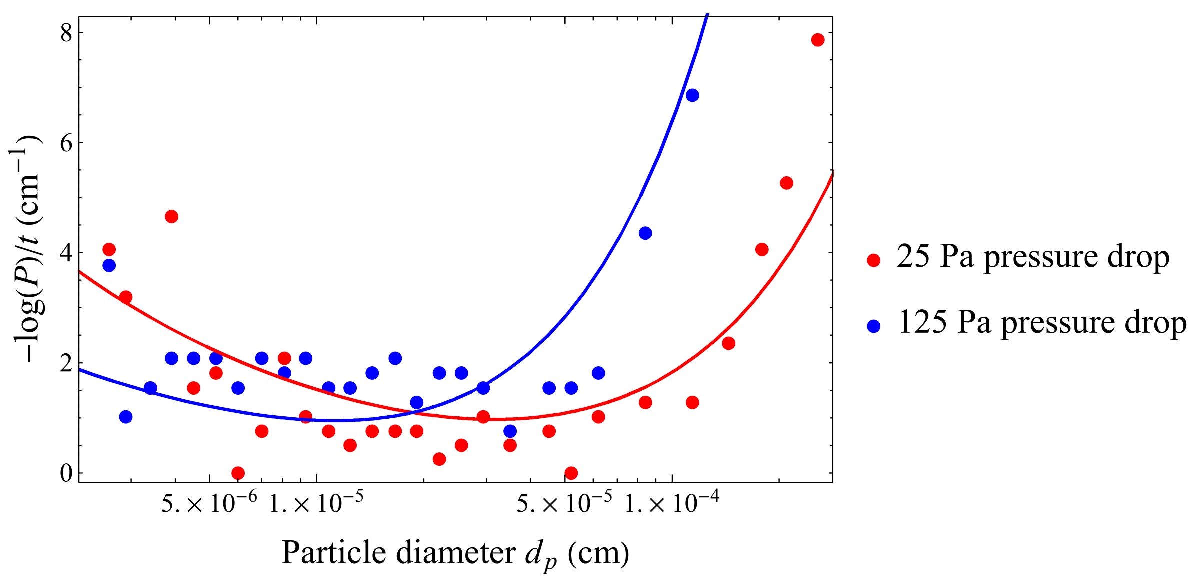
```
ploty25m = ListLogLinearPlot[data1m, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
ploty125m = ListLogLinearPlot[data2m, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
Show[ploty25m, ploty125m, ploty25theor, ploty125theor,
 BaseStyle → {FontFamily → "Times New Roman", FontSize → 14},
 Frame → True,
 FrameLabel → {Style["Particle diameter dp (cm)", FontSize → 18],
   Style["-log(P)/t (cm^-1)", FontSize → 18]}, ImageSize → 72. * 6]
```

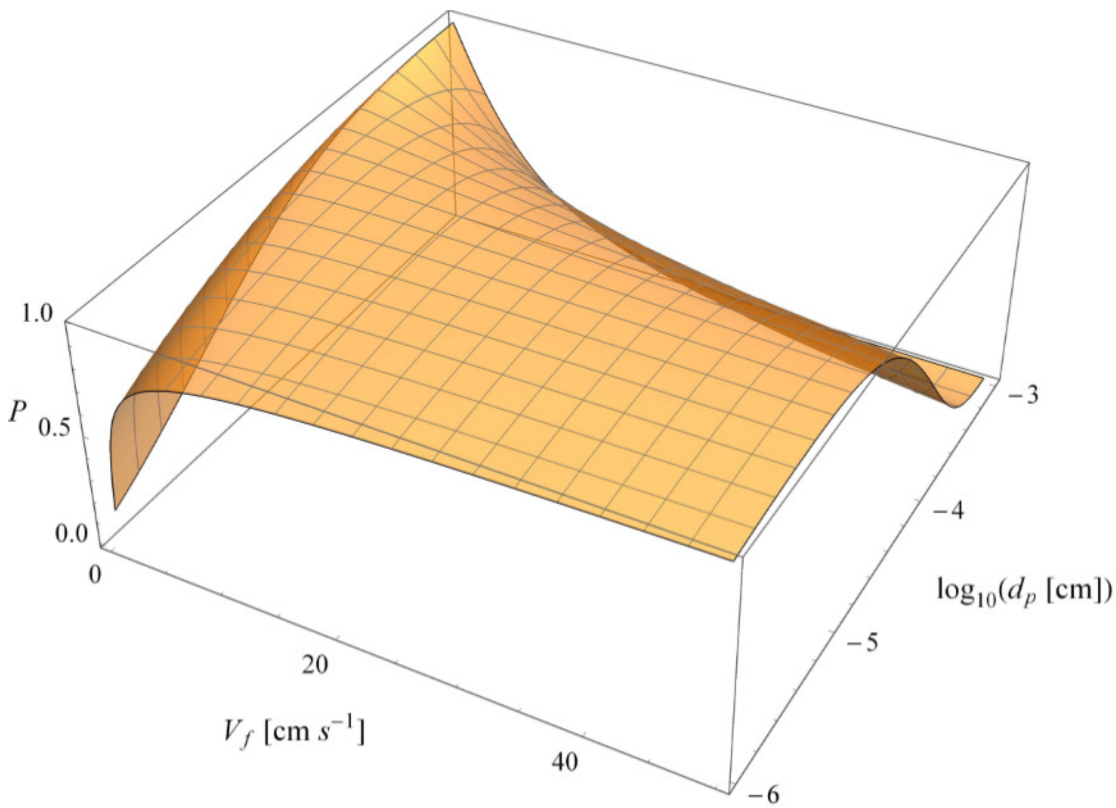



```
(*-----------------------------------------------------------------------------*)
```

Visualization in terms of a 3-D surface plot

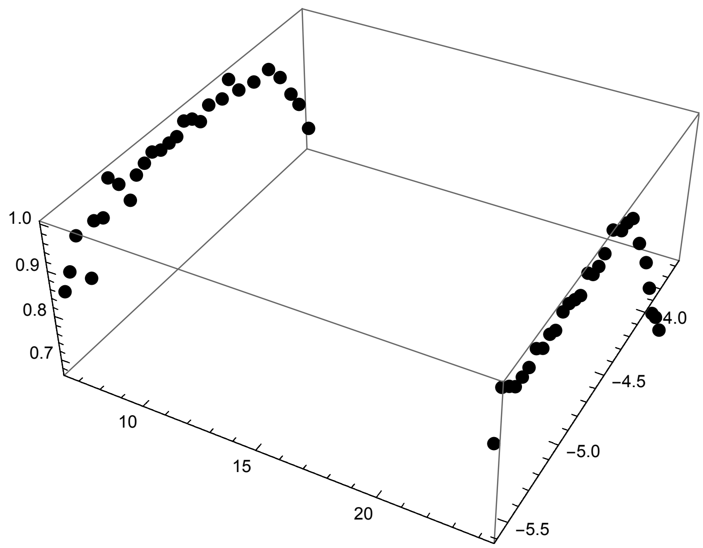
```
(* Construct 3-D plot of penetration probability using fitted model function *)

(* Face velocity in cm s^-1 *)
Vfaxis = Range[0.1, 50, 0.1];
 (* Common logarithm of particle diameter in cm *)
LogDpaxis = Range[-6., -3, 0.05];
```

```
(* Sample the penetration probability as a function of
 the face velocity Vf (cm s^-1) and particle diameter dp (cm) *)

datavals = Flatten[Outer[{#1, #2, Exp[-t model[#1, 10^#2]]} &, Vfaxis, LogDpaxis], 1];

(* Use the sampled data set to plot the penetration probability surface *)

penePlot3D =
 ListPlot3D[datavals, BaseStyle → {FontFamily → "Times New Roman", FontSize → 14, Black},
  AxesLabel → {Style["Vf  [cm s^-1]", Black, FontSize → 16], Style["log10(dp  [cm])",
     Black, FontSize → 16], Style["P", Black, FontSlant → Italic, FontSize → 16]},
  PlotStyle → {Opacity[0.6]}, PlotTheme → "GrayMesh", ImageSize → Large]
```



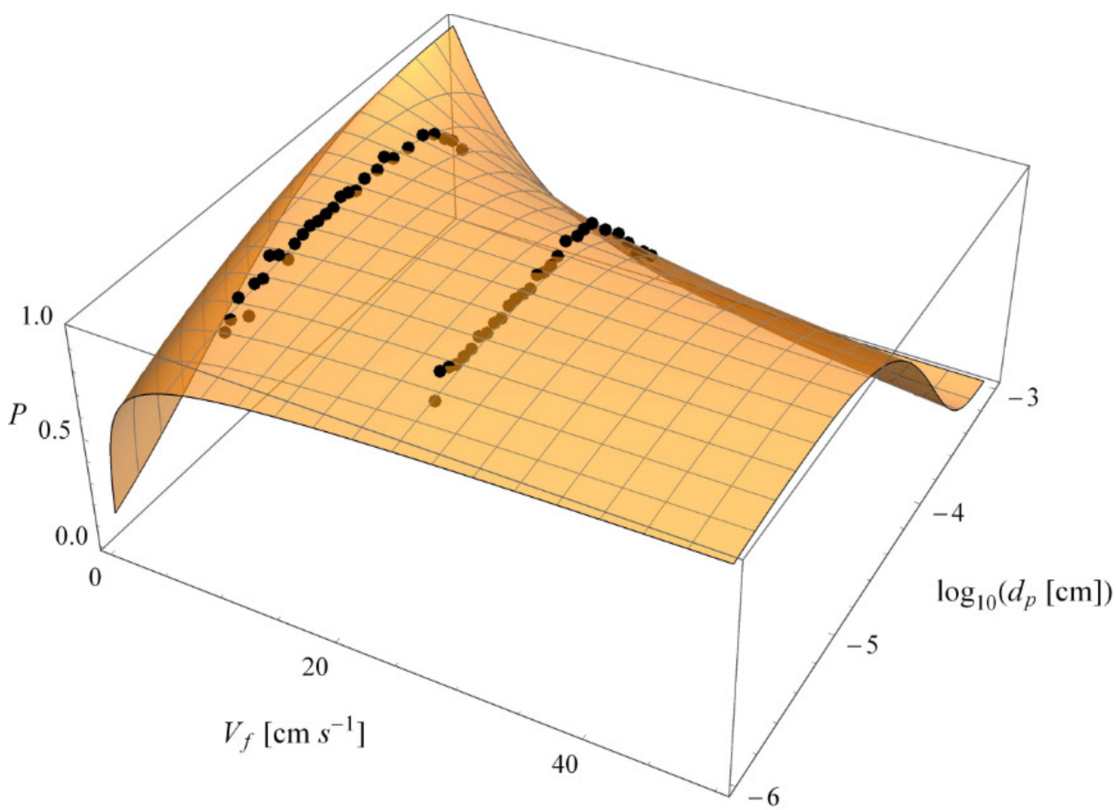

```
(* Plot the penetration data points in 3-D space *)

pene25m = Transpose[{vf25Vec, Log[10, diam * 10.^-4], pene25}];
pene125m = Transpose[{vf125Vec, Log[10, diam * 10.^-4], pene125}];
peneAllm = Join[pene25m, pene125m];
```

```
penePlot3Ddata = ListPointPlot3D[Style[peneAllm, Black, PointSize[Large]]]
```




```
(* Superimpose the model for penetration probability
 with measured values for penetration probability *)
```

```
Show[penePlot3D, penePlot3Ddata]
```



Summary

The key parameters of the penetration model for the Combat Uniform are as follows.

The material thickness t (cm) = 0.04. The effective fiber diameter d_f (cm) = 1.0×10^{-4}.
The model coefficients a, b, c, d are:

```
{a, b, c, d}
```

```
{0.101359, -0.519135, 0.000444615, 1.05104}
```

```
(*+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++*)
(*=============================================================================*)
```

Horizon I Material System

The first step is to provide the data that can be used to determine the coefficients a, b, c, and d for the penetration model.

Define the thickness of the material system for Horizon I material system.

```
(* Thickness of material system (t) *)
t = 1.30 * 0.1;    (* converted from mm to cm *)
```

Extraction and Visualization of Penetration Data

- First, let us import the data file containing penetration data through Horizon I material system at two different pressure drops obtained from swatch-level testing. The columns in the data file are as follows:
  - column 1 : particle diameter (μm)
  - column 2 : penetration probability (for 25 Pa pressure drop across the filter)
  - column 3 : penetration probability (for 125 Pa pressure drop across the filter)

```
data = Import["C:\\Deposition on Humans Project\\Aerosol Deposition
    Project - Persons\\Fabrics\\Horizon 1\\peneHorz1.txt", "Table"];
```

Display the penetration data for the Horizon I material system as table.

```
dataFormatted =
  {NumberForm[#[[1]], {5, 3}], NumberForm[#[[2]], {4, 2}], NumberForm[#[[3]], {4, 2}]} & /@ data;
colLabels = Style[#, Bold] & /@ {"Dp  (μm)", "P(at 25 Pa)", "P  (at 125 Pa)"};
Grid[Join[{colLabels}, dataFormatted],
 Dividers → {{1 → True, 2 → True, 3 → True, 4 → True}, {1 → True, 2 → True, -1 → True}},
 Alignment → Center,
 Spacings → {4.5, 0.5}]
```

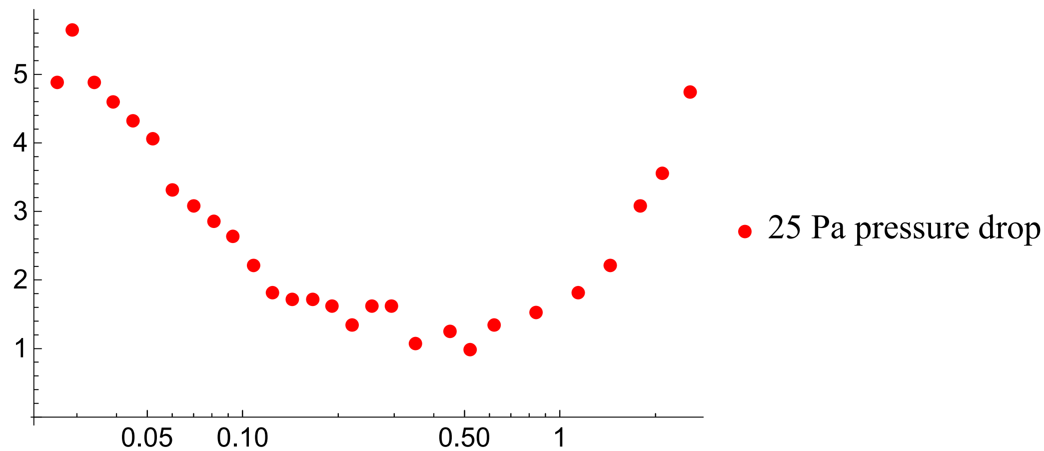
D_p (μm)	P(at 25 Pa)	P (at 125 Pa)
0.026	0.53	0.76
0.029	0.48	0.79
0.034	0.53	0.74
0.039	0.55	0.77
0.045	0.57	0.78
0.052	0.59	0.80
0.060	0.65	0.80
0.070	0.67	0.82
0.081	0.69	0.81
0.093	0.71	0.82
0.108	0.75	0.82
0.124	0.79	0.85
0.143	0.80	0.84
0.166	0.80	0.85
0.191	0.81	0.87
0.221	0.84	0.86
0.255	0.81	0.87
0.294	0.81	0.88
0.350	0.87	0.91
0.450	0.85	0.86
0.520	0.88	0.86
0.620	0.84	0.86
0.840	0.82	0.76
1.140	0.79	0.67
1.440	0.75	0.55
1.790	0.67	0.40
2.100	0.63	0.31
2.570	0.54	0.22

- Next, we transform the imported penetration data into a form that can be used for nonlinear model fitting.

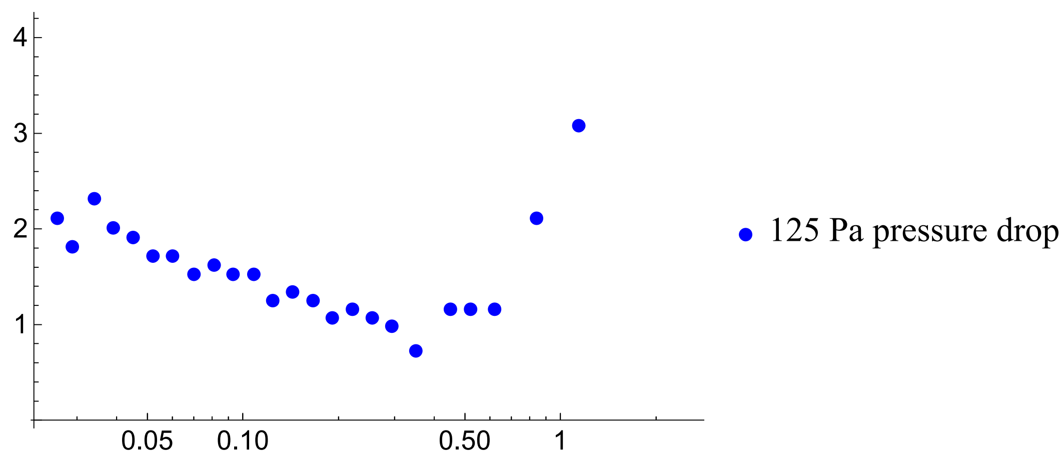
```
dimData = Dimensions[data];
vf25 = 3.33;
(* face velocity for 25 Pa pressure drop across material system in cm s^-1  *)
vf125 = 15.37;
(* face velocity for 125 Pa pressure drop across material system in cm s^-1 *)
vf25Vec = Table[vf25, dimData[[1]]];
vf125Vec = Table[vf125, dimData[[1]]];
(* Form vectors for particle diameter, penetration at 25 Pa pressure drop,
and penetration at 125 Pa pressure drop *)
{diam, pene25, pene125} = {data[[All, 1]], data[[All, 2]], data[[All, 3]]};

(* Compute the transformed penetration data *)
(* Transformed penetration probability y = -(1/t) log(P),
where P is the penetration probability *)
(* y has dimensions of cm^-1 *)
(* y for pressure drop of 25 Pa across material system *)
y25 = -Log[pene25] / t;
(* y for pressure drop of 125 Pa across material system *)
y125 = -Log[pene125] / t;

(* Construct data structure for nonlinear least squares fitting *)
(* Note that particle diameter is converted from μm to cm *)
(* Each data triple consists of face velocity (cm s^-1), particle diameter (cm),
and transformed penetration probability y = (-1/t) log(P) (cm^-1) *)
data1ToFit = Transpose[{vf25Vec,  diam * 10.^(-4), y25}];
data2ToFit = Transpose[{vf125Vec, diam * 10.^(-4), y125}];
dataToFit = Join[data1ToFit, data2ToFit];
(* Total penetration data set {{V_f, D_p, y}..} *)
```

- Visualization of transformed penetration data

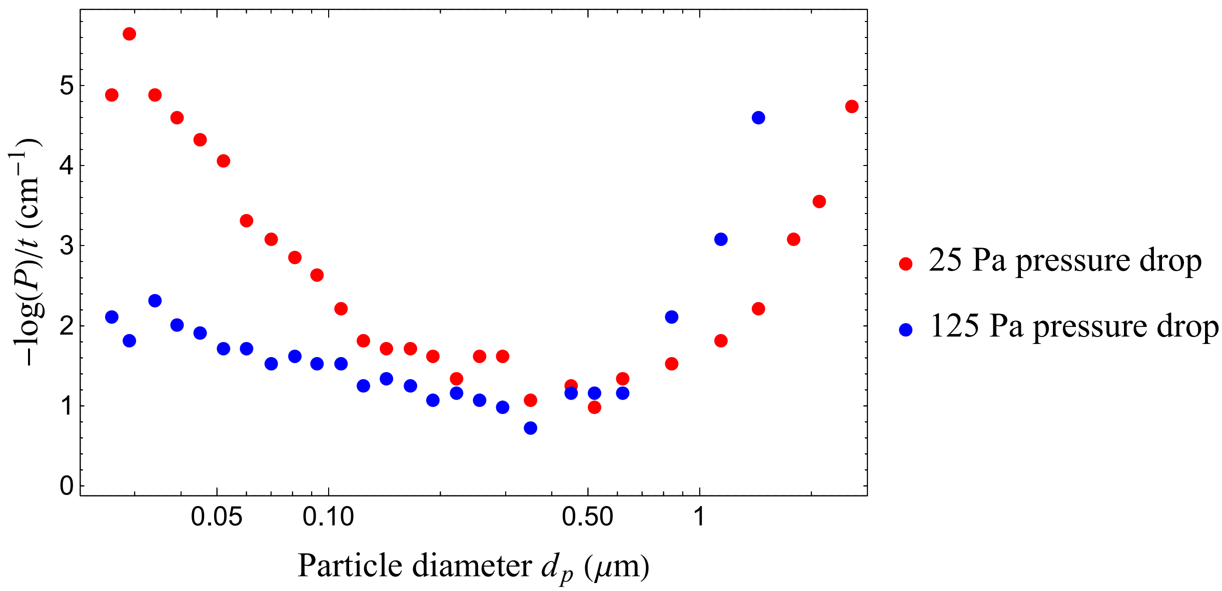
```
ploty25 = ListLogLinearPlot[{diam, y25}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
ploty125 = ListLogLinearPlot[{diam, y125}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
Show[ploty25, ploty125,
 Frame → True,
 BaseStyle -> {"TimesNewRoman", 14},
 FrameLabel → {Style["Particle diameter d_p (μm)", FontFamily → "Times New Roman", 18],
   Style["-log(P)/t (cm^-1)", FontFamily → "Times New Roman", 18]},
 ImageSize → 450]
```



Determination of Coefficients for Penetration Model for Horizon I Material System

In this sub-section,we use the penetration data obtained in the last sub-section to determine the coefficients for the penetration model for the Horizon I material system using nonlinear least-squares fitting.

```
(* Nonlinear fitting of transformed penetration probability model to the data *)
(* For the fitting, it is necessary to choose a reasonable fibre diameter df *)

df = 1.0 × 10^-4;  (* fiber diameter in cm *)
Clear[a, b, c, d];
nlm = NonlinearModelFit[dataToFit, model[v, x], {a, b, c, d}, {v, x}];
(* Extract the best fit parameters *)
{a, b, c, d} = {a, b, c, d} /. nlm["BestFitParameters"]
(* Display table of estimated parameter statistics *)
nlm["ParameterTable"]
```

```
{4.52095, 0.792578, 9.64952, -0.384131}
```

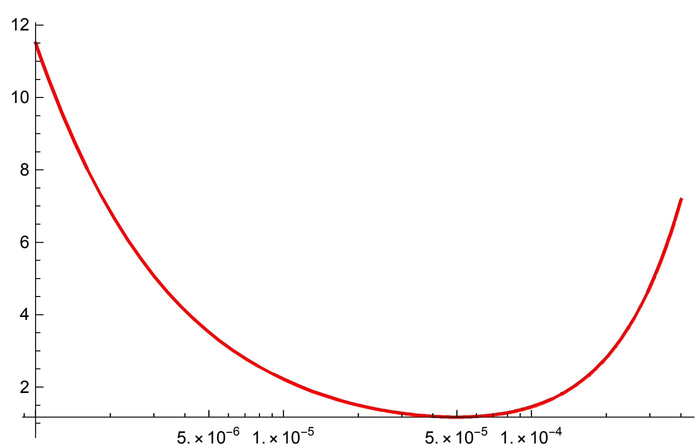
	Estimate	Standard Error	t-Statistic	P-Value
4.52095	4.52095	0.166675	27.1243	2.32511×10^{-32}
0.792578	0.792578	0.0370312	21.403	1.9125×10^{-27}
9.64952	9.64952	0.674395	14.3084	1.1446×10^{-19}
-0.384131	-0.384131	0.0235863	-16.2861	4.56264×10^{-22}

Visualization of the Fit of Model to Data

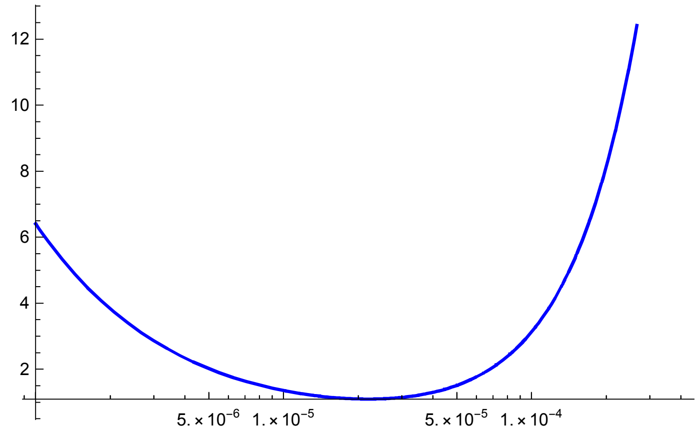
```
(* Provide plot showing the predicted transformed penetration probability and the
   measured transformed penetration probability *)
(*--------------------------------------------------------------------------
                                                  --*)
```

First visualization in terms of 2-D line plot

```
Vf = vf25;
ploty25theor =
 LogLinearPlot[model[Vf, x], {x, 1.0 × 10^(-6), 4.0 × 10^(-4)}, PlotStyle → Red]
```

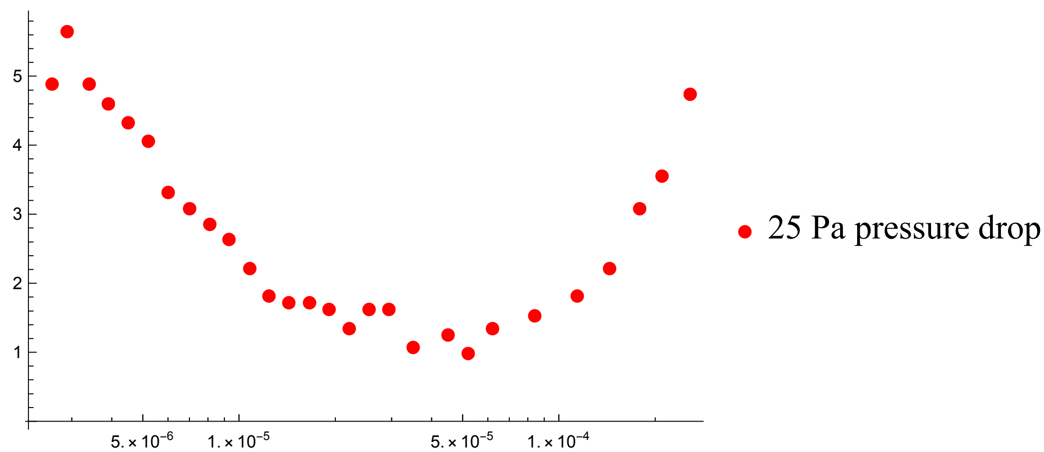


```
Vf = vf125;
ploty125theor = LogLinearPlot[model[Vf, x], {x, 1.0×10^-6, 4.0×10^-4}, PlotStyle → Blue]
```

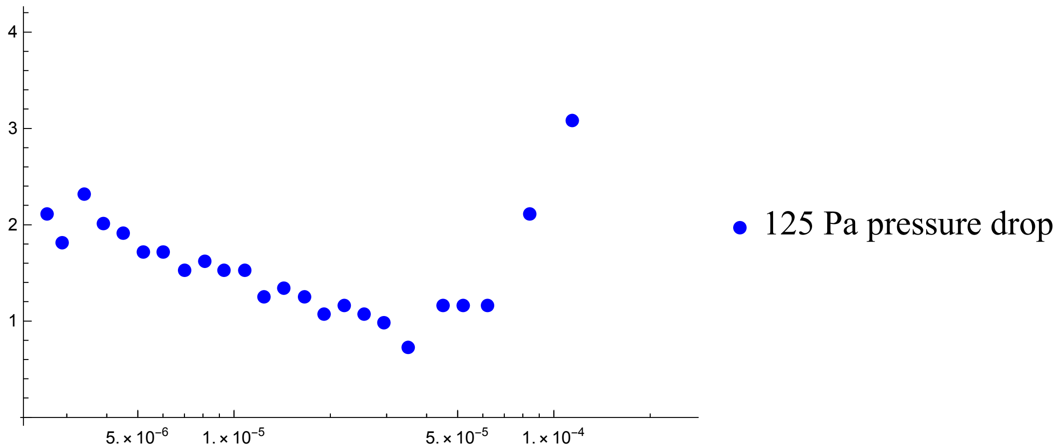



```
data1m = Transpose[{diam * 1.0×10^(-4), y25}];
data2m = Transpose[{diam * 1.0×10^-4, y125}];
```

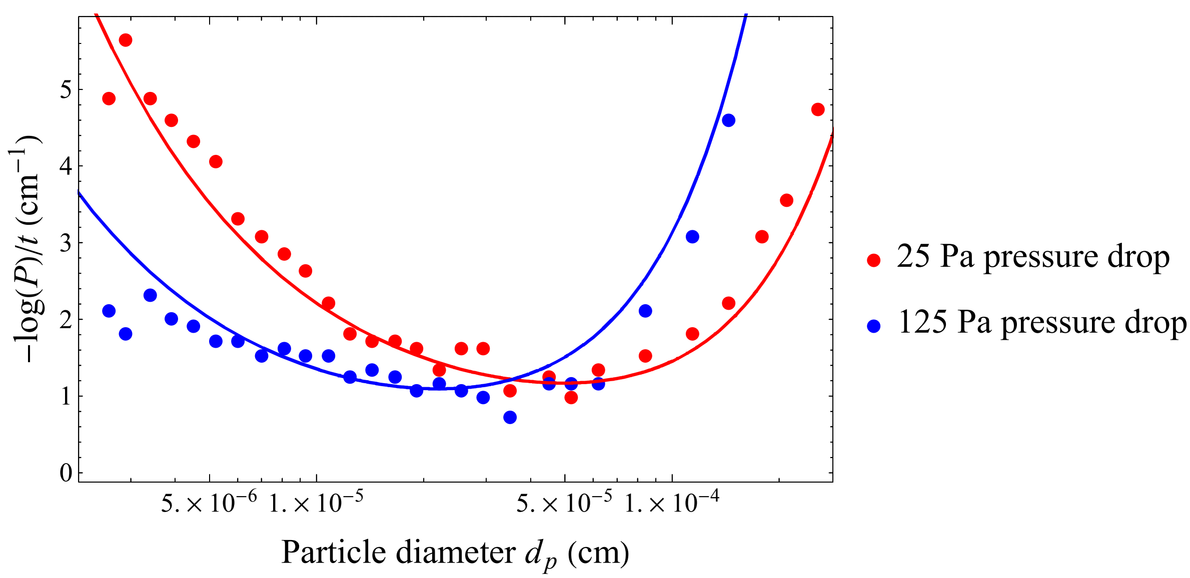
```
ploty25m = ListLogLinearPlot[data1m, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
ploty125m = ListLogLinearPlot[data2m, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
Show[ploty25m, ploty125m, ploty25theor, ploty125theor,
 BaseStyle → {FontFamily → "Times New Roman", FontSize → 14},
 Frame → True,
 FrameLabel → {Style["Particle diameter d_p (cm)", FontSize → 18],
   Style["-log(P)/t (cm^-1)", FontSize → 18]}, ImageSize → 72. * 6]
```

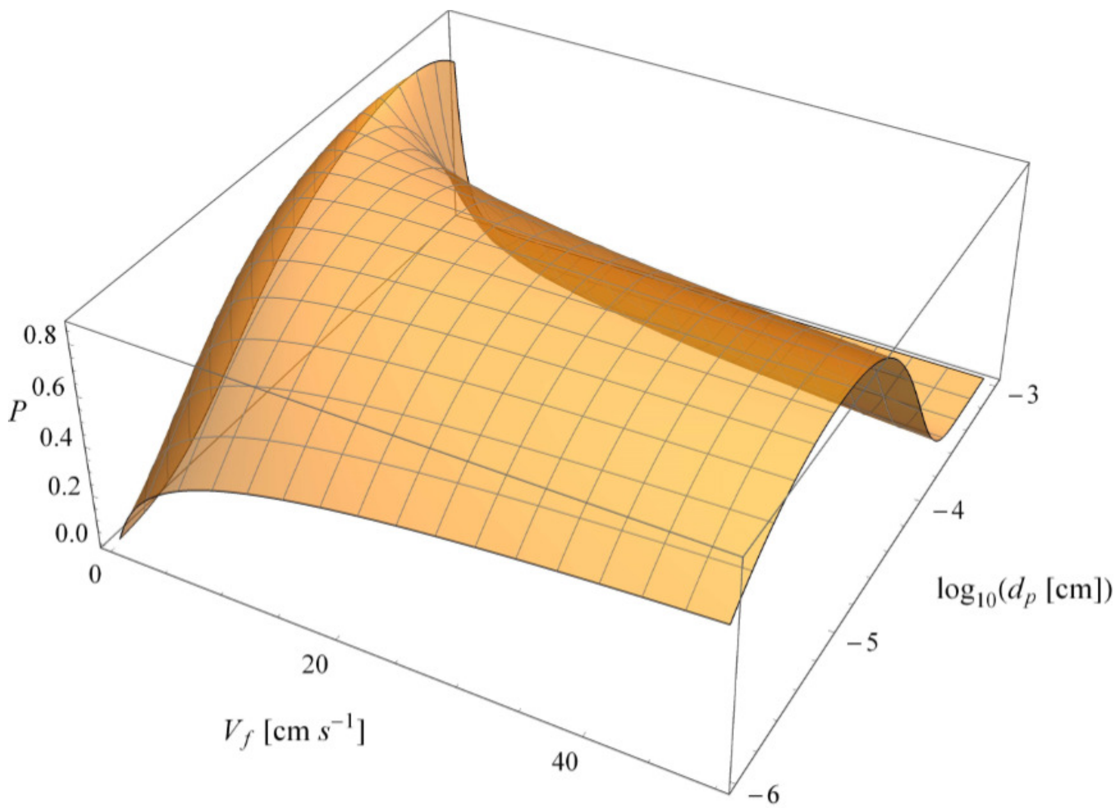



```
(*---------------------------------------------------------------------------*)
```

Visualization in terms of a 3-D surface plot

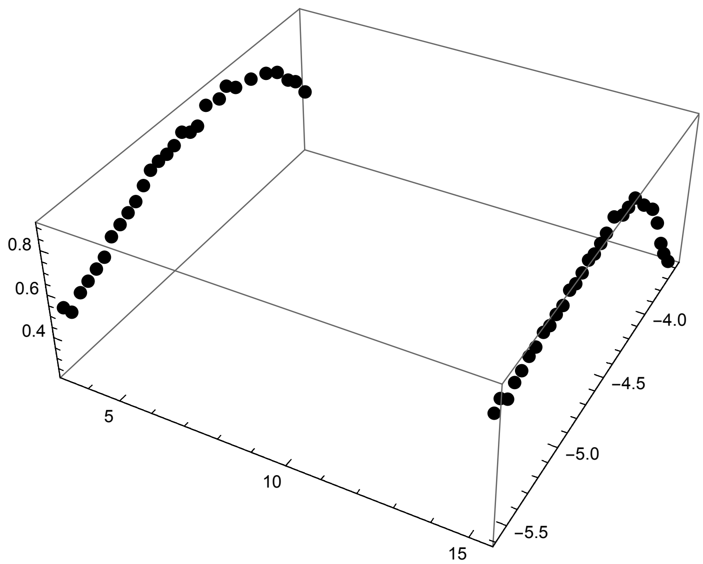
```
(* Construct 3-D plot of penetration probability using fitted model function *)

(* Face velocity in cm s^-1 *)
Vfaxis = Range[0.1, 50, 0.1];
 (* Common logarithm of particle diameter in cm *)
LogDpaxis = Range[-6., -3, 0.05];
```

```
(* Sample the penetration probability as a function of
 the face velocity Vf (cm s^-1) and particle diameter dp (cm) *)

datavals = Flatten[Outer[{#1, #2, Exp[-t model[#1, 10^#2]]} &, Vfaxis, LogDpaxis], 1];

(* Use the sampled data set to plot the penetration probability surface *)

penePlot3D =
 ListPlot3D[datavals, BaseStyle → {FontFamily → "Times New Roman", FontSize → 14, Black},
  AxesLabel → {Style["Vf [cm s^-1]", Black, FontSize → 16], Style["log10(dp [cm])",
     Black, FontSize → 16], Style["P", Black, FontSlant → Italic, FontSize → 16]},
  PlotStyle → {Opacity[0.6]}, PlotTheme → "GrayMesh", ImageSize → Large]
```

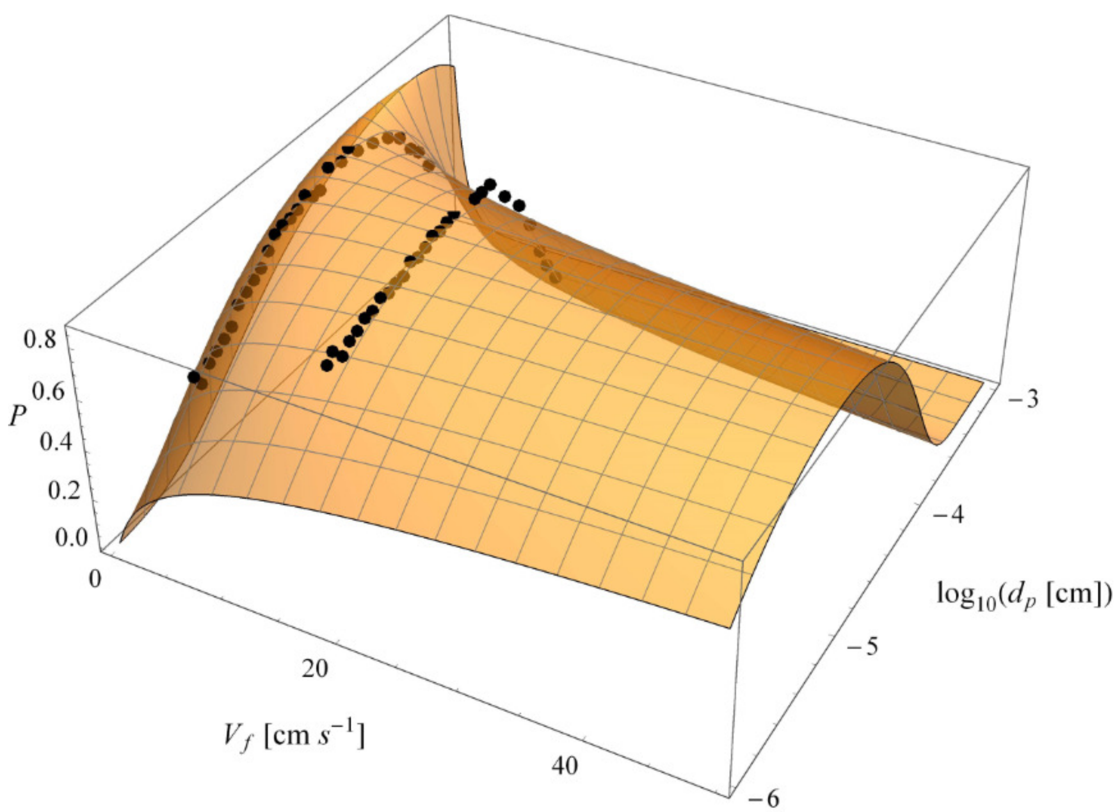



```
(* Plot the penetration data points in 3-D space *)

pene25m = Transpose[{vf25Vec, Log[10, diam * 10.^-4], pene25}];
pene125m = Transpose[{vf125Vec, Log[10, diam * 10.^-4], pene125}];
peneAllm = Join[pene25m, pene125m];
```

```
penePlot3Ddata = ListPointPlot3D[Style[peneAllm, Black, PointSize[Large]]]
```




```
(* Superimpose the model for penetration probability
 with measured values for penetration probability *)

Show[penePlot3D, penePlot3Ddata]
```



Summary

The key parameters of the penetration model for the Horizon I material system are as follows.

The material thickness t (cm) = 0.13. The effective fiber diameter d_f (cm) = 1.0×10^{-4}.
The model coefficients a, b, c, d are:

```
{a, b, c, d}
```

```
{4.52095, 0.792578, 9.64952, -0.384131}
```

```
(*++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++*)
(*==========================================================================*)
```

CPCU MkIII Material System

The first step is to provide the data that can be used to determine the coefficients a, b, c, and d for the penetration model.

Define the thickness of the material system for CPCU MkIII material system.

```
(* Thickness of material system (t) *)
t = 1.22 * 0.1;    (* converted from mm to cm *)
```

Extraction and Visualization of Penetration Data

- First, let us import the data file containing penetration data through CPCU MkIII material system at two different pressure drops obtained from swatch-level testing. The columns in the data file are as follows:
  - column 1 : particle diameter (μm)
  - column 2 : penetration probability (for 25 Pa pressure drop across the filter)
  - column 3 : penetration probability (for 125 Pa pressure drop across the filter)

```
data = Import["C:\\Deposition on Humans Project\\Aerosol Deposition
    Project - Persons\\Fabrics\\CPCU MkIII\\peneMkIIIMod.txt", "Table"];
```

Display the penetration data for the CPCU MkIII material system as table.

```
dataFormatted =
  {NumberForm[#[[1]], {5, 3}], NumberForm[#[[2]], {4, 3}], NumberForm[#[[3]], {4, 3}]} & /@ data;
colLabels = Style[#, Bold] & /@ {"Dp  (μm)", "P(at 25 Pa)", "P  (at 125 Pa)"};
Grid[Join[{colLabels}, dataFormatted],
 Dividers → {{1 → True, 2 → True, 3 → True, 4 → True}, {1 → True, 2 → True, -1 → True}},
 Alignment → Center,
 Spacings → {4.5, 0.5}]
```

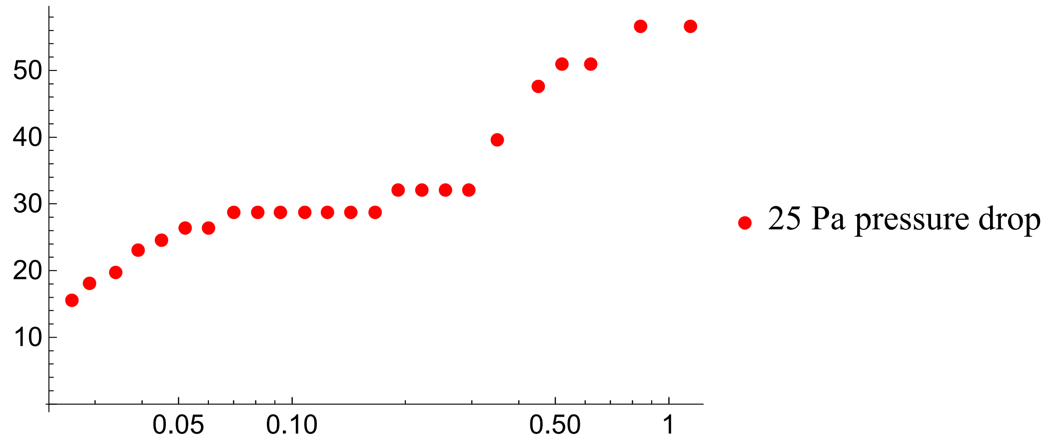
D_p (μm)	P(at 25 Pa)	P (at 125 Pa)
0.026	0.150	0.250
0.029	0.110	0.210
0.034	0.090	0.170
0.039	0.060	0.160
0.045	0.050	0.150
0.052	0.040	0.160
0.060	0.040	0.170
0.070	0.030	0.170
0.081	0.030	0.160
0.093	0.030	0.160
0.108	0.030	0.150
0.124	0.030	0.130
0.143	0.030	0.110
0.166	0.030	0.090
0.191	0.020	0.080
0.221	0.020	0.060
0.255	0.020	0.050
0.294	0.020	0.050
0.350	0.008	0.013
0.450	0.003	0.004
0.520	0.002	0.002
0.620	0.002	0.002
0.840	0.001	0.001
1.140	0.001	0.001

- Next, we transform the imported penetration data into a form that can be used for nonlinear model fitting.

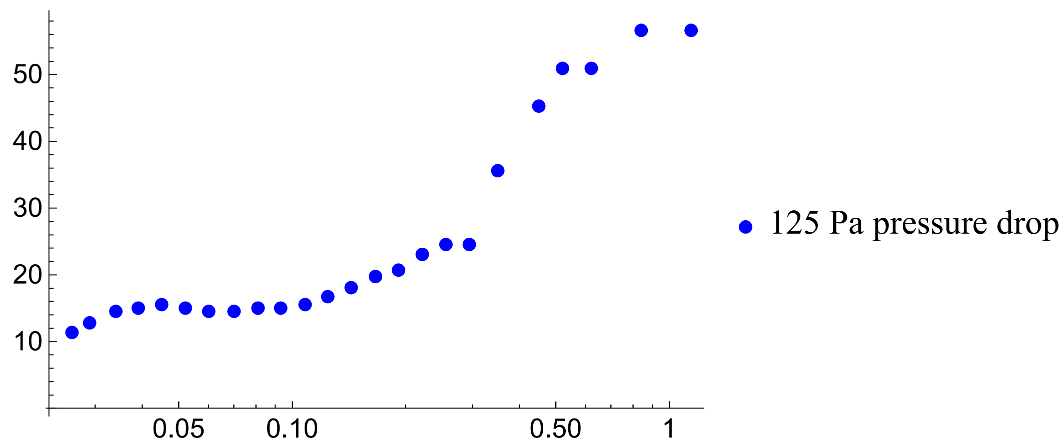
```
dimData = Dimensions[data];
vf25 = 0.8965;
(* face velocity for 25 Pa pressure drop across material system in cm s^-1  *)
vf125 = 4.25;
(* face velocity for 125 Pa pressure drop across material system in cm s^-1 *)
vf25Vec = Table[vf25, dimData[[1]]];
vf125Vec = Table[vf125, dimData[[1]]];
(* Form vectors for particle diameter, penetration at 25 Pa pressure drop,
and penetration at 125 Pa pressure drop *)
{diam, pene25, pene125} = {data[[All, 1]], data[[All, 2]], data[[All, 3]]};

(* Compute the transformed penetration data *)
(* Transformed penetration probability y = -(1/t)log(P),
where P is the penetration probability *)
(* y has dimensions of cm^-1 *)
(* y for pressure drop of 25 Pa across material system *)
y25 = -Log[pene25] / t;
(* y for pressure drop of 125 Pa across material system *)
y125 = -Log[pene125] / t;

(* Construct data structure for nonlinear least squares fitting *)
(* Note that particle diameter is converted from μm to cm *)
(* Each data triple consists of face velocity (cm s^-1), particle diameter (cm),
and transformed penetration probability y = (-1/t)log(P) (cm^-1) *)
data1ToFit = Transpose[{vf25Vec,  diam * 10.^(-4), y25}];
data2ToFit = Transpose[{vf125Vec, diam * 10.^(-4), y125}];
dataToFit = Join[data1ToFit, data2ToFit];
(* Total penetration data set {{V_f, D_p, y}..} *)
```

- Visualization of transformed penetration data

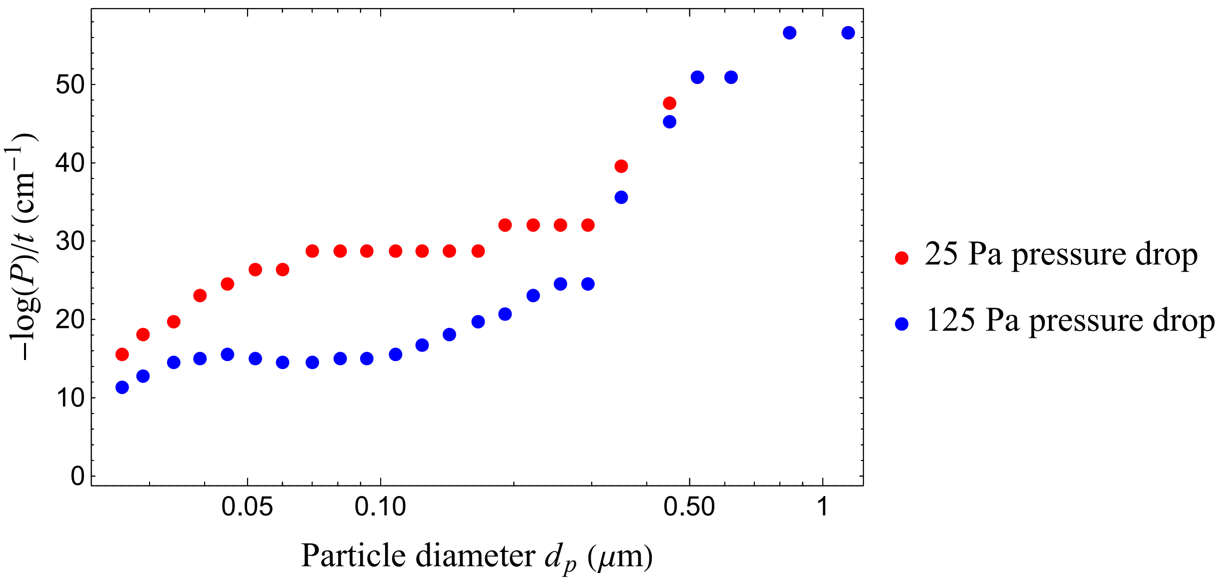
```
ploty25 = ListLogLinearPlot[{diam, y25}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
ploty125 = ListLogLinearPlot[{diam, y125}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
Show[ploty25, ploty125,
 Frame → True,
 BaseStyle -> {"TimesNewRoman", 14},
 FrameLabel → {Style["Particle diameter d_p (μm)", FontFamily → "Times New Roman", 18],
   Style["-log(P)/t (cm^-1)", FontFamily → "Times New Roman", 18]},
 ImageSize → 450]
```



Determination of Coefficients for Penetration Model for CPCU MkIII Material System

In this sub-section,we use the penetration data obtained in the last sub-section to determine the coefficients for the penetration model for the CPCU MkIII material system using nonlinear least-squares fitting.

```
(* Nonlinear fitting of transformed penetration probability model to the data *)
(* For the fitting, it is necessary to choose a reasonable fibre diameter df *)

df = 0.1 × 10^-4;  (* fiber diameter in cm *)
Clear[a, b, c, d];
nlm = NonlinearModelFit[dataToFit, model[v, x], {a, b, c, d}, {v, x}];
(* Extract the best fit parameters *)
{a, b, c, d} = {a, b, c, d} /. nlm["BestFitParameters"]
(* Display table of estimated parameter statistics *)
nlm["ParameterTable"]
```

{0.413873, -0.559138, 14.472, 0.274692}

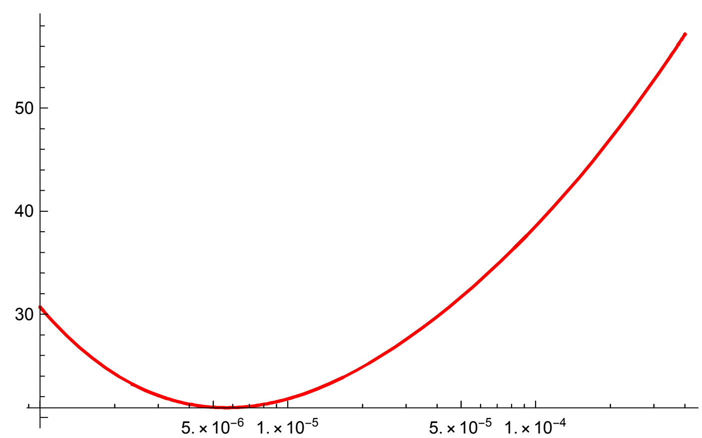
	Estimate	Standard Error	t-Statistic	P-Value
0.413873	0.413873	2.32196	0.178243	0.85935
-0.559138	-0.559138	0.852299	-0.656034	0.515218
14.472	14.472	7.90435	1.83089	0.0738944
0.274692	0.274692	0.115131	2.38591	0.0214059

Visualization of the Fit of Model to Data

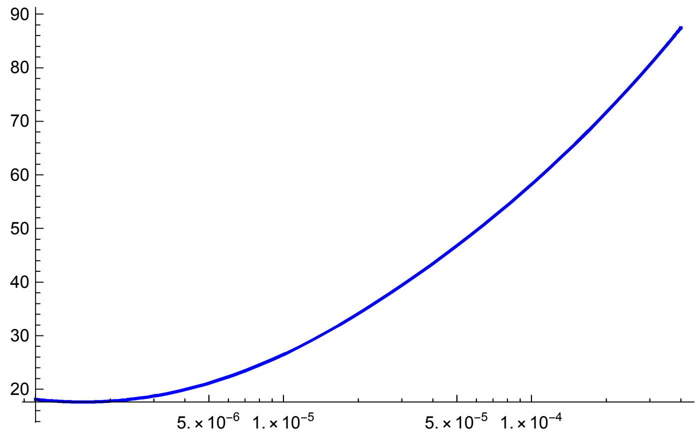
```
(* Provide plot showing the predicted transformed penetration probability and the
   measured transformed penetration probability *)
(*-------------------------------------------------------------------------------
                                           --*)
```

First visualization in terms of 2-D line plot

```
Vf = vf25;
ploty25theor =
 LogLinearPlot[model[Vf, x], {x, 1.0 × 10^(-6), 4.0 × 10^(-4)}, PlotStyle → Red]
```

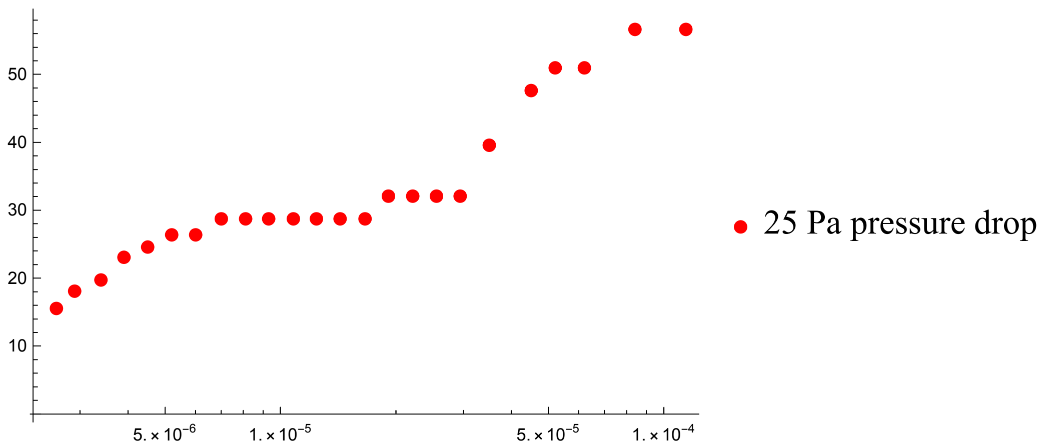


```
Vf = vf125;
ploty125theor = LogLinearPlot[model[Vf, x], {x, 1.0 × 10^-6, 4.0 × 10^-4}, PlotStyle → Blue]
```

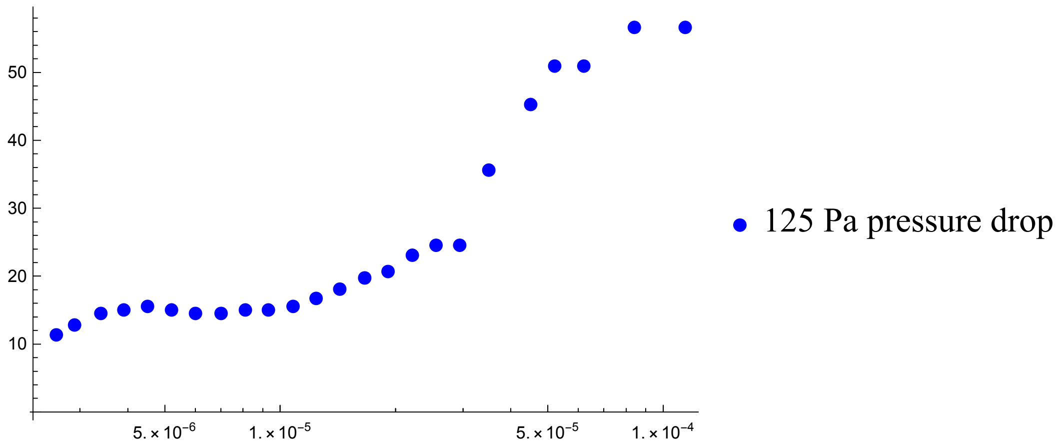



```
data1m = Transpose[{diam * 1.0 × 10^(-4), y25}];
data2m = Transpose[{diam * 1.0 × 10^-4, y125}];
```

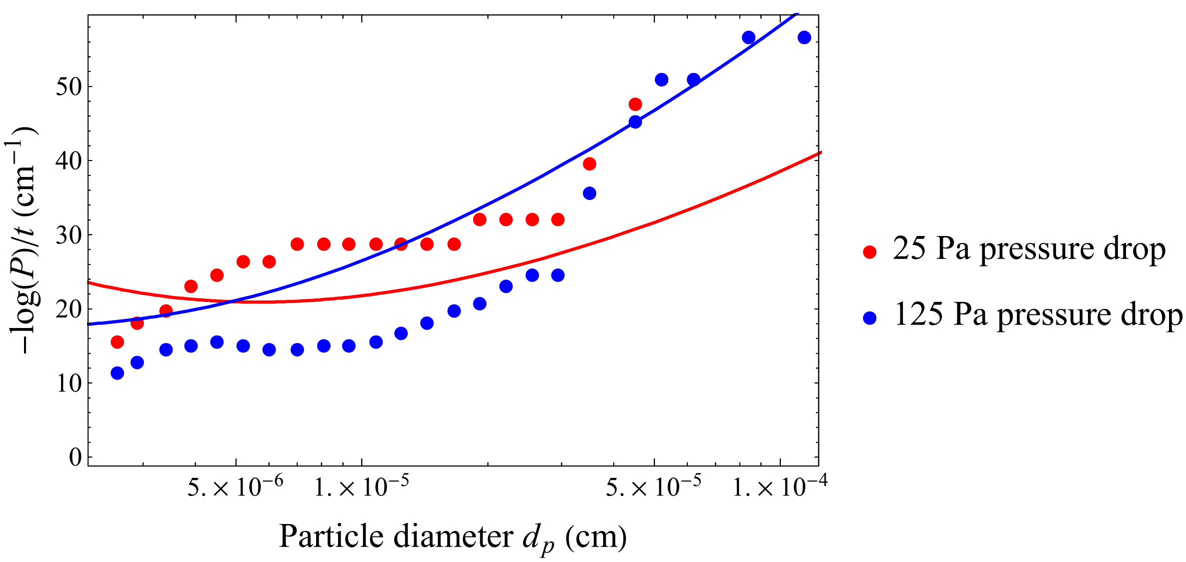
```
ploty25m = ListLogLinearPlot[data1m, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
ploty125m = ListLogLinearPlot[data2m, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
Show[ploty25m, ploty125m, ploty25theor, ploty125theor,
 BaseStyle → {FontFamily → "Times New Roman", FontSize → 14},
 Frame → True,
 FrameLabel → {Style["Particle diameter dp (cm)", FontSize → 18],
   Style["-log(P)/t (cm^-1)", FontSize → 18]}, ImageSize → 72. * 6]
```

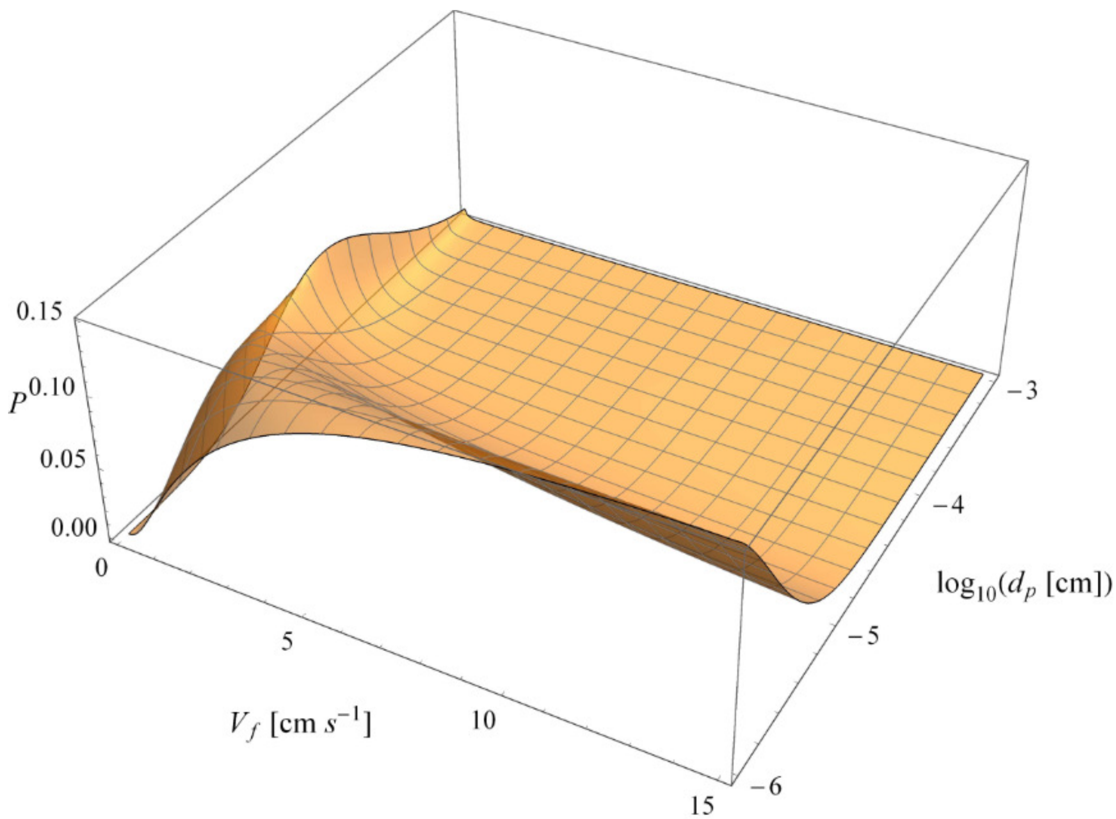



```
(*------------------------------------------------------------------------*)
```

Visualization in terms of a 3-D surface plot

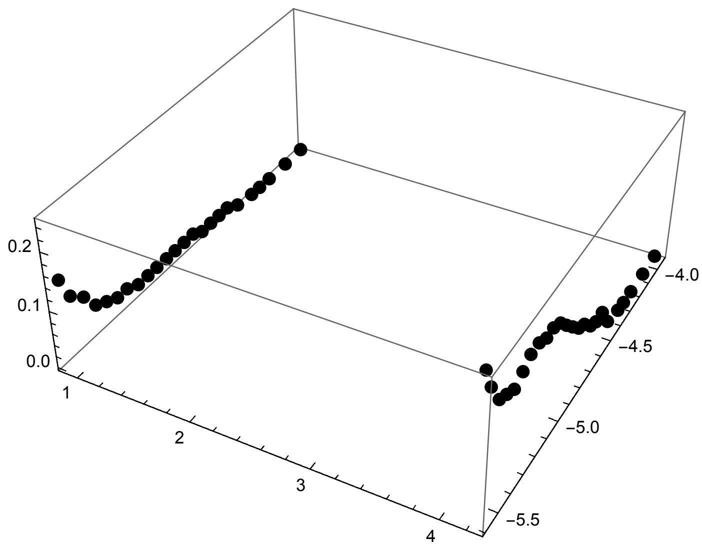
```
(* Construct 3-D plot of penetration probability using fitted model function *)

(* Face velocity in cm s^-1 *)
Vfaxis = Range[0.1, 15., 0.1];
 (* Common logarithm of particle diameter in cm *)
LogDpaxis = Range[-6., -3, 0.05];
```

```
(* Sample the penetration probability as a function of
 the face velocity V_f (cm s^-1) and particle diameter d_p (cm) *)

datavals = Flatten[Outer[{#1, #2, Exp[-t model[#1, 10^#2]]} &, Vfaxis, LogDpaxis], 1];

(* Use the sampled data set to plot the penetration probability surface *)

penePlot3D =
 ListPlot3D[datavals, BaseStyle → {FontFamily → "Times New Roman", FontSize → 14, Black},
  AxesLabel → {Style["V_f [cm s^-1]", Black, FontSize → 16], Style["log_10(d_p [cm])",
     Black, FontSize → 16], Style["P", Black, FontSlant → Italic, FontSize → 16]},
  PlotStyle → {Opacity[0.6]}, PlotTheme → "GrayMesh", ImageSize → Large]
```

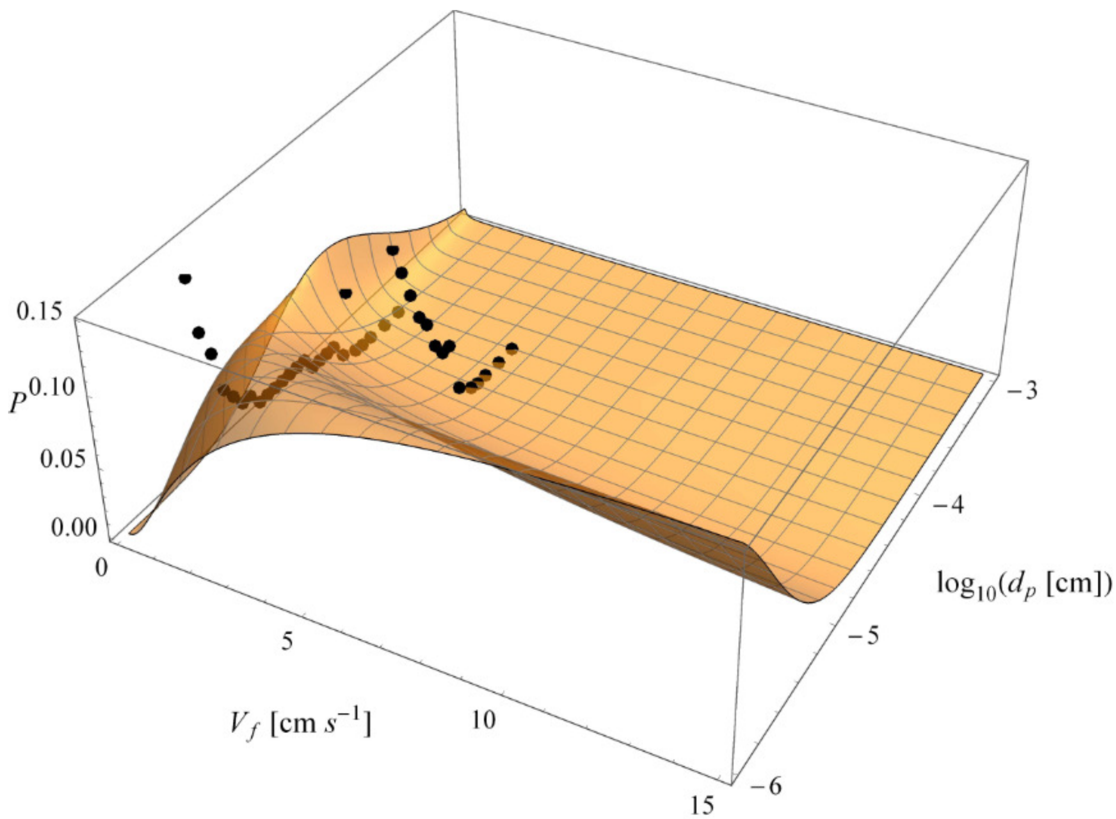



```
(* Plot the penetration data points in 3-D space *)

pene25m = Transpose[{vf25Vec, Log[10, diam * 10.^-4], pene25}];
pene125m = Transpose[{vf125Vec, Log[10, diam * 10.^-4], pene125}];
peneAllm = Join[pene25m, pene125m];
```

```
penePlot3Ddata = ListPointPlot3D[Style[peneAllm, Black, PointSize[Large]]]
```




```
(* Superimpose the model for penetration probability
 with measured values for penetration probability *)

Show[penePlot3D, penePlot3Ddata]
```



Summary

The key parameters of the penetration model for the CPCU MkIII material system are as follows.

The material thickness t (cm) = 0.122. The effective fiber diameter d_f (cm) = 0.1×10^{-4}.
The model coefficients a, b, c, d are:

```
{a, b, c, d}
```

```
{0.413873, -0.559138, 14.472, 0.274692}
```

```
(*++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++*)
(*==========================================================================*)
```

CPCU MkIV Material System

The first step is to provide the data that can be used to determine the coefficients a, b, c, and d for the penetration model.

Define the thickness of the material system for CPCU MkIV material system.

```
(* Thickness of material system (t) *)
t = 1.33 * 0.1;    (* converted from mm to cm *)
```

Extraction and Visualization of Penetration Data

- First, let us import the data file containing penetration data through CPCU MkIV material system at two different pressure drops obtained from swatch-level testing. The columns in the data file are as follows:
  - column 1 : particle diameter (μm)
  - column 2 : penetration probability (for either 25 and 125 Pa pressure drop across the filter)

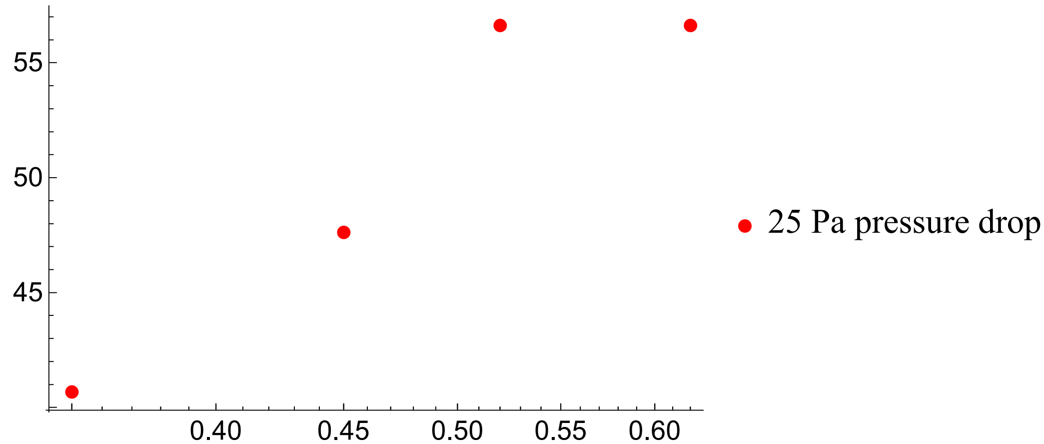
```
(* penetration data for 25 Pa pressure drop *)
data25 = Import["C:\\Deposition on Humans Project\\Aerosol Deposition Project
     - Persons\\Fabrics\\CPCU MkIV\\peneMkIV25.txt", "Table"];
(* penetration data for 125 Pa pressure drop *)
data125 = Import["C:\\Deposition on Humans Project\\Aerosol Deposition Project
     - Persons\\Fabrics\\CPCU MkIV\\peneMkIV125.txt", "Table"];
```

- Next, we transform the imported penetration data into a form that can be used for nonlinear model fitting.

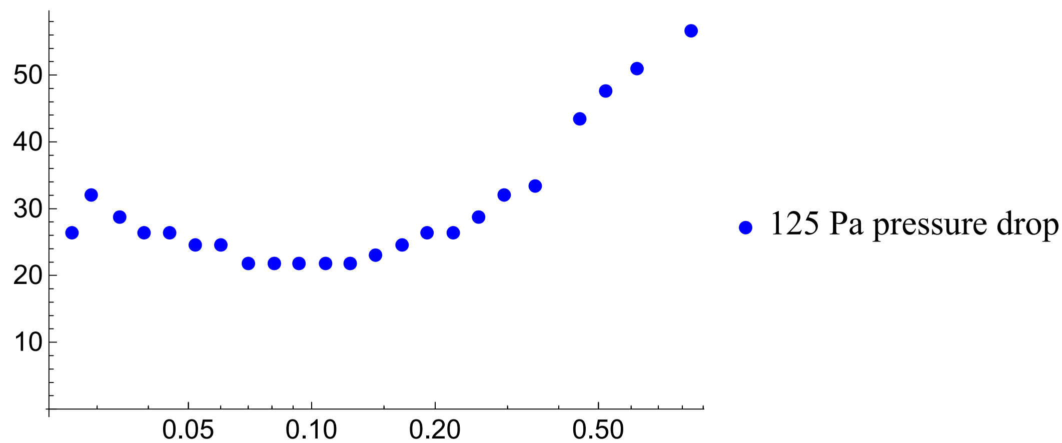
```
(* Face velocity (cm s^-1) associated with the pressure drops of 25 Pa and 125 Pa *)
dimData25 = Dimensions[data25];
dimData125 = Dimensions[data125];
vf25 = 0.64;
(* face velocity for 25 Pa pressure drop across material system in cm s^-1 *)
vf125 = 3.24;
(* face velocity for 125 Pa pressure drop across material system in cm s^-1 *)
vf25Vec = Table[vf25, dimData25[[1]]];
vf125Vec = Table[vf125, dimData125[[1]]];

(* Extract particle diameters (μm) and penetration probabilities
 for data associated with pressure drops of 25 and 125 Pa *)

d25 = data25[[All, 1]];
d125 = data125[[All, 1]];
pene25 = data25[[All, 2]];
pene125 = data125[[All, 2]];

(* Transformed penetration probability y = -(1/t) Log(P),
where P is the penetration probability *)
(* y has dimensions of cm^-1 *)

 (* y for pressure drop of 25 Pa across material system *)
y25 = -Log[pene25] / t ;
(* y for pressure drop of 125 Pa across material system *)
y125 = -Log[pene125] / t;

(* Construct data structure for nonlinear least squares fitting *)
(* Note that particle diameter is converted from μm to cm *)
(* Each data triple is face velocity (cm s^-1), particle diameter (cm),
and transformed penetration probability y = (-1/t) log(P) (cm^-1) *)
data1ToFit = Transpose[{vf25Vec, d25 * 10.^(-4), y25}];
data2ToFit = Transpose[{vf125Vec, d125 * 10.^(-4), y125}];
(* Total penetration data set {{Vf, Dp, y}..} *)
dataToFit = Join[data1ToFit, data2ToFit] ;
```

- Visualization of transformed penetration data

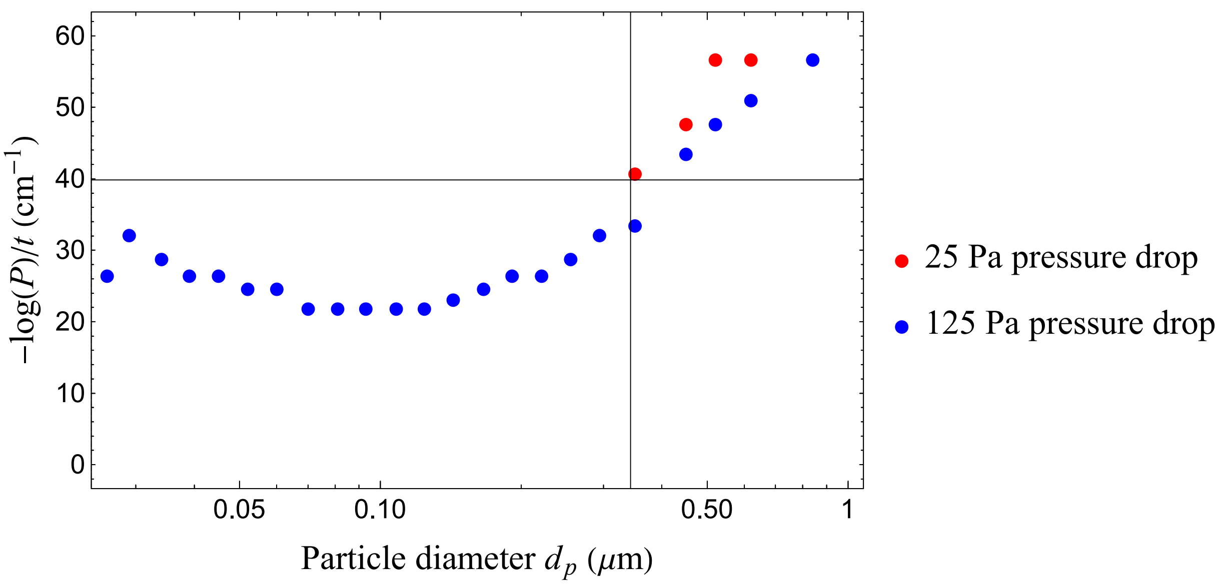
```
ploty25 = ListLogLinearPlot[{d25, y25}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
ploty125 = ListLogLinearPlot[{d125, y125}ᵀ,
  BaseStyle -> {"Times New Roman", 14}, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
Show[ploty25, ploty125,
 Frame → True,
 BaseStyle -> {"TimesNewRoman", 14},
 PlotRange -> {0, 60},
 FrameLabel → {Style["Particle diameter dp (μm)", FontFamily → "Times New Roman", 18],
   Style["-log(P)/t (cm^-1)", FontFamily → "Times New Roman", 18]},
 ImageSize → 450]
```



Determination of Coefficients for Penetration Model for CPCU MkIV Material System

In this sub-section,we use the penetration data obtained in the last sub-section to determine the coefficients for the penetration model for the CPCU MkIV material system using nonlinear least-squares fitting.

```
(* Nonlinear fitting of transformed penetration probability model to the data *)
(* For the fitting, it is necessary to choose a reasonable fibre diameter d_f *)

df = 0.25 × 10^-4;  (* fiber diameter in cm *)
Clear[a, b, c, d];
nlm = NonlinearModelFit[dataToFit, model[v, x], {a, b, c, d}, {v, x}];
(* Extract the best fit parameters *)
{a, b, c, d} = {a, b, c, d} /. nlm["BestFitParameters"]
(* Display table of estimated parameter statistics *)
nlm["ParameterTable"]
```

```
{67.3268, 0.229111, 10.278, -0.894001}
```

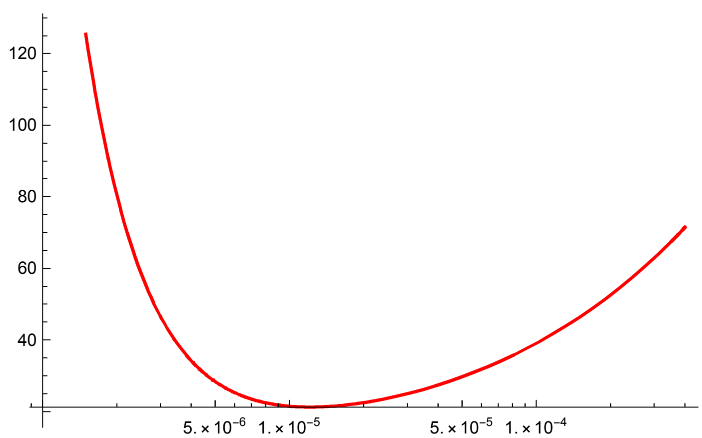
	Estimate	Standard Error	t-Statistic	P-Value
67.3268	67.3268	13.2894	5.06623	0.0000395861
0.229111	0.229111	0.0893191	2.56509	0.0173079
10.278	10.278	7.50262	1.36992	0.183937
-0.894001	-0.894001	1.79725	-0.497428	0.623609

Visualization of the Fit of Model to Data

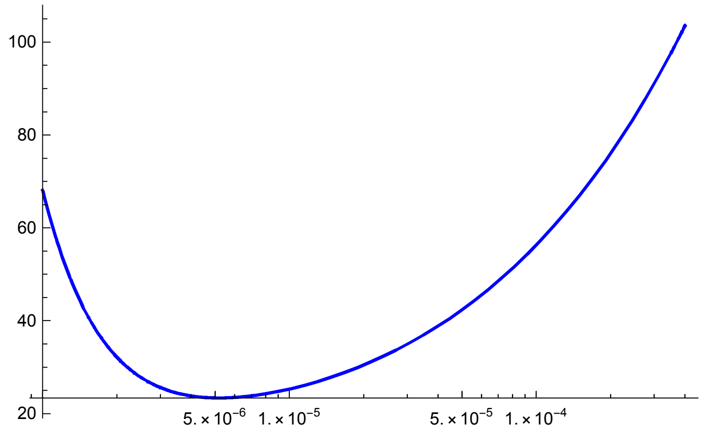
```
(* Provide plot showing the predicted transformed penetration probability and the
   measured transformed penetration probability *)
(*---------------------------------------------------------------------------------
                                                  --*)
```

First visualization in terms of 2-D line plot

```
Vf = vf25;
ploty25theor =
 LogLinearPlot[model[Vf, x], {x, 1.0 × 10^(-6), 4.0 × 10^(-4)}, PlotStyle → Red]
```

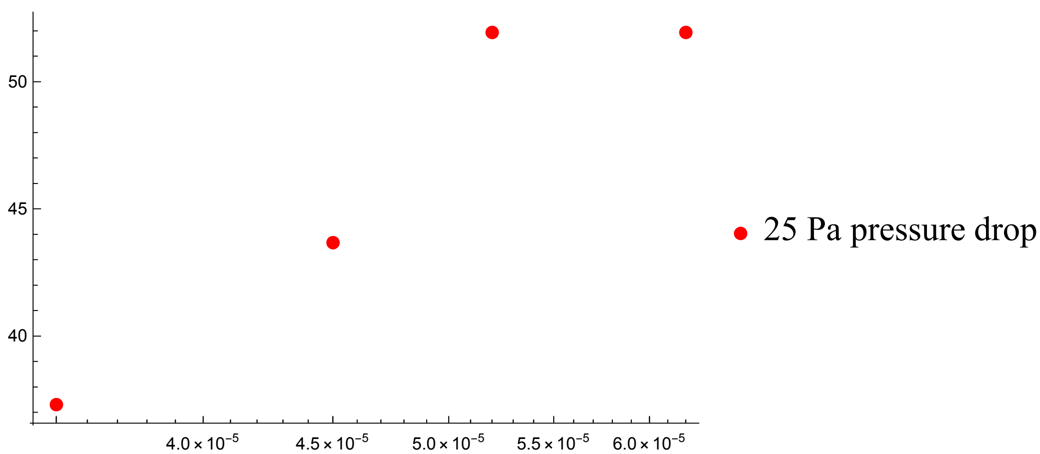


```
Vf = vf125;
ploty125theor = LogLinearPlot[model[Vf, x], {x, 1.0 × 10^-6, 4.0 × 10^-4}, PlotStyle → Blue]
```

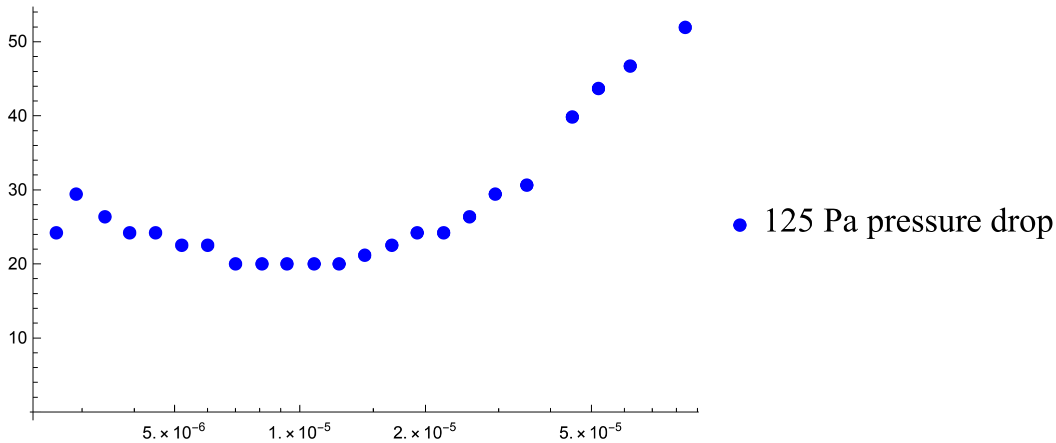



```
data1m = Transpose[{d25 * 1.0 × 10^(-4), y25}];
data2m = Transpose[{d125 * 1.0 × 10^-4, y125}];
```

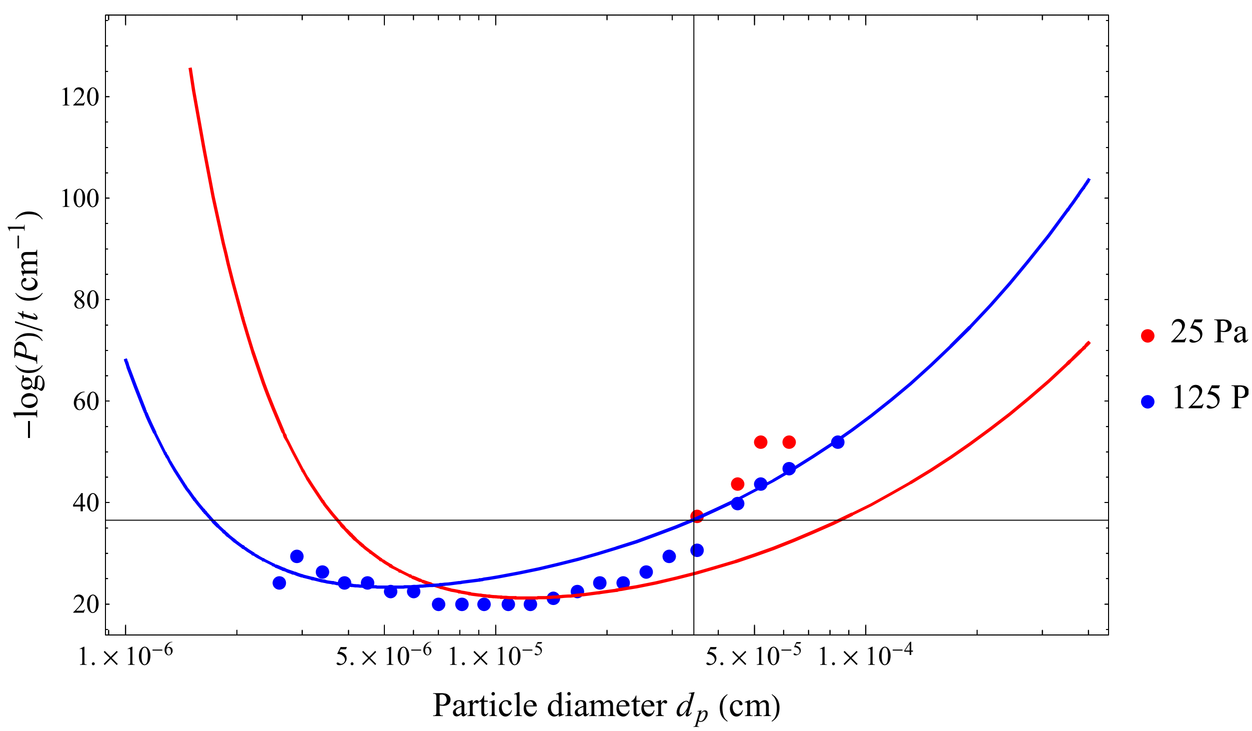
```
ploty25m = ListLogLinearPlot[data1m, PlotStyle → {Red, PointSize[Large]},
  PlotLegends → {Style["25 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```



```
ploty125m = ListLogLinearPlot[data2m, PlotStyle → {Blue, PointSize[Large]},
  PlotLegends → {Style["125 Pa pressure drop", FontFamily → "Times New Roman", 18]}]
```




```
Show[ploty25m, ploty125m, ploty25theor, ploty125theor,
 BaseStyle → {FontFamily → "Times New Roman", FontSize → 14},
 PlotRange → {20, 130},
 Frame → True,
 FrameLabel → {Style["Particle diameter dp (cm)", FontSize → 18],
   Style["-log(P)/t (cm^-1)", FontSize → 18]}, ImageSize → 72. * 8]
```

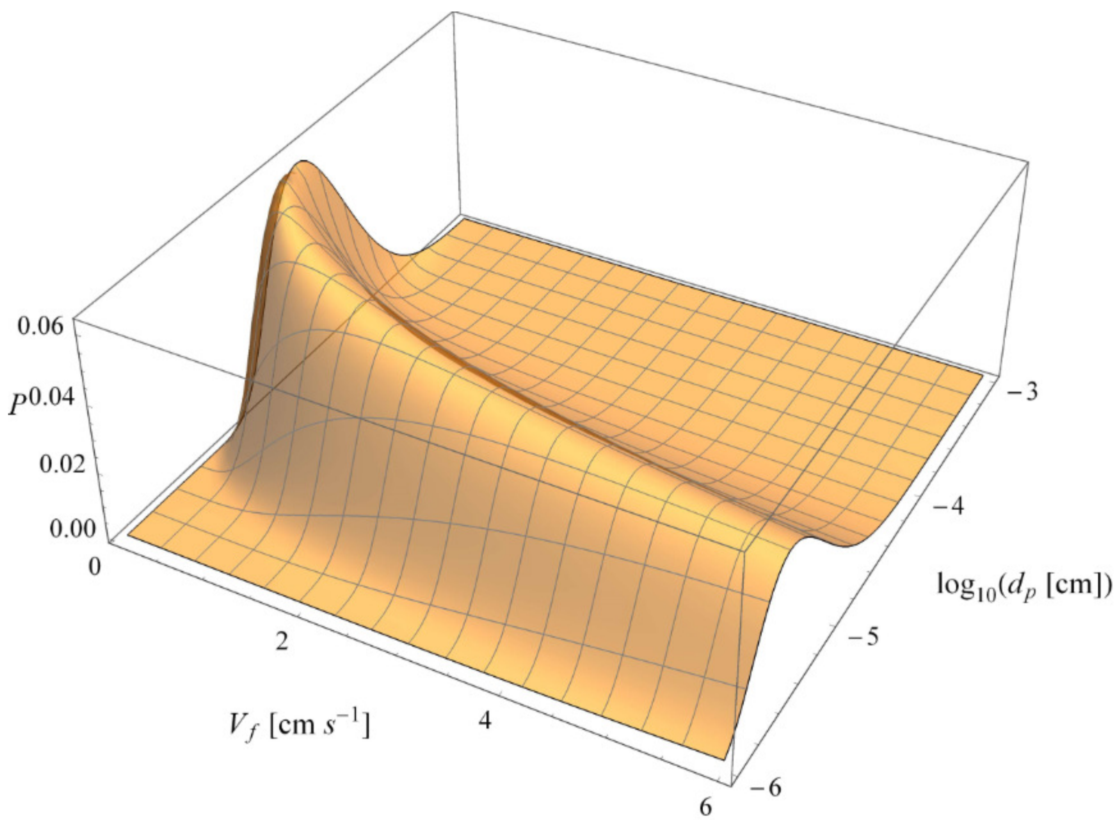



```
(*--------------------------------------------------------------------------*)
```

Visualization in terms of a 3-D surface plot

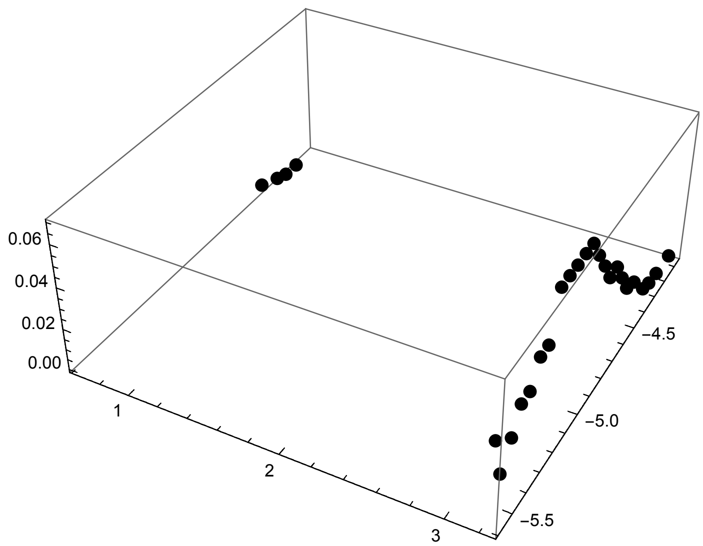
```
(* Construct 3-D plot of penetration probability using fitted model function *)
```

```
(* Face velocity in cm s^-1 *)
Vfaxis = Range[0.1, 6., 0.1];
 (* Common logarithm of particle diameter in cm *)
LogDpaxis = Range[-6., -3, 0.05];

(* Sample the penetration probability as a function of
 the face velocity Vf (cm s^-1) and particle diameter dp (cm) *)

datavals = Flatten[Outer[{#1, #2, Exp[-t model[#1, 10^#2]]} &, Vfaxis, LogDpaxis], 1];

(* Use the sampled data set to plot the penetration probability surface *)

penePlot3D =
 ListPlot3D[datavals, BaseStyle → {FontFamily → "Times New Roman", FontSize → 14, Black},
  AxesLabel → {Style["Vf  [cm s^-1]", Black, FontSize → 16], Style["log10(dp  [cm])",
     Black, FontSize → 16], Style["P", Black, FontSlant → Italic, FontSize → 16]},
  PlotStyle → {Opacity[0.6]}, PlotTheme → "GrayMesh", ImageSize → Large]
```



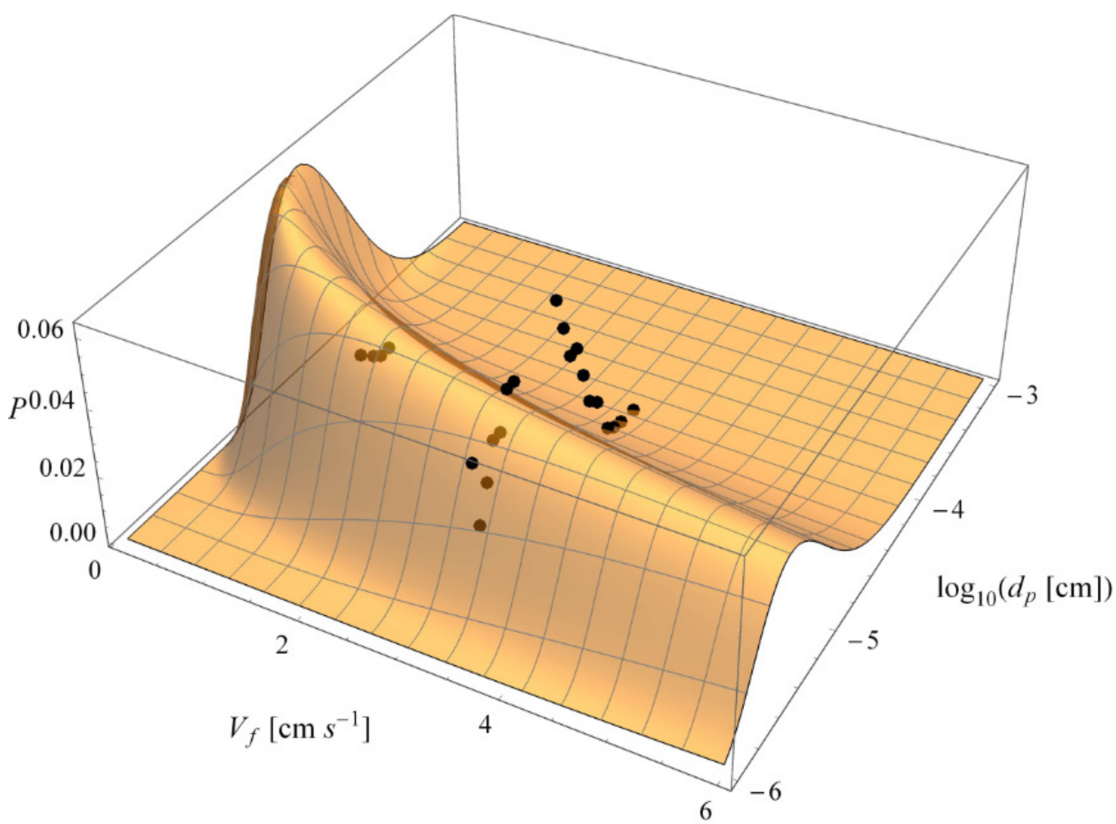

```
(* Plot the penetration data points in 3-D space *)

pene25m = Transpose[{vf25Vec, Log[10, d25 * 10.^-4], pene25}];
pene125m = Transpose[{vf125Vec, Log[10, d125 * 10.^-4], pene125}];
peneAllm = Join[pene25m, pene125m];
```

```
penePlot3Ddata = ListPointPlot3D[Style[peneAllm, Black, PointSize[Large]]]
```




```
(* Superimpose the model for penetration probability
 with measured values for penetration probability *)
```

```
Show[penePlot3D, penePlot3Ddata]
```



Summary

The key parameters of the penetration model for the CPCU MkIV material system are as follows.

The material thickness t (cm) = 0.133. The effective fiber diameter d_f (cm) = 0.25×10^{-4}.
The model coefficients a, b, c, d are:

```
{a, b, c, d}
```

```
{67.3268, 0.229111, 10.278, -0.894001}
```

```
(*+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++*)
(*=================================================================================*)
```