

# Supplement

Technical Note: Curve fitting algorithm for multimodal particle size distributions – a theoretical basis

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Source code for SMPS read functions are housed here <https://github.com/christopher-rapp/scripts-multimodal.git>

## 1 Setup

- 1.1 Retrieve Read Functions**
- 1.2 Retrieve Example Data**
- 1.3 Import Libraries**
- 1.4 User Paths**

These must be changed if trying with your own data!

```
log.path = '~/Library/CloudStorage/Box-Box/Multimodal Curve Fitting/log/'  
  
import.path.BMI = '~/Library/CloudStorage/Box-Box/Multimodal Curve Fitting/example/BMI/'  
import.path.TSI = '~/Library/CloudStorage/Box-Box/Multimodal Curve Fitting/example/TSI/'  
import.path.NC = '~/Library/CloudStorage/Box-Box/Multimodal Curve Fitting/example/netCDF/'  
import.path.NAS = '~/Library/CloudStorage/Box-Box/Multimodal Curve Fitting/example/NASA-AMES/'
```

## 2 Formatting Data

### 2.1 Brechtel Manufacturing Inc. (BMI) Data

```
BMI.data.ls <- readPSD_BMI(import.path.BMI, tz = "US/Eastern")

# Read functions export data as a list to account for multiple files in a directory
dataPSD.BMI <- BMI.data.ls[[1]]

head(dataPSD.BMI)

##           Local Time          UTC Time #StartDate      StartTime EndDate
##             <POSc>            <POSc>    <int>       <char>   <int>
## 1: 2023-10-31 18:15:23 2023-10-31 22:15:23    231031 18:15:23.757 231031
## 2: 2023-10-31 18:17:47 2023-10-31 22:17:47    231031 18:17:47.862 231031
## 3: 2023-10-31 18:20:11 2023-10-31 22:20:11    231031 18:20:11.965 231031
## 4: 2023-10-31 18:22:36 2023-10-31 22:22:36    231031 18:22:36.078 231031
## 5: 2023-10-31 18:25:00 2023-10-31 22:25:00    231031 18:25:00.193 231031
## 6: 2023-10-31 18:27:24 2023-10-31 22:27:24    231031 18:27:24.307 231031
##           EndTime StartSecs EndSecs Temp(K) Press(hPa) NumBins 10.16 10.49
##             <char>    <int>    <int>  <num>     <num>    <int>    <num>    <num>
## 1: 18:17:23.748        21      141  26.490    950.521     120 3420.58 3734.03
## 2: 18:19:47.858        165     285  26.466    950.415     120 3159.37 3015.60
## 3: 18:22:11.968        309     429  26.455    950.511     120 7291.97 8002.41
## 4: 18:24:36.083        453     573  26.435    950.417     120 7145.41 7368.59
## 5: 18:27:00.195        597     717  26.412    950.458     120 7046.85 7546.17
## 6: 18:29:24.306        742     862  26.409    950.604     120 2208.41 2063.78
##      10.82 11.17 11.53 11.90 12.28 12.68 13.09 13.51 13.94
##      <num> <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 3931.78 4285.83 4785.94 5211.06 5268.06 4873.85 4272.60 3827.94 3760.99
## 2: 4087.27 4818.65 5183.06 5336.76 5346.21 5206.69 4998.48 4886.98 4944.24
## 3: 7251.37 6337.08 5376.83 4597.65 4178.56 4153.40 4396.36 4713.25 4961.93
## 4: 6523.60 5940.70 5641.67 5455.18 5259.88 5029.63 4781.73 4578.09 4466.42
## 5: 6556.28 5675.03 5022.23 4626.64 4408.62 4239.64 4075.71 3978.30 3973.91
## 6: 2907.14 3777.76 4616.84 5205.54 5305.98 4937.05 4398.17 4000.95 3931.87
##      14.40 14.86 15.34 15.84 16.35 16.88 17.43 17.99 18.57
##      <num> <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 4106.44 4786.17 5649.61 6422.93 6777.77 6717.27 6708.59 7177.82 7989.92
## 2: 5049.88 5048.12 4945.73 4856.21 4877.03 5118.77 5683.88 6476.23 7140.36
## 3: 5073.22 5027.45 4903.05 4873.84 5070.76 5554.36 6386.57 7467.70 8367.67
## 4: 4424.22 4408.08 4513.98 4953.89 5805.99 6829.31 7542.95 7696.56 7641.66
## 5: 3991.92 3976.83 4005.68 4224.04 4727.91 5535.34 6520.87 7310.20 7577.44
## 6: 4208.82 4651.85 5008.29 5245.93 5548.47 6031.69 6648.09 7249.82 7612.15
##      19.18 19.80 20.45 21.11 21.80 22.51 23.25 24.01
##      <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 8548.47 8733.28 9211.15 10457.97 12012.68 12841.21 12669.16 12648.49
## 2: 7514.08 8066.04 9179.75 10343.19 11042.74 11890.38 13214.68 14357.91
## 3: 8732.85 8759.77 8792.58 9051.57 9983.58 12063.36 14492.67 15392.67
## 4: 7942.76 8795.73 9750.65 10256.04 10502.03 11103.43 12314.28 13682.46
## 5: 7667.47 8289.82 9573.20 11022.25 12169.90 13114.89 14118.46 14922.20
## 6: 7639.78 7705.24 8208.07 9024.83 9942.67 11218.32 12955.83 14377.35
##      24.79 25.61 26.45 27.31 28.21 29.14 30.10 31.10
##      <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 13986.12 16129.58 17227.65 17045.35 17272.03 18938.52 21684.38 23692.69
```

```

## 2: 15183.52 15898.18 16213.41 16797.10 18398.39 20293.99 21057.08 21117.08
## 3: 14657.90 14021.72 14551.29 15970.48 17511.27 19085.68 21431.74 23555.15
## 4: 15083.17 16876.54 18452.55 19452.92 20586.91 21894.61 22498.43 23233.30
## 5: 15221.22 15556.25 16922.90 19208.62 21415.54 23383.32 24749.90 24420.52
## 6: 14636.24 14337.90 14894.69 16789.12 19050.79 20696.30 21733.00 22751.64
##      32.13    33.19    34.29    35.43    36.61    37.83    39.10    40.41
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 23181.99 22953.61 25254.42 27887.39 30067.61 32229.90 32671.72 32868.48
## 2: 23213.38 26595.63 27721.17 28408.51 29796.26 29939.27 31497.24 32851.97
## 3: 23757.11 24485.96 27037.65 29302.56 31065.86 32441.37 33273.56 34834.62
## 4: 25760.26 28023.02 27012.32 26622.12 30856.78 34567.88 34071.72 34225.12
## 5: 23573.56 24717.11 27277.00 28911.48 30296.23 32413.12 33819.28 34148.55
## 6: 24186.33 25943.83 28263.17 30151.38 30477.61 28989.20 27230.35 27257.49
##      41.76    43.17    44.62    46.13    47.69    49.31    50.98    52.72
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 35450.00 38604.59 38953.14 39872.12 43913.64 45240.86 46239.88 47895.46
## 2: 32848.97 36334.22 38330.20 37851.80 39612.10 41868.67 43626.08 44671.76
## 3: 36850.88 38143.57 40412.24 41480.42 41738.99 42380.16 44951.39 47878.62
## 4: 35305.43 36483.99 40160.20 40913.30 41338.65 43762.25 45823.24 47474.99
## 5: 35653.22 39005.12 40350.96 41288.66 41667.12 41604.13 42420.06 44916.30
## 6: 29868.46 34058.13 38195.04 41527.81 40805.77 40652.88 41817.84 43309.53
##      54.52    56.39    58.33    60.34    62.43    64.59    66.84    69.18
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 48281.58 50674.20 52528.16 50908.68 50761.38 49602.70 50528.73 52279.97
## 2: 45577.47 46407.03 46156.82 47093.80 49093.31 50892.83 50109.76 54196.07
## 3: 47918.56 47875.31 49415.92 48505.99 47098.50 48811.16 50357.77 51081.66
## 4: 48298.86 50519.05 53224.56 50885.04 47354.77 50035.90 51154.73 50535.06
## 5: 46813.32 49133.65 49786.21 51540.26 50666.08 54057.69 57616.11 54979.51
## 6: 44099.67 44213.12 43783.88 49945.58 53104.36 52352.23 55076.31 51120.83
##      71.60    74.12    76.74    79.46    82.29    85.24    88.30    91.49
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 50352.99 48915.17 49036.42 47895.21 45138.51 42063.32 41833.62 41722.89
## 2: 53978.99 50493.50 48187.22 44805.96 43748.55 43132.88 41691.31 39140.19
## 3: 52832.49 50063.21 47126.57 47528.52 45807.05 46552.90 45463.66 43382.42
## 4: 49539.02 49384.89 47012.91 47039.31 48432.25 47355.53 43283.66 42326.72
## 5: 54723.19 54407.00 54407.02 51001.54 47072.40 48224.70 42988.93 42028.12
## 6: 53844.64 54517.47 47695.84 48707.64 49135.27 45931.29 44152.33 41760.10
##      94.80    98.26   101.86   105.61   109.52   113.60   117.86   122.30
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 39969.75 35038.72 32446.79 32587.17 30219.92 33671.06 33991.86 31547.75
## 2: 37680.04 31840.54 34578.53 32434.63 36885.01 36445.42 34801.38 31460.89
## 3: 38850.88 36612.29 36634.99 35406.63 34316.29 35955.79 32048.60 30834.88
## 4: 41253.58 37798.44 36200.26 34462.05 33798.13 35368.46 35001.89 31128.95
## 5: 39703.71 36910.56 34052.27 36365.87 38649.88 35738.99 35325.53 31006.84
## 6: 36851.33 35329.81 35153.62 33348.54 37888.60 35243.59 34359.17 34295.79
##      126.94   131.79   136.85   142.15   147.69   153.49   159.56   165.93
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 27432.75 28020.87 31142.28 32206.87 33388.63 31906.87 27556.64 21712.79
## 2: 27405.51 26126.54 27194.69 31262.51 31840.73 29377.42 25640.83 20579.79
## 3: 30856.82 27673.98 28863.90 30873.96 33176.87 33095.38 27237.82 20676.43
## 4: 31438.97 28104.94 28422.75 31550.96 32987.19 33022.69 26099.18 21490.21
## 5: 31225.77 28995.79 30330.49 32069.83 32074.74 33180.79 28002.80 21229.33
## 6: 34255.16 31391.69 32262.48 35523.92 36315.22 34053.78 30792.82 24445.10
##      172.59   179.59   186.92   194.62   202.71   211.21   220.14   229.54

```

```

##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 19280.14 20543.98 20651.60 19030.09 16269.33 12139.91 8732.44 4561.59
## 2: 20773.91 21115.16 20380.08 19801.21 18840.94 14031.73 9938.76 6253.27
## 3: 21683.90 23658.16 25327.43 23842.45 19942.16 16333.91 12696.32 7650.79
## 4: 19329.21 20022.26 20520.26 22393.30 20091.52 15331.79 10676.07 6659.61
## 5: 21184.50 22315.74 24783.85 24756.46 19801.98 15676.01 10671.15 6076.28
## 6: 20811.07 23654.21 23256.48 25116.91 18546.70 13154.91 11376.66 8653.37
##      239.44 249.85 260.82 272.39 284.59 297.45 311.03 325.37
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 2873.65 3003.38 5532.21 17202.01 40744.48 60474.39 73052.66 67931.15
## 2: 3858.99 3109.18 5901.98 18149.35 39104.25 62219.36 72902.43 68268.13
## 3: 3905.74 3666.30 7276.22 20093.63 37902.27 61023.07 74393.81 66100.27
## 4: 4263.19 4177.95 7186.87 16972.94 40544.63 61328.13 70400.53 65854.64
## 5: 4027.26 4348.13 6070.95 17347.98 37584.21 61411.90 73498.74 67506.95
## 6: 5734.11 4079.36 6781.74 17969.24 40607.33 63940.04 77308.55 68125.98
##      340.52 356.53 373.46 391.36 410.30 430.34 451.56 474.03 497.83
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 48048.68 31763.35 18487.14 9178.38 5363.63 3381.23 3259.09 4331.26 5111.66
## 2: 47841.06 30071.61 16786.55 9125.37 5836.74 3570.41 2698.44 3306.43 4627.42
## 3: 46664.94 32120.27 17603.53 10592.59 5481.44 3070.19 2597.24 3497.24 3810.38
## 4: 47402.11 33812.84 19663.36 9710.91 5916.86 3928.15 2984.95 3203.95 4999.13
## 5: 49807.95 31643.16 18237.92 9933.42 6239.27 2752.77 3720.83 4089.52 4663.98
## 6: 48837.00 33299.19 19291.92 11030.60 6025.11 3592.56 4514.76 5593.17 4698.33
##      523.04 549.76 578.09 608.12 639.96 673.74 709.57 747.59 787.94 830.76
##      <num>    <num>    <num>    <num>    <num>    <num>    <num>    <num>
## 1: 3996.63 3495.25 2421.18 1041.61 542.10 457.46 490.19 136.88 34.25 157.63
## 2: 4165.94 3149.61 1438.42 1009.10 601.28 536.62 359.14 235.85 224.78 62.12
## 3: 3624.72 3009.17 1071.64 587.13 234.54 398.96 410.90 213.38 332.68 76.72
## 4: 3769.93 3194.02 1893.51 914.24 547.04 365.28 169.72 221.69 199.39 40.96
## 5: 3670.90 2798.97 1762.13 449.38 586.24 773.44 398.76 164.58 80.64 134.43
## 6: 4794.93 2871.07 1847.37 956.91 858.19 510.44 478.79 310.43 381.14 36.52
##      876.23 NumFlag    Units Size Range
##      <num>    <int>    <char>    <num>
## 1: 77.70        0 dNdlogDp   866.07
## 2: 58.30        0 dNdlogDp   866.07
## 3: 57.90        0 dNdlogDp   866.07
## 4: 5.39         0 dNdlogDp   866.07
## 5: 18.44        0 dNdlogDp   866.07
## 6: 3.90         0 dNdlogDp   866.07

```

## 2.2 TSI Data

Use example data from Storm Peak Laboratory for a new particle formation event (NPF) on 2022-03-23 MDT.

```

TSI.data.ls <- readPSD_TSI(import.path.TSI, tz = "US/Mountain")

# Read functions export data as a list to account for multiple files in a directory
dataPSD.TSI <- TSI.data.ls[[1]]

head(dataPSD.TSI)

##          Local Time            UTC Time Sample #      Date Start Time
##          <POSc>            <POSc>    <int>    <char>    <char>
## 1: 2022-03-23 00:03:41 2022-03-23 06:03:41 22042 03/23/22 00:03:41

```

```

## 2: 2022-03-23 00:08:40 2022-03-23 06:08:40      22043 03/23/22 00:08:40
## 3: 2022-03-23 00:13:40 2022-03-23 06:13:40      22044 03/23/22 00:13:40
## 4: 2022-03-23 00:18:41 2022-03-23 06:18:41      22045 03/23/22 00:18:41
## 5: 2022-03-23 00:23:41 2022-03-23 06:23:41      22046 03/23/22 00:23:41
## 6: 2022-03-23 00:28:41 2022-03-23 06:28:41      22047 03/23/22 00:28:41
##   Sample Temp(C) Sample Pressure(kPa) Mean Free Path(m) Gas Viscosity(Pa*s)
##   <num>           <num>           <num>           <num>           <num>
## 1:    21.8           65.0       1.042800e-07  1.826716e-05
## 2:    21.8           64.9       1.044406e-07  1.826716e-05
## 3:    21.7           65.0       1.042511e-07  1.826237e-05
## 4:    21.8           65.0       1.042961e-07  1.826716e-05
## 5:    21.6           65.0       1.042061e-07  1.825759e-05
## 6:    21.8           65.1       1.042319e-07  1.826716e-05
##   Diameter Midpoint  9.14  9.47  9.82 10.2   10.6   10.9   11.3   11.8
##   <lgcl> <num> <num> <num> <num> <num> <num> <num> <num>
## 1:      NA     0     0     0     0   0.000 197.349 165.190  0.000
## 2:      NA     0     0     0     0   0.000   0.000   0.000 139.885
## 3:      NA     0     0     0     0   0.000   0.000   0.000   0.000
## 4:      NA     0     0     0     0   0.000   0.000   0.000 139.686
## 5:      NA     0     0     0     0 239.221   0.000 165.063 139.563
## 6:      NA     0     0     0     0   0.000 197.246   0.000   0.000
##   12.2   12.6   13.1   13.6   14.1   14.6   15.1   15.7
##   <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 119.149 205.893 537.7770 1100.4600 731.200 1264.100 1272.090 1045.530
## 2:  0.000  0.000  89.7529  865.7820 695.574  534.916  817.785 1075.470
## 3: 238.234 205.841 896.0800  78.5859 972.367  827.438  696.483  846.219
## 4: 476.667 308.884 448.2090 393.0710 555.828  864.461  536.244  910.998
## 5: 238.134 308.638 716.5930 549.9040 555.448  802.190  870.332 1057.760
## 6: 238.190 102.902 627.1480 892.1420 600.387 1278.010  845.519  946.997
##   16.3   16.8   17.5   18.1   18.8   19.5   20.2   20.9
##   <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 945.511 705.087 750.964 1029.850 1136.800 1121.590  798.448 811.939
## 2: 585.939 662.720 853.130 1087.340 1063.430  978.252  824.356 778.284
## 3: 810.294 746.247 825.571 1014.800  788.091  714.964  755.608 822.320
## 4: 1497.180 1022.380 1423.590  947.111 1008.230  818.397  800.194 931.906
## 5: 1266.740 852.461 1021.970 1116.670 1166.100 1222.520  971.384 1035.850
## 6: 1169.030 746.401 924.198 1007.570  900.127  993.537 1021.950 538.486
##   21.7   22.5   23.3   24.1   25.0   25.9   26.9   27.9   28.9
##   <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 552.977 936.257 772.250 753.779  970.894  991.501  821.234 912.458 994.252
## 2: 686.882 787.487 885.758 771.547 1064.100  516.136  673.900  963.984 852.055
## 3: 893.441 948.449 942.425 746.502  739.741  982.018  874.202 1071.140 1079.850
## 4: 748.017 534.817 780.669 896.600  986.982  870.489  989.264  893.928 1139.280
## 5: 847.582 796.664 942.216 864.329  818.518  901.165  894.329 1050.530 1009.270
## 6: 793.556 892.247 710.593 817.135  759.351 1218.100 1062.580 1030.360 881.614
##   30.0   31.1   32.2   33.4   34.6   35.9   37.2   38.5
##   <num> <num> <num> <num> <num> <num> <num> <num>
## 1: 1101.620 1059.470 1051.010 1110.000  874.964  772.121  923.254 830.352
## 2: 810.815 982.204 1129.770 1156.650 1147.190 1030.990  927.985 740.158
## 3: 814.663 1103.450 1130.750  995.607 1097.650 1117.610  871.307 764.166
## 4: 1222.570 824.732 1097.810 896.415  898.849  909.217 1095.970 714.966
## 5: 1164.170 1033.240 893.356 911.370 1023.610 1028.900  778.422 642.334
## 6: 904.722 940.746 883.367 1218.180 1000.030  989.585  751.879 784.413
##   40.0   41.4   42.9   44.5   46.1   47.8   49.6   51.4   53.3

```

```

##      <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>
## 1: 704.077 543.343 532.085 413.761 340.885 192.353 203.8520 149.168 199.1210
## 2: 589.793 597.713 440.377 322.472 258.539 266.625 214.3630 199.551 160.5590
## 3: 655.200 517.612 335.643 361.668 248.236 249.078 149.7990 114.920 124.5500
## 4: 803.899 539.732 422.166 350.520 360.424 266.994 97.3948 193.785 105.5690
## 5: 663.602 580.939 464.785 251.628 277.625 220.313 169.5690 212.348 109.7310
## 6: 647.183 477.660 506.529 327.103 286.743 264.709 214.7340 159.438 79.7374
##      55.2     57.3     59.4     61.5     63.8     66.1     68.5     71.0     73.7
##      <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>
## 1: 97.9716 106.3630 154.9910 153.8300 145.934 233.5010 232.727 184.466 155.427
## 2: 146.3700 112.1270 137.2040 118.8250 122.510 80.3680 152.510 103.625 209.588
## 3: 105.6750 54.4646 101.7230 104.1780 152.435 134.3620 196.023 186.525 139.293
## 4: 93.0872 121.1920 81.2171 99.5188 141.156 94.9131 223.259 135.609 184.474
## 5: 74.0632 131.2950 132.4830 115.4640 175.797 71.8226 167.940 169.304 141.137
## 6: 126.9810 134.5350 113.8760 126.8410 109.639 123.8490 128.060 108.854 278.049
##      76.4     79.1     82.0     85.1     88.2     91.4     94.7     98.2     101.8
##      <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>
## 1: 160.150 190.965 210.829 258.099 297.700 253.898 288.489 330.759 301.084
## 2: 152.934 234.367 185.909 185.675 245.477 339.798 348.205 333.769 382.287
## 3: 151.405 241.164 232.721 235.929 248.013 329.950 258.245 407.918 293.789
## 4: 134.784 215.345 229.982 320.966 335.539 328.506 239.511 310.813 301.674
## 5: 187.564 254.811 249.418 340.641 278.084 221.111 205.900 296.925 257.330
## 6: 148.768 231.010 165.701 228.159 256.833 301.819 242.626 262.261 279.860
##      105.5    109.4    113.4    117.6    121.9    126.3    131.0    135.8    140.7
##      <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>
## 1: 365.322 304.885 315.507 288.473 305.216 231.640 195.869 192.862 249.229
## 2: 350.268 326.903 391.164 310.955 336.524 325.825 337.661 283.029 295.786
## 3: 325.951 370.892 273.395 309.865 265.613 261.247 320.133 288.952 284.883
## 4: 283.761 310.761 297.287 348.271 267.395 312.350 319.894 226.978 297.472
## 5: 319.653 334.636 303.913 309.348 275.987 301.593 247.608 227.335 250.395
## 6: 393.031 245.679 301.759 252.979 342.495 265.423 250.865 321.399 233.386
##      145.9    151.2    156.8    162.5    168.5    174.7    181.1    187.7    194.6
##      <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>
## 1: 260.072 201.171 204.748 175.090 238.277 136.991 111.7630 138.5130 83.9202
## 2: 226.807 230.971 237.514 202.594 146.391 153.754 165.2710 92.9477 107.3920
## 3: 229.934 188.236 195.393 181.404 105.471 167.408 127.0000 156.6190 98.8299
## 4: 262.732 249.206 235.344 233.248 185.762 167.274 148.6380 95.8195 115.1420
## 5: 185.565 232.205 198.869 164.970 137.844 158.655 92.3299 92.2701 98.3238
## 6: 255.239 207.533 171.502 119.280 205.706 153.636 126.0880 117.4170 107.6480
##      201.7    209.1    216.7    224.7    232.9    241.4    250.3    259.5    269.0
##      <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>   <num>
## 1: 109.3220 121.7440 33.8008 81.0674 35.7504 20.1837 31.8373 15.79130 5.33835
## 2: 104.8160 71.4689 71.1985 33.6003 20.4320 25.8819 10.4397 15.79370 16.01750
## 3: 98.0943 81.5530 58.8758 52.8620 23.3219 35.7559 16.1332 5.26366 16.01470
## 4: 80.5776 108.6790 77.5540 28.2422 21.6584 39.6153 21.4253 8.87974 17.68660
## 5: 92.7493 73.5486 82.7527 38.1945 15.3207 20.7012 25.0776 22.07870 5.33805
## 6: 68.0021 43.5719 65.3531 47.8294 18.1787 31.0521 20.8752 10.52700 4.46073
##      278.8    289.0    299.6    310.6    322.0    333.8    346.0 Scan Up Time(s) Retrace Time(s)
##      <int> <int> <int> <int> <int> <int> <int> <int> <int>
## 1:     0     0     0     0     0     0     0     280     10
## 2:     0     0     0     0     0     0     0     280     10
## 3:     0     0     0     0     0     0     0     280     10
## 4:     0     0     0     0     0     0     0     280     10
## 5:     0     0     0     0     0     0     0     280     10

```

```

## 6:      0      0      0      0      0      0      0      280      10
##   Down Scan First Scans Per Sample Impactor Type(cm) Sheath Flow(lpm)
##           <lgcl>          <int>          <num>          <int>
## 1:    FALSE           1     0.0457           10
## 2:    FALSE           1     0.0457           10
## 3:    FALSE           1     0.0457           10
## 4:    FALSE           1     0.0457           10
## 5:    FALSE           1     0.0457           10
## 6:    FALSE           1     0.0457           10
##   Aerosol Flow(lpm) CPC Inlet Flow(lpm) CPC Sample Flow(lpm) Low Voltage
##           <int>          <int>          <int>          <num>
## 1:           1           1           1     10.6730
## 2:           1           1           1     10.6568
## 3:           1           1           1     10.6732
## 4:           1           1           1     10.6714
## 5:           1           1           1     10.6749
## 6:           1           1           1     10.6779
##   High Voltage Lower Size(nm) Upper Size(nm) Density(g/cc) Title Status Flag
##           <num>          <num>          <num>          <num>  <lgcl>  <char>
## 1: 9855.99       8.97687     352.269        1.2    NA Normal Scan
## 2: 9848.78       8.97687     352.269        1.2    NA Normal Scan
## 3: 9854.71       8.97687     352.269        1.2    NA Normal Scan
## 4: 9855.27       8.97687     352.269        1.2    NA Normal Scan
## 5: 9854.15       8.97687     352.269        1.2    NA Normal Scan
## 6: 9858.15       8.97687     352.269        1.2    NA Normal Scan
##   td(s)    tf(s) D50(nm) Median(nm) Mean(nm) Geo.Mean(nm) Mode(nm)
##           <num>  <num>  <num>  <num>  <num>  <num>  <num>
## 1: 1.779 2.25624 265.182  28.1484 43.6574 32.2018 15.1247
## 2: 1.779 2.25624 265.018  30.2327 46.9183 34.8112 33.3762
## 3: 1.779 2.25624 265.163  29.0698 45.3157 33.6499 32.1968
## 4: 1.779 2.25624 265.166  28.6246 45.0059 33.1420 16.2531
## 5: 1.779 2.25624 265.160  27.3360 42.4647 31.5314 16.2531
## 6: 1.779 2.25624 265.231  27.7849 43.3304 32.1639 14.5902
##   Geo.Std. Dev. Total Conc.(#/cc) Comment    Units Size Range
##           <num>          <num>  <lgcl>  <char>  <num>
## 1: 2.04694       638.399    NA dNdlogDp 336.86
## 2: 2.04897       589.268    NA dNdlogDp 336.86
## 3: 2.03663       598.152    NA dNdlogDp 336.86
## 4: 2.05389       626.208    NA dNdlogDp 336.86
## 5: 2.02267       634.772    NA dNdlogDp 336.86
## 6: 2.02913       615.324    NA dNdlogDp 336.86

```

## 2.3 netCDF Data

Data were obtained from the Atmospheric Radiation Measurement (ARM) User Facility, a U.S. Department of Energy (DOE) Office of Science user facility managed by the Biological and Environmental Research Program.

Kuang, C., Singh, A., Howie, J., Salwen, C., & Hayes, C. Scanning mobility particle sizer (AOSSMPS), 2016-11-15 to 2025-06-23, Southern Great Plains (SGP), Lamont, OK (Extended and Co-located with C1) (E13). Atmospheric Radiation Measurement (ARM) User Facility. <https://doi.org/10.5439/1476898>

```
NC.data.ls <- readPSD_NC(import.path.NC)
```

```
# Read functions export data as a list to account for multiple files in a directory
```

```
dataPSD.NC <- NC.data.ls[[1]]
```

```
head(dataPSD.NC)
```

```
##          Time 10.55 10.9 11.3 11.75 12.2 12.65 13.1
## 1 2023-07-19 00:00:01 229.408 548.848 262.211 884.073 530.819 794.500 763.913
## 2 2023-07-19 00:05:00 114.746 299.476 218.582 461.397 597.981 531.017 921.694
## 3 2023-07-19 00:10:00 230.551 451.271 526.986 502.107 579.764 938.770 849.747
## 4 2023-07-19 00:15:00 115.809 352.599 397.037 310.385 445.339 1003.796 908.580
## 5 2023-07-19 00:20:00 114.704 249.476 305.913 768.758 543.062 753.482 818.479
## 6 2023-07-19 00:25:00 347.944 353.094 309.220 388.476 411.583 639.520 854.460
##      13.55 14.05 14.6 15.15 15.7 16.25 16.85 17.5
## 1 1121.157 1130.514 1211.083 1389.714 1453.444 1709.798 1621.780 1876.027
## 2 736.839 1214.537 1172.016 1166.224 1471.679 1399.218 1331.886 1919.116
## 3 964.090 993.853 1014.759 1132.285 1231.431 1539.507 1618.466 1654.262
## 4 1106.781 1338.346 1124.499 1145.662 1598.000 1301.520 1320.362 1795.484
## 5 682.445 1086.181 929.296 1274.957 1257.640 1441.239 1507.432 1662.602
## 6 738.635 1046.237 923.729 1389.188 1166.476 1297.628 1539.155 1552.144
##      18.1 18.75 19.45 20.15 20.9 21.7 22.5 23.3
## 1 1764.448 2429.017 2329.730 2320.435 2426.032 2144.505 2953.922 2892.823
## 2 2078.902 1784.736 2238.934 2599.956 2238.237 2729.816 2568.009 2865.300
## 3 1978.002 1924.727 2113.580 2389.900 2136.968 2457.808 2574.584 2803.770
## 4 1702.826 2441.895 1930.326 2193.416 2250.921 2491.292 2514.423 2778.490
## 5 1730.383 2237.354 1960.943 2203.576 2214.458 2177.672 2251.208 2567.292
## 6 1842.513 2022.649 1957.764 2218.728 2282.920 2335.917 2350.628 2576.894
##      24.15 25.05 25.95 26.9 27.9 28.9 29.95 31.05
## 1 3023.508 3295.483 3538.897 3728.871 4002.189 4419.072 4430.606 4916.476
## 2 2921.435 3019.030 3655.349 3642.867 4121.817 4351.931 4344.164 4808.162
## 3 2863.671 2955.779 3165.180 3597.900 3835.769 4206.578 4491.183 4772.361
## 4 2950.127 3041.181 3033.596 3525.306 3764.251 4518.231 4226.971 4906.754
## 5 2842.133 2832.622 3096.053 3368.349 3519.172 4116.027 4131.004 4908.662
## 6 3193.599 2849.140 3278.841 3570.402 3492.563 3708.533 4139.758 4553.236
##      32.2 33.4 34.6 35.85 37.2 38.55 39.95 41.45
## 1 5183.347 5586.184 5627.987 5668.352 6305.616 5850.432 5525.757 4909.097
## 2 4940.063 5348.845 5788.506 6273.896 6252.516 5840.920 5754.282 5006.534
## 3 5333.142 5527.131 5553.507 6158.542 6319.847 6255.833 5876.435 5583.143
## 4 5182.285 5376.875 5981.352 6303.903 6453.669 6093.425 6367.504 6294.676
## 5 5283.231 5743.592 5555.021 6240.056 6650.838 6758.908 6682.508 6402.453
## 6 5036.475 5258.476 6059.448 6698.119 6786.079 7332.025 7485.635 7316.705
##      42.95 44.5 46.15 47.85 49.6 51.4 53.25 55.2
## 1 4626.498 3861.933 3801.762 3259.180 3058.614 2875.609 3132.449 3321.056
## 2 4518.195 3963.110 3345.568 3221.533 2945.356 3083.876 3290.623 3431.242
## 3 4825.924 4435.265 4056.036 3627.474 3482.259 3395.029 3427.702 3578.296
## 4 5848.510 5260.221 4673.045 4295.160 3913.575 3708.291 3756.823 3770.353
## 5 6157.749 5815.503 4749.304 4416.361 4045.551 3734.515 3659.251 3759.374
## 6 6902.182 6340.164 5786.006 5161.751 4537.692 3820.945 3991.784 3805.736
##      57.25 59.35 61.5 63.75 66.1 68.55 71.05 73.65
## 1 3756.458 4388.521 4840.560 5370.918 5533.685 5802.646 5955.583 5348.883
## 2 3676.774 4480.724 4916.737 5357.544 5836.761 6005.729 5812.702 5457.548
## 3 3809.919 4494.913 4679.721 5719.344 5860.879 6114.155 5822.916 5876.069
## 4 4157.233 4528.021 4867.136 5398.713 5804.219 6060.933 5897.384 6031.204
## 5 3965.716 4435.867 4905.022 5539.349 5624.933 5966.754 6137.991 5788.471
## 6 4081.439 4503.414 4585.815 5276.229 5883.960 6018.710 5708.181 5926.518
##      76.35 79.15 82.05 85.05 88.2 91.45 94.8 98.25
```

```

## 1 5257.314 4937.997 4372.268 4001.376 3502.182 2896.232 2984.634 2654.561
## 2 5160.905 4876.296 4356.225 3935.288 3555.791 3108.744 2785.382 2623.546
## 3 5419.656 4842.824 4316.584 4053.013 3371.008 3159.801 2864.063 2725.578
## 4 5485.083 5166.305 4567.694 4043.328 3539.274 3090.468 2876.918 2712.535
## 5 5460.610 5072.785 4481.935 4258.757 3668.452 3413.873 2842.041 2818.431
## 6 5873.427 5388.537 4906.322 4201.384 3908.009 3508.810 3069.931 2626.065
##      102    105.5     109     113    117.5     122    126.5     131
## 1 2538.021 2247.618 2274.669 1937.595 1853.359 1793.009 1756.517 1516.367
## 2 2465.159 2274.896 2123.226 2074.377 1854.472 1834.397 1711.330 1537.152
## 3 2554.263 2208.979 2153.753 2129.170 2077.445 1777.651 1621.750 1664.572
## 4 2421.829 2391.145 2377.817 2051.115 2080.636 1810.110 1731.530 1682.714
## 5 2466.716 2399.010 2210.243 2042.621 2006.983 1916.026 1796.339 1709.397
## 6 2698.418 2556.055 2142.996 2162.599 2093.221 1889.757 1784.344 1628.241
##      135.5    140.5     146    151.5     157    162.5    168.5     175
## 1 1402.989 1393.854 1201.337 1232.041 1038.491 842.605 966.673 986.092
## 2 1600.321 1296.363 1412.774 1154.705 1301.814 1052.601 898.659 931.269
## 3 1698.079 1398.789 1364.831 1237.431 1172.154 977.313 1076.738 959.608
## 4 1493.433 1420.170 1301.576 1294.773 1008.620 980.325 919.513 884.260
## 5 1602.446 1392.331 1289.403 1233.346 1106.326 1178.849 859.516 979.881
## 6 1557.199 1451.036 1401.997 1243.497 1236.863 1098.424 945.006 943.942
##      181    187.5    194.5    201.5     209     217    225    233    241.5
## 1 857.364 883.544 765.581 729.769 715.337 639.000 553.750 524.392 506.776
## 2 780.790 739.892 708.611 613.622 645.240 647.817 573.260 570.102 456.216
## 3 825.174 794.066 722.401 691.995 677.901 616.601 589.802 455.427 422.744
## 4 789.248 792.965 712.277 696.179 617.265 596.020 530.092 581.154 524.253
## 5 832.008 773.040 660.379 805.312 632.536 592.711 585.909 544.394 443.887
## 6 899.463 770.290 748.299 757.026 702.633 707.764 621.278 612.352 564.387
##      250.5    259.5     269     279     289    299.5    310.5     322     334
## 1 463.636 396.987 368.449 291.418 276.257 233.573 246.820 186.964 169.124
## 2 410.224 427.664 415.029 288.641 261.489 219.244 191.458 201.809 138.921
## 3 449.623 450.036 341.147 335.495 283.009 252.993 260.690 233.852 174.338
## 4 460.110 413.281 387.842 331.133 320.346 260.985 273.399 238.332 207.620
## 5 493.967 376.266 346.639 313.250 269.700 270.287 252.098 211.557 157.856
## 6 407.486 389.319 419.432 311.440 263.083 266.570 234.922 254.118 248.421
##      346    358.5     372    385.5    399.5    414.5    429.5     445    461.5    478.5
## 1 160.291 101.170 105.324 107.734 68.150 79.852 60.160 39.428 51.185 26.116
## 2 159.808 152.503 99.196 84.170 54.522 69.440 38.929 35.846 32.906 29.848
## 3 163.470 101.103 106.541 111.226 85.528 45.314 59.347 40.653 51.390 41.204
## 4 144.812 147.345 116.648 64.477 48.086 54.477 51.485 37.128 61.633 18.804
## 5 153.238 130.405 128.471 67.953 84.560 72.909 49.544 32.259 32.905 41.040
## 6 158.702 135.787 93.337 81.461 82.450 59.505 46.381 43.364 44.232 30.091
##      496     514
## 1 49.166 11.587
## 2 26.475 34.763
## 3 18.986 27.145
## 4 38.122 19.466
## 5 34.038 11.587
## 6 41.942 23.364

```

## 2.4 NASA-AMES Data

Data obtained from <https://ebas-data.nilu.no/DataSets.aspx?stations=US9050R&InstrumentTypes=smpls&fromDate=1970-01-01&toDate=2025-12-31>.

The EBAS database has largely been funded by the UN-ECE CLRTAP (EMEP), AMAP and through NILU

internal resources. Specific developments have been possible due to projects like EUSAAR (EU-FP5)(EBAS web interface), EBAS-Online (Norwegian Research Council INFRA) (upgrading of database platform) and HTAP (European Commission DG-ENV)(import and export routines to build a secondary repository in support of [www.htap.org](http://www.htap.org)). A large number of specific projects have supported development of data and meta data reporting schemes in dialog with data providers (EU)(CREATE, ACTRIS and others).

```
NAS.data.ls <- readPSD_NAS(import.path.NAS)

# Read functions export data as a list to account for multiple files in a directory
dataPSD.NAS <- NAS.data.ls[[1]]

head(dataPSD.NAS)

##          starttime        endtime pressure (hPa) temperature (K)  9.14
## 1 2022-03-22 00:00:00 2022-03-22 01:00:00       646.33      299.72 474.24
## 2 2022-03-22 01:00:00 2022-03-22 01:59:59       646.83      299.25 84.12
## 3 2022-03-22 01:59:59 2022-03-22 03:00:00       646.58      298.76 0.00
## 4 2022-03-22 03:00:00 2022-03-22 04:00:00       647.00      298.46 0.00
## 5 2022-03-22 04:00:00 2022-03-22 04:59:59       646.83      298.20 0.00
## 6 2022-03-22 04:59:59 2022-03-22 06:00:00       647.08      297.82 0.00
##    9.47    9.82   10.2   10.6   10.9   11.3   11.8   12.2   12.6
## 1 957.28 2867.13 3583.47 5114.35 6310.64 7191.34 7549.04 8580.99 8822.77
## 2 298.20  916.45 1245.15 1485.14 2468.77 2897.71 3331.94 3617.07 4289.60
## 3 120.74  189.00  529.25  605.65  796.45 1144.47 1584.89 1746.31 2045.49
## 4   0.00   94.34  133.73   75.24  198.43  312.59  320.85  275.00  400.82
## 5   0.00   31.36   25.14   40.92  168.13  238.74  299.34  346.10  351.32
## 6   0.00    0.00   25.07  122.19  151.01  210.47  278.15  342.93  542.03
##    13.1    13.6   14.1   14.6   15.1   15.7   16.3   16.8   17.5
## 1 7952.76 8010.82 8162.86 7990.85 7451.82 7584.54 7593.25 7594.88 7001.90
## 2 4424.07 4447.83 4597.11 4500.57 4620.33 4802.66 4865.29 4819.59 5048.73
## 3 2123.54 2227.72 2054.91 2302.66 2327.27 2574.78 2489.49 2572.97 2945.02
## 4  441.17  583.74  626.55  646.45  752.25  845.95  818.85  881.72 1049.40
## 5  475.65  438.01  612.68  584.59  726.27  692.28  805.44  880.78  923.34
## 6  468.29  766.36  774.15  798.08  919.40  972.99 1031.76 1092.83 1195.97
##    18.1    18.8   19.5   20.2   20.9   21.7   22.5   23.3   24.1
## 1 7125.60 7862.48 8124.80 8159.64 8364.12 8668.43 9002.40 9461.98 9622.86
## 2 5513.54 5543.39 5945.24 6631.56 6552.99 7130.38 7386.48 7614.73 7806.07
## 3 3080.90 3204.40 3573.71 3759.66 4030.89 4260.40 4499.01 4618.08 4902.01
## 4 1049.61 1210.46 1189.02 1250.51 1195.23 1263.97 1262.21 1328.49 1260.05
## 5  997.21 1153.40 1169.85 1226.61 1239.19 1358.63 1385.03 1447.41 1496.10
## 6 1343.78 1458.61 1407.93 1530.73 1582.33 1734.30 1774.63 1756.64 1859.80
##    25     25.9   26.9   27.9   28.9     30   31.1   32.2
## 1 9946.65 10164.08 10489.97 10751.10 10815.08 10605.00 10928.09 10570.33
## 2 8382.28  8610.70  8977.47  8990.91  9017.20  9184.89  9058.58  8908.22
## 3 5232.13  5463.19  5566.40  5534.47  5708.35  5517.94  5529.11  5402.95
## 4 1305.21  1373.60  1372.72  1341.94  1378.23  1410.03  1323.68  1346.79
## 5 1459.50  1536.34  1602.51  1622.83  1670.06  1636.87  1661.84  1692.39
## 6 1908.20  2064.13  2066.88  2153.87  2184.21  2167.84  2311.34  2311.05
##    33.4    34.6   35.9   37.2   38.5     40   41.4   42.9   44.5
## 1 10358.50 9783.52 9459.79 8558.29 7695.16 6851.74 5834.16 4942.83 4192.25
## 2 8438.41 8037.41 7532.57 7088.88 6175.92 5608.94 4724.73 4034.35 3385.69
## 3 4980.05 4867.38 4367.58 3831.24 3402.95 2974.85 2467.29 2100.91 1787.02
## 4 1428.47 1320.27 1200.93 1190.69 1150.40 1097.74 982.27 910.10 800.29
## 5 1676.72 1646.94 1566.61 1531.97 1458.84 1378.62 1266.97 1189.41 1029.79
## 6 2285.59 2436.51 2321.06 2303.95 2236.54 2069.25 1980.24 1747.04 1582.02
```

```

##      46.1    47.8    49.6    51.4    53.3    55.2    57.3    59.4    61.5    63.8
## 1 3382.34 2716.13 2182.88 1793.04 1464.58 1209.39 998.06 848.05 734.84 592.79
## 2 2784.91 2355.69 1772.08 1507.75 1253.15 1031.68 854.03 758.11 595.86 523.25
## 3 1423.36 1228.62 971.92 828.83 676.32 537.27 482.39 431.73 326.24 292.78
## 4 754.27 612.65 572.04 513.85 407.18 363.87 281.49 258.54 228.20 192.09
## 5 900.15 769.38 664.89 586.86 527.89 403.64 344.26 297.05 259.85 248.29
## 6 1388.00 1162.01 1037.57 901.58 715.39 633.97 520.10 452.40 379.16 336.34
##      66.1    68.5     71    73.7    76.4    79.1     82    85.1    88.2    91.4    94.7
## 1 512.72 445.46 378.32 318.03 290.38 284.55 252.50 260.34 251.02 273.03 214.79
## 2 449.11 415.56 338.35 324.20 283.20 251.22 217.34 224.30 231.22 236.16 241.40
## 3 247.59 220.45 185.24 181.72 189.66 174.19 179.05 163.21 191.91 181.62 226.92
## 4 171.30 169.45 163.22 155.08 177.27 178.84 179.88 182.70 171.43 184.97 215.76
## 5 217.41 197.53 161.24 159.57 178.57 168.03 160.96 162.04 184.80 183.87 181.94
## 6 280.22 261.75 232.72 202.27 217.25 203.28 195.96 203.14 209.34 204.90 221.08
##      98.2   101.8   105.5   109.4   113.4   117.6   121.9   126.3   131   135.8   140.7
## 1 258.38 259.50 256.63 268.92 259.48 258.36 280.98 289.10 302.29 298.64 321.96
## 2 244.99 241.06 253.38 269.55 286.54 308.75 283.43 329.53 308.09 333.24 350.34
## 3 192.55 212.90 217.24 215.47 232.49 232.15 248.19 245.20 264.20 252.14 262.13
## 4 204.90 207.46 223.79 208.16 201.93 246.67 232.52 236.46 265.16 293.46 278.25
## 5 176.06 216.26 226.13 227.97 230.01 247.26 247.21 256.99 296.23 264.36 287.18
## 6 244.08 234.17 265.16 264.20 260.05 271.70 287.46 316.44 309.72 320.14 308.20
##      145.9   151.2   156.8   162.5   168.5   174.7   181.1   187.7   194.6   201.7   209.1
## 1 335.77 353.06 328.67 362.97 360.43 363.98 350.93 346.04 332.69 320.46 298.03
## 2 329.74 352.83 367.66 350.14 357.34 364.43 327.49 334.80 338.99 293.30 288.43
## 3 290.72 276.36 318.40 294.14 301.60 310.36 297.91 285.13 275.97 266.37 233.51
## 4 281.34 291.47 291.63 275.51 286.84 307.70 264.72 247.35 218.87 204.69 159.03
## 5 273.42 293.82 296.25 292.59 307.69 297.63 286.49 273.43 247.65 197.44 170.20
## 6 311.86 322.37 339.79 318.80 334.50 342.54 300.79 297.08 250.80 249.10 211.09
##      216.7   224.7   232.9   241.4   250.3   259.5   269   278.8   289   299.6   310.6
## 1 261.44 243.50 190.16 151.17 123.31 92.10 72.33     0     0     0     0
## 2 249.12 208.33 170.19 147.77 115.52 91.64 74.70     0     0     0     0
## 3 210.80 169.81 144.35 118.50 88.52 80.92 59.73     0     0     0     0
## 4 143.56 110.82 90.40 78.33 53.16 38.25 30.68     0     0     0     0
## 5 150.52 120.76 101.64 68.88 58.16 44.93 36.39     0     0     0     0
## 6 168.26 141.73 117.16 85.99 76.30 55.52 42.99     0     0     0     0
##      numflag, no unit
## 1          0
## 2          0
## 3          0
## 4          0
## 5          0
## 6          0

```

### 3 Running multimodal

Let's run multimodal on an example dataset using a Brechtel SEMS (Model 2002). Note the log path will need to be changed to whatever location you'd like it sent to!

#### 3.1 Example 1 - Laboratory Data

```

# Frequency is null here because I already grouped data above
result <- multimodal.fitting(dataPSD.BMI,
                               log.path = log.path,

```

```

frequency = NULL,
labeling = T,
max.iterations = 20,
max.modes = 6,
lower.limit = 10,
upper.limit = 1500,
NMRSE.threshold = 0.05,
FVU.threshold = 20,
verbose = T)

## [1] "Current Dataset Time: 2023-10-31 22:15:23 UTC"
## [1] "Dataset sampling frequency is 2.4 min"
## [1] "2023-10-31 22:15:23: Current Loop Iteration: 1, Remaining Variance: 94.93%, Number of Modes: 1"
## [1] "2023-10-31 22:15:23: Current Loop Iteration: 2, Remaining Variance: 3.93%, Number of Modes: 2"
## [1] "2023-10-31 22:15:23: Current Loop Iteration: 3, Remaining Variance: 2.57%, Number of Modes: 3"
## [1] "2023-10-31 22:15:23: Current Loop Iteration: 4, Remaining Variance: 1.63%, Number of Modes: 4"
## [1] "2023-10-31 22:15:23: Current Loop Iteration: 5, Remaining Variance: 1.34%, Number of Modes: 5"
## [1] "2023-10-31 22:15:23: Current Loop Iteration: 6, Remaining Variance: 1.3%, Number of Modes: 6"
## [1] "Concentration RMSE: 2132.57 n/cc"

# As there is only 1 data file for this set, we will flatten the list

result <- flatten(result)

```

## 3.2 Outputs

The first element of result is a pass flag i.e. T or F

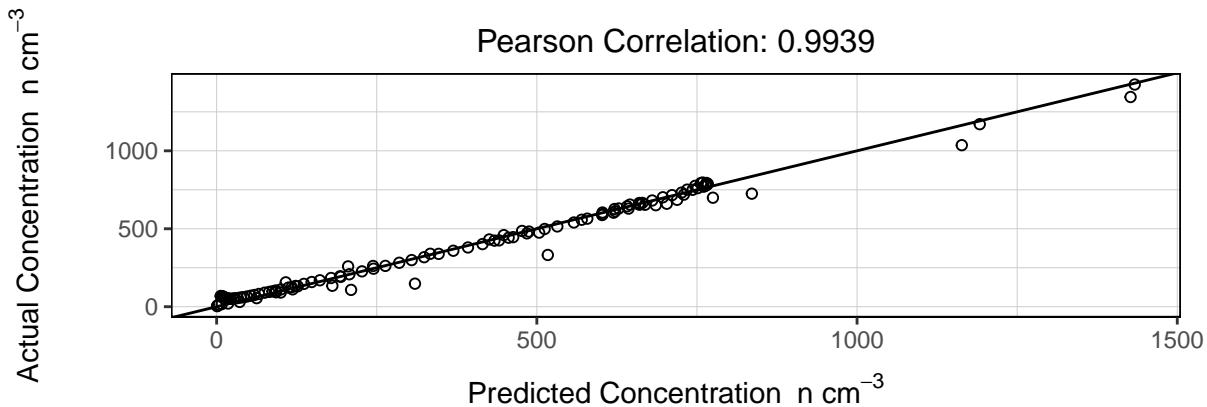
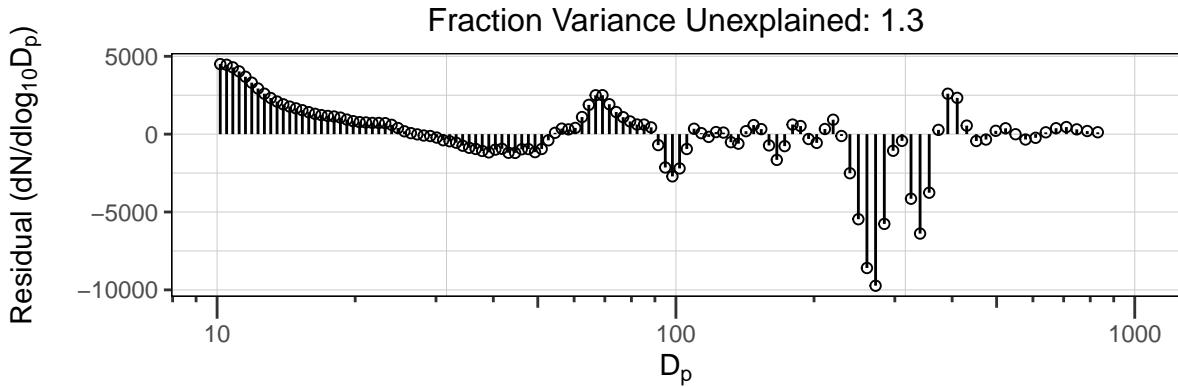
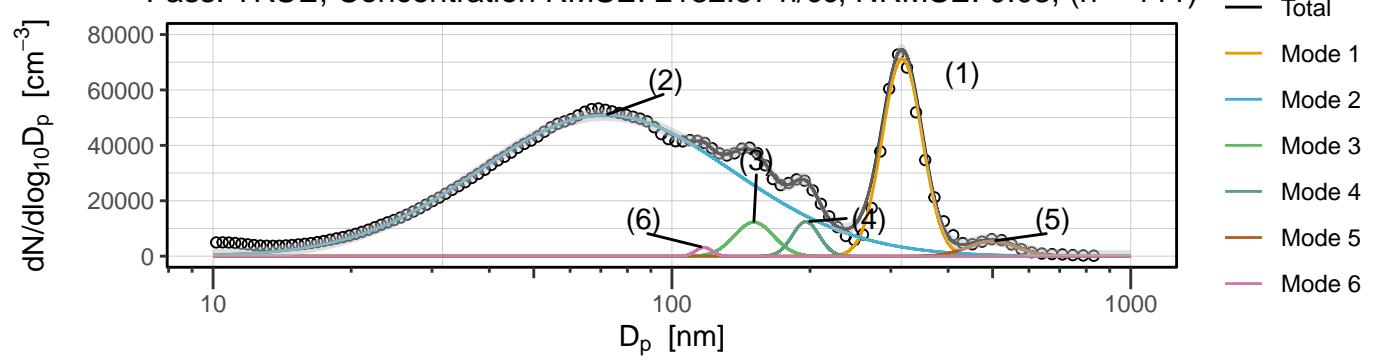
```
result$pass
```

```
## [1] TRUE
```

The second is the plot which consists of three panels

2023-10-31 22:15:23 – 2023-11-01 02:39:36

Pass: TRUE, Concentration RMSE: 2132.57 n/cc, NRMSE: 0.03, (n = 111)



The remaining outputs are predicted data, the data used to plot curves, and evaluation parameters

```
head(result[[3]])
```

	D <sub>p</sub>	Predicted dN/dlogD <sub>p</sub>	Predicted dN	Actual dN	dN/dlogD <sub>p</sub>	Actual dN
## 1	10.16	453.91	6.301079	4952.512	68.74969	
## 2	10.49	529.09	7.117198	4985.419	67.06273	
## 3	10.82	612.31	8.465744	4903.316	67.79281	
## 4	11.17	709.75	9.777611	4740.169	65.30121	
## 5	11.53	820.21	11.251357	4507.124	61.82717	
## 6	11.90	944.94	12.899759	4250.884	58.03054	

```

##      Residual dNdlogDp Residual dN      Ratio
## 1        4498.602    62.44861 0.09165247
## 2        4456.329    59.94553 0.10612748
## 3        4291.006    59.32707 0.12487672
## 4        4030.419    55.52360 0.14973093
## 5        3686.914    50.57581 0.18198080
## 6        3305.944    45.13078 0.22229260

head(result[[4]])

##      Dp Mode 1 Mode 2 Mode 3 Mode 4 Mode 5 Mode 6 dNdlogDp
## 1 10.00    0 420.26    0    0    0    0    0 420.26
## 2 10.01    0 422.31    0    0    0    0    0 422.31
## 3 10.02    0 424.37    0    0    0    0    0 424.37
## 4 10.03    0 426.43    0    0    0    0    0 426.43
## 5 10.04    0 428.50    0    0    0    0    0 428.50
## 6 10.05    0 430.58    0    0    0    0    0 430.58

head(result[[5]])

##      Mode Label      N      GSD      Dpg      Max Mode Lower Upper Width
## 1    Mode 1 7709.7021 1.104493 317.61847 72801.737 311.03 249.85 451.56 13
## 2    Mode 2 35219.1406 1.888153 71.61388 53335.797 69.18 13.51 105.61 62
## 3    Mode 3 1299.9919 1.102360 150.90879 12544.712 147.69 126.94 172.59 8
## 4    Mode 4 906.6612 1.069269 195.75567 12079.366 194.62 165.93 272.39 12
## 5    Mode 5 715.3382 1.128914 499.31587 5631.458 497.83 430.34 830.76 13
## 6    Mode 6 140.9658 1.042290 117.38486 2934.445 117.86 98.26 136.85 9
##      BIC      RSS      TSS      R2 N T pval GSD T pval Dpg T pval
## 1 276.9295 150254441 8174258916 0.9816186 5e-12 2.3e-22 2.16e-22
## 2 1087.2011 88575112 19969539592 0.9955645 1e-65 1.1e-75 1.16e-73
## 3 152.9817 4783910 93721539 0.9489561 8e-07 2.7e-12 1.13e-12
## 4 262.9294 210120965 618259998 0.6601414 4e-03 3.1e-13 3.04e-13
## 5 212.3369 1489699 53034863 0.9719109 2e-10 2.0e-19 5.82e-20
## 6 179.0575 13928215 32875106 0.5763294 4e-02 2.1e-10 2.12e-10

result[[6]]

##      Pearson Correlation      RMSE      NRMSE dN RMSE      dN NRMSE Students T Test
## [1,]              0.9939 2132.57 0.02935411 37.15 0.02613263 0.8524
##      Chi-Squared
## [1,]          0.2391

```

### 3.3 Example 2 - Storm Peak Laboratory

```

## [1] "Current Dataset Time: 2022-03-23 06:03:41 UTC"
## [1] "Dataset sampling frequency is 5 min"
## [1] "2022-03-23 06:03:41: Error, please modify lower and upper limits to accomodate data set"

```

Notice the failure message? This is because the dataset begins for bin diameter 9.14. Now we can retry with adjusted limits.

```

## [1] "Current Dataset Time: 2022-03-23 06:03:41 UTC"
## [1] "Dataset sampling frequency is 5 min"
## [1] "2022-03-23 06:03:41: Current Loop Iteration: 1, Remaining Variance: 1.11%, Number of Modes: 1"
## [1] "2022-03-23 06:03:41: Current Loop Iteration: 2, Remaining Variance: 0.82%, Number of Modes: 2"
## [1] "Concentration RMSE: 354.11 n/cc"

```

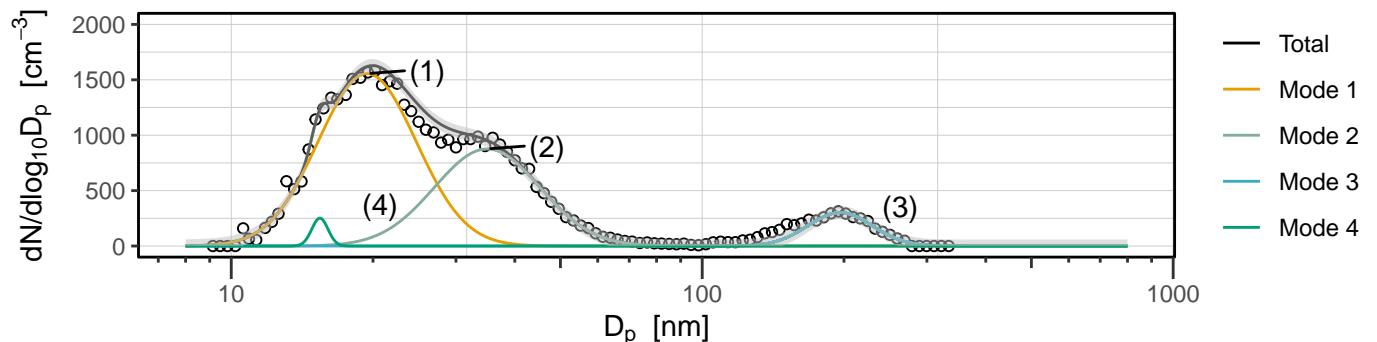
For this file there is a NPF event, but currently the averaging across the entire day removes all temporal

variation. We will instead select times between 07:00 and 15:00 and use an hourly frequency.

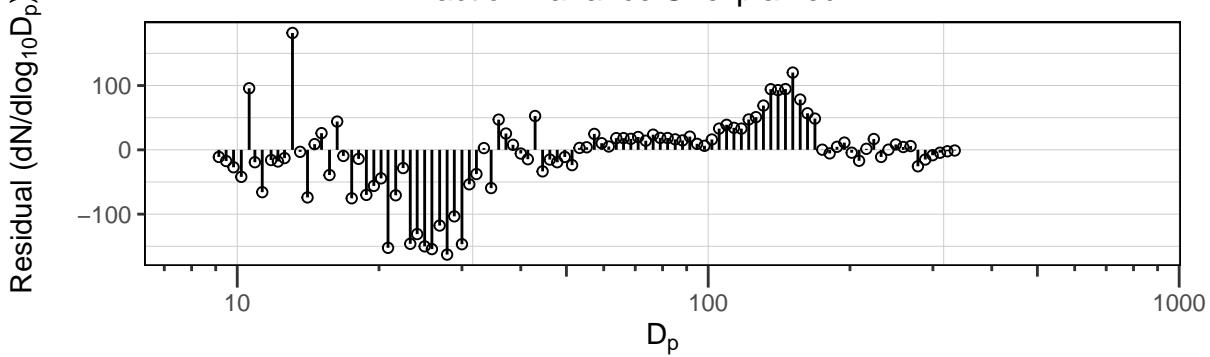
```
## $`2022-03-23 11:00:00`
```

2022-03-23 11:03:40 – 2022-03-23 11:28:41

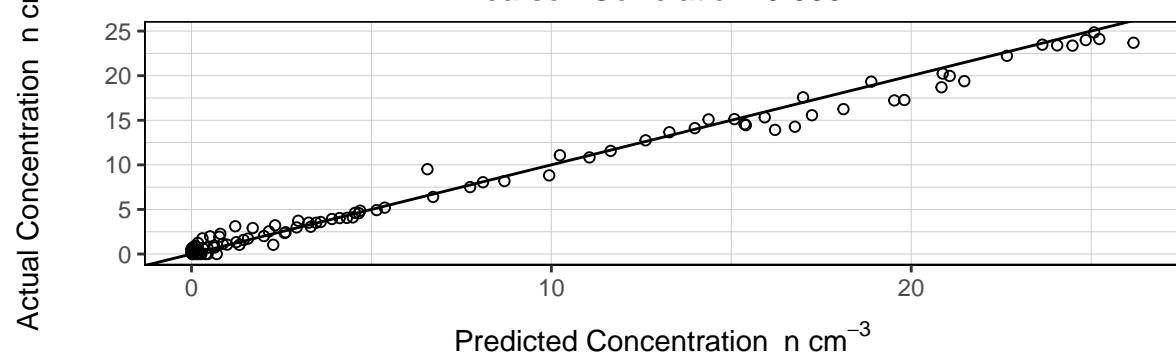
Pass: TRUE, Concentration RMSE: 59.11 n/cc, NRMSE: 0.04, (n = 6)



Fraction Variance Unexplained: 1.41



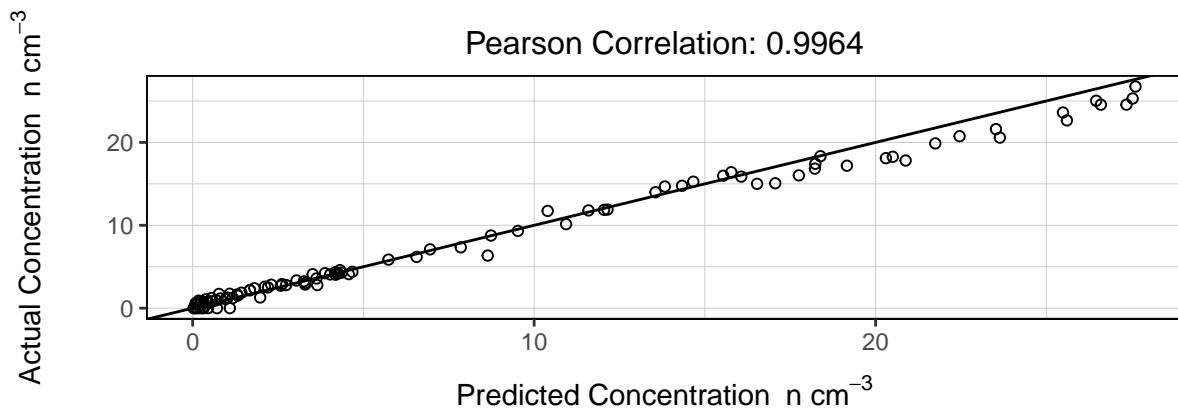
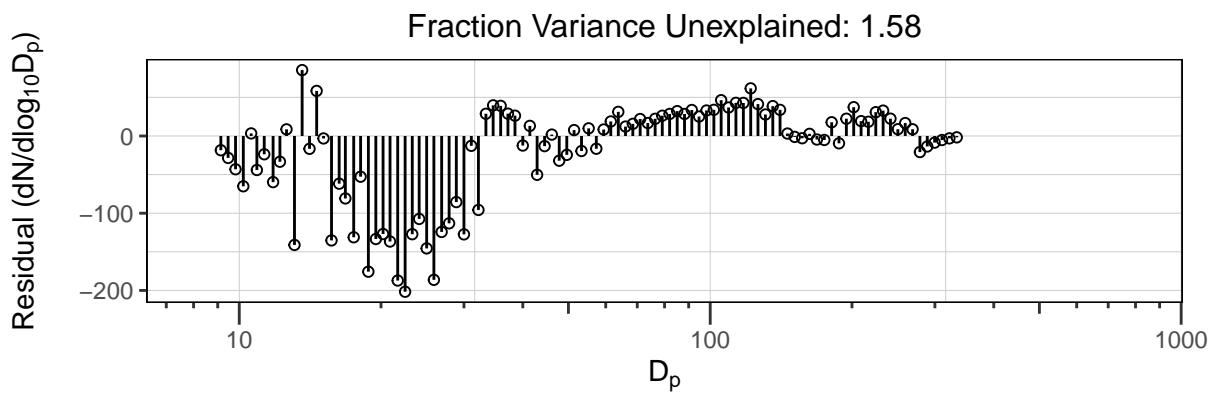
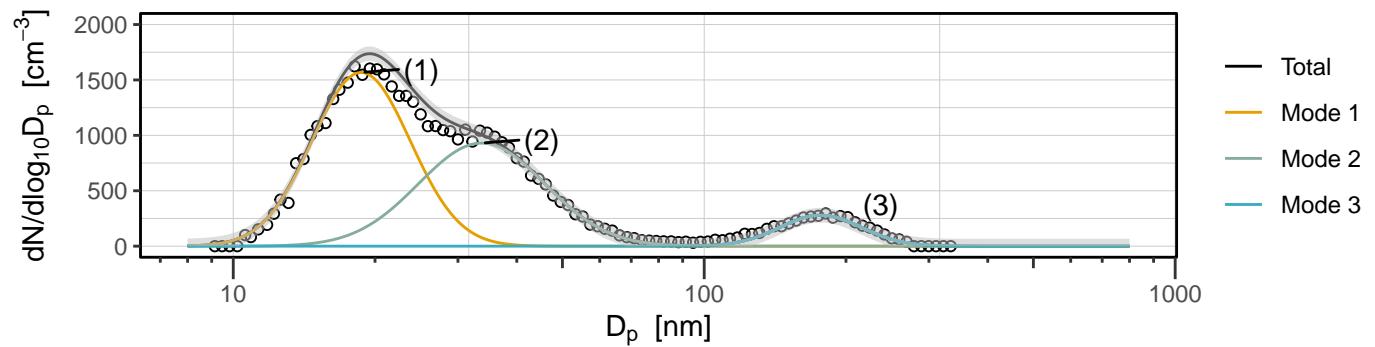
Pearson Correlation: 0.9954



```
##
```

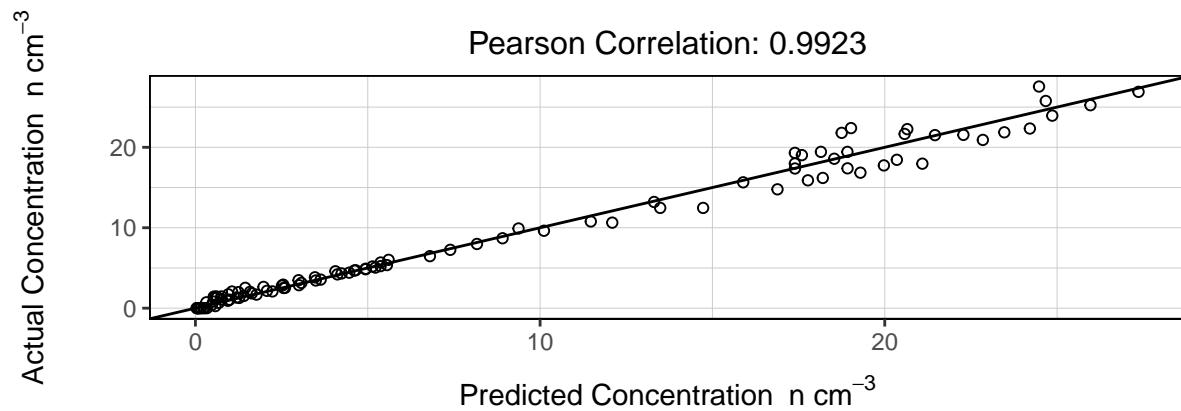
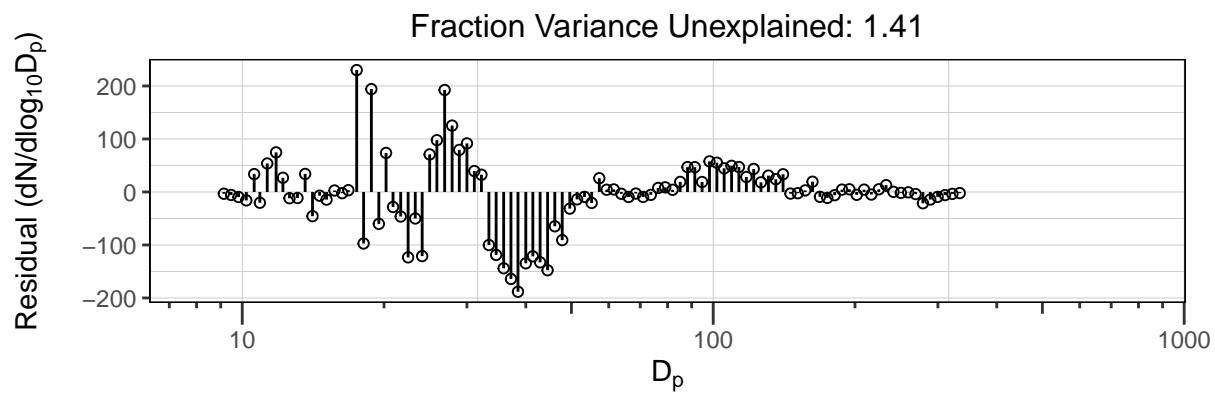
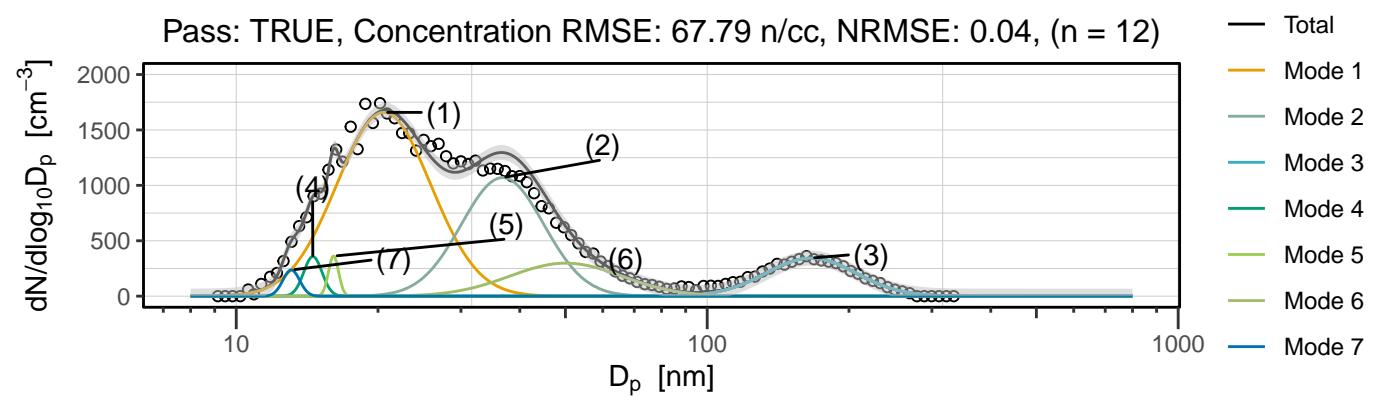
```
## $`2022-03-23 12:00:00`
```

2022-03-23 11:33:41 – 2022-03-23 12:28:41  
Pass: TRUE, Concentration RMSE: 66.16 n/cc, NRMSE: 0.04, (n = 12)



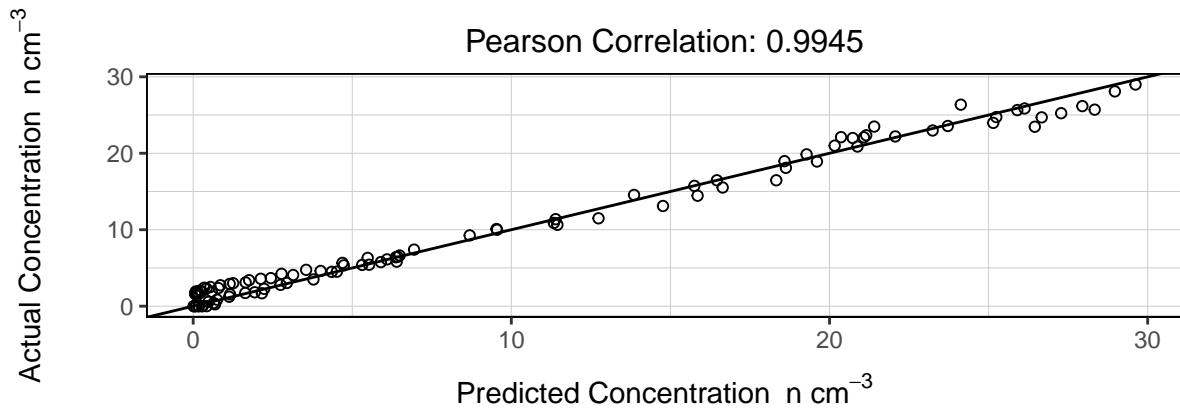
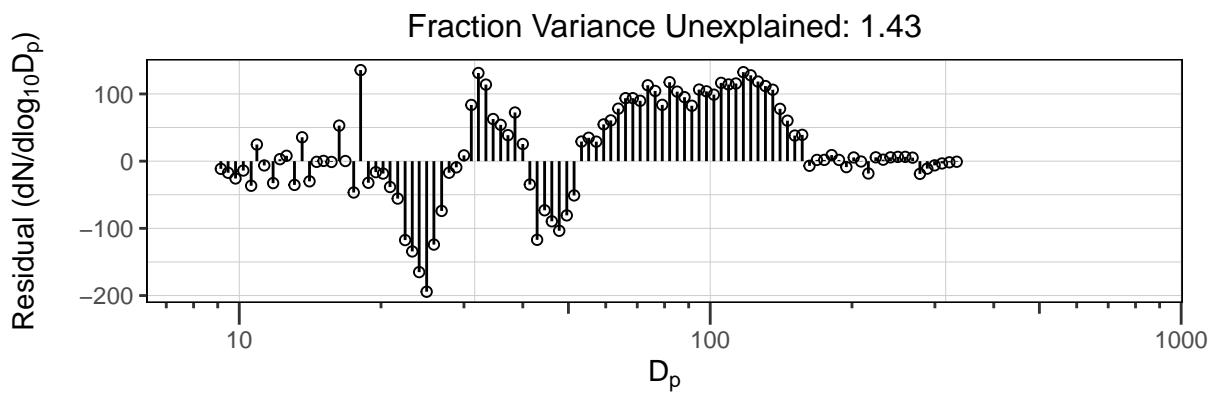
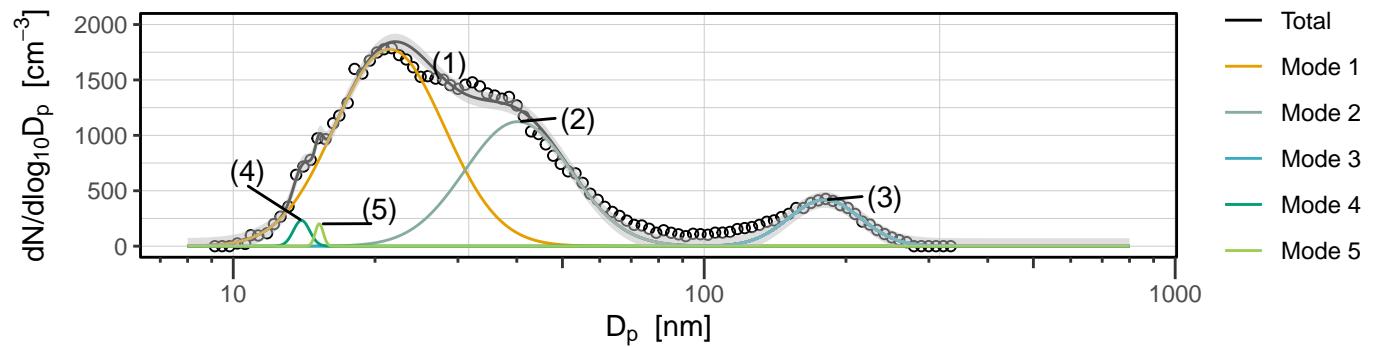
```
##  
## $`2022-03-23 13:00:00`
```

2022-03-23 12:33:41 – 2022-03-23 13:28:41  
 Pass: TRUE, Concentration RMSE: 67.79 n/cc, NRMSE: 0.04, (n = 12)



```
##  
## $`2022-03-23 14:00:00`
```

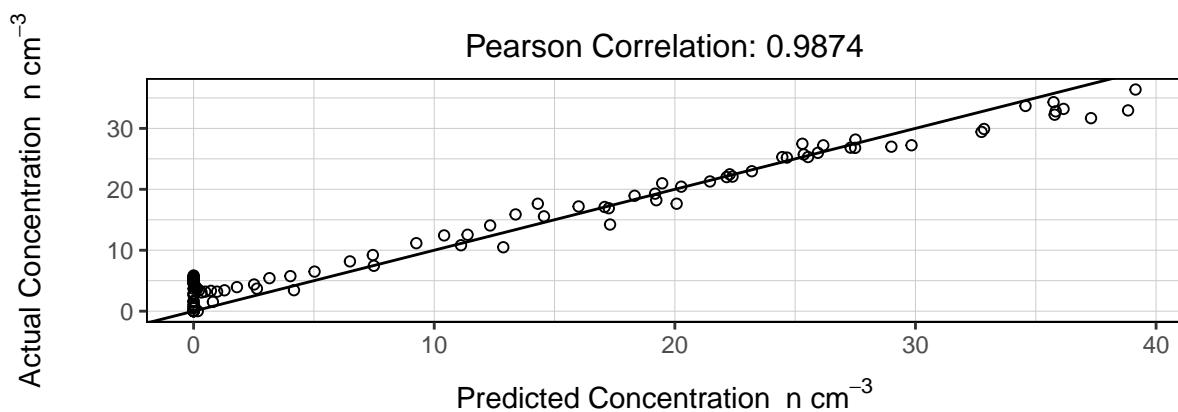
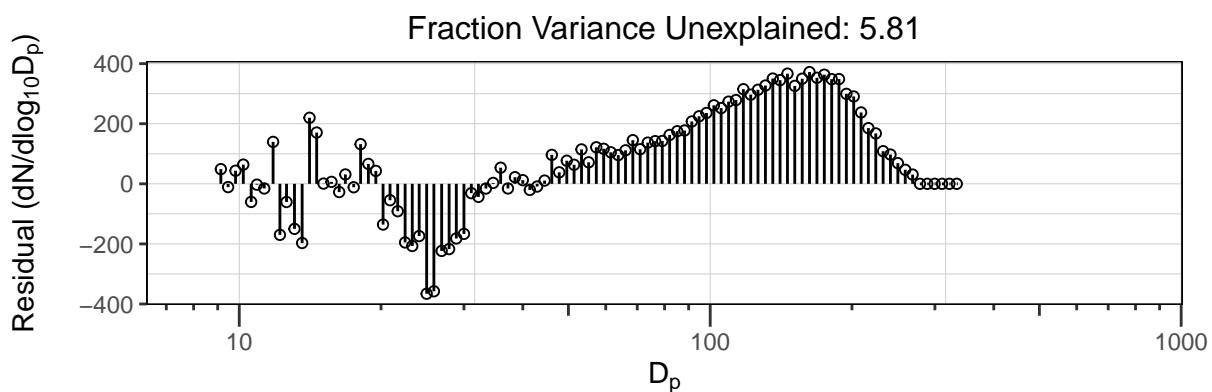
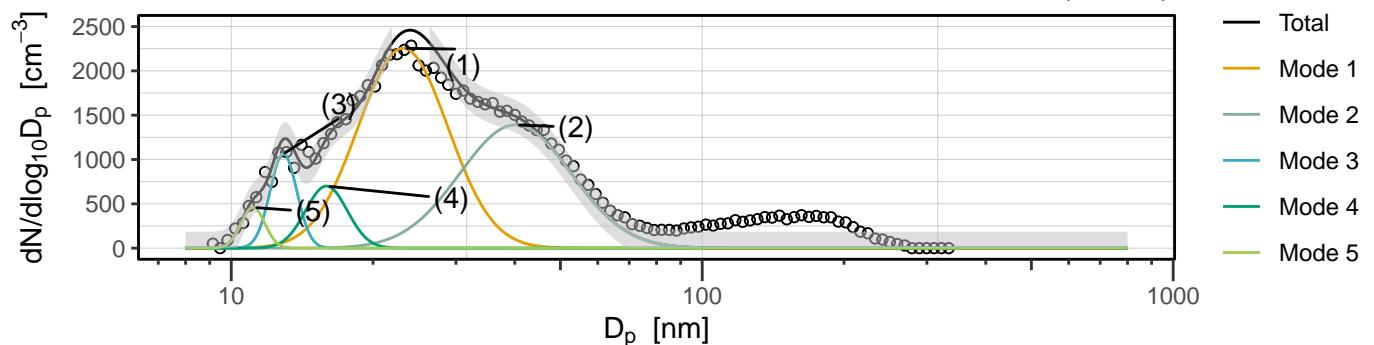
2022-03-23 13:33:40 – 2022-03-23 14:28:41  
 Pass: TRUE, Concentration RMSE: 72.09 n/cc, NRMSE: 0.04, (n = 12)



```
##  
## $`2022-03-23 15:00:00`
```

2022-03-23 14:33:40 – 2022-03-23 15:28:40

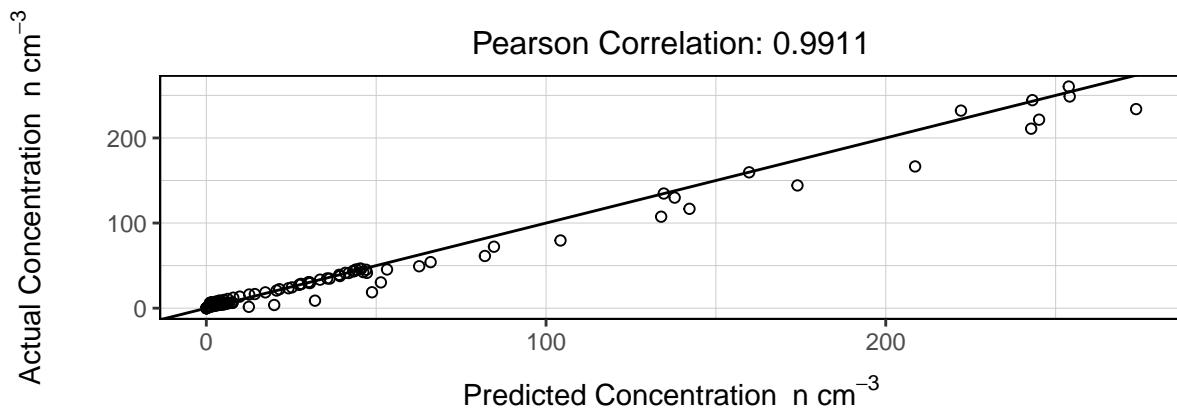
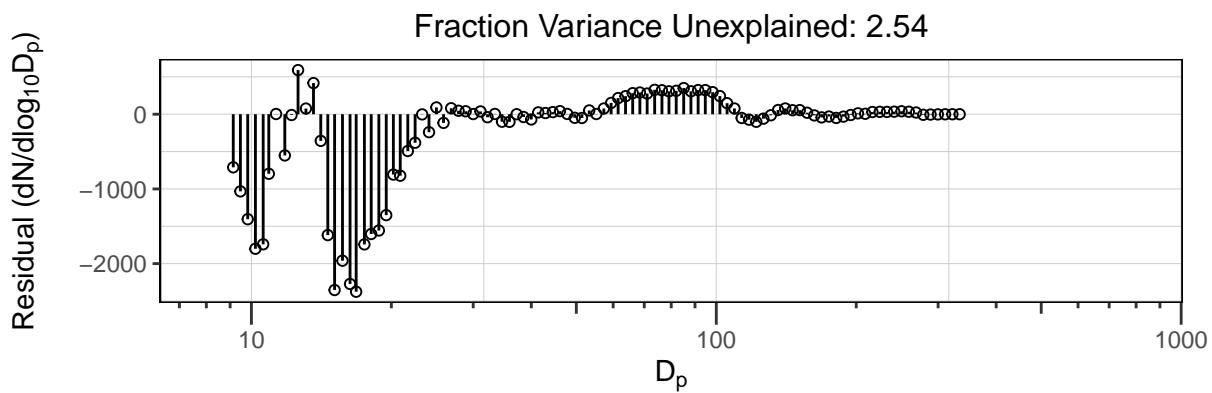
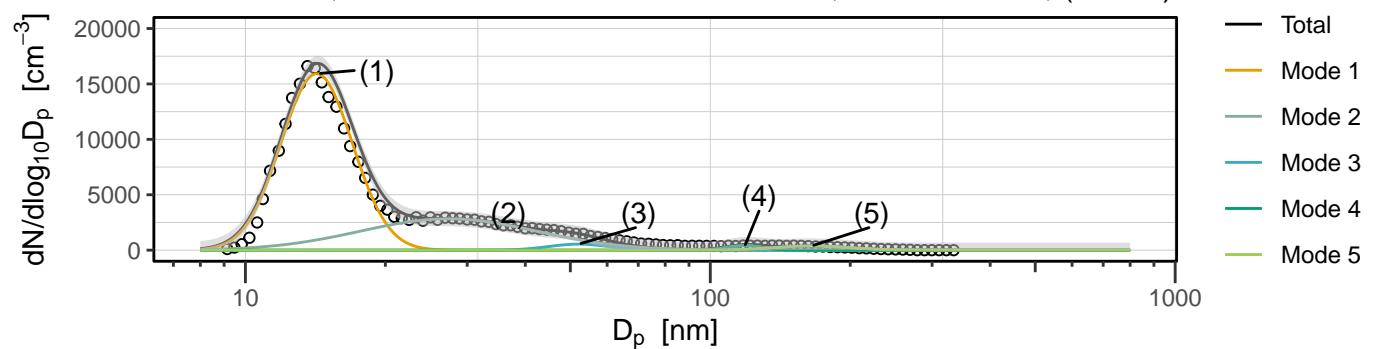
Pass: FALSE, Concentration RMSE: 185.32 n/cc, NRMSE: 0.08, (n = 12)



```
##  
## $`2022-03-23 16:00:00`
```

2022-03-23 15:33:40 – 2022-03-23 16:28:41

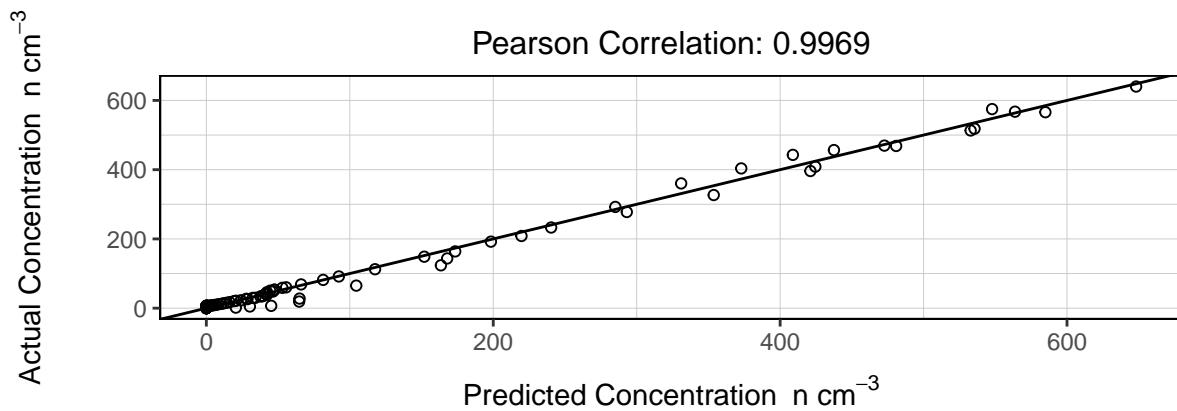
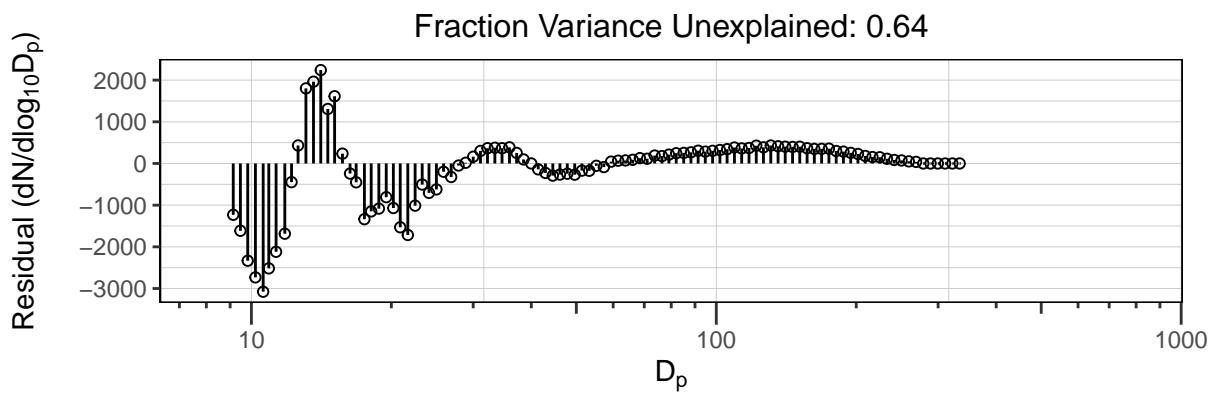
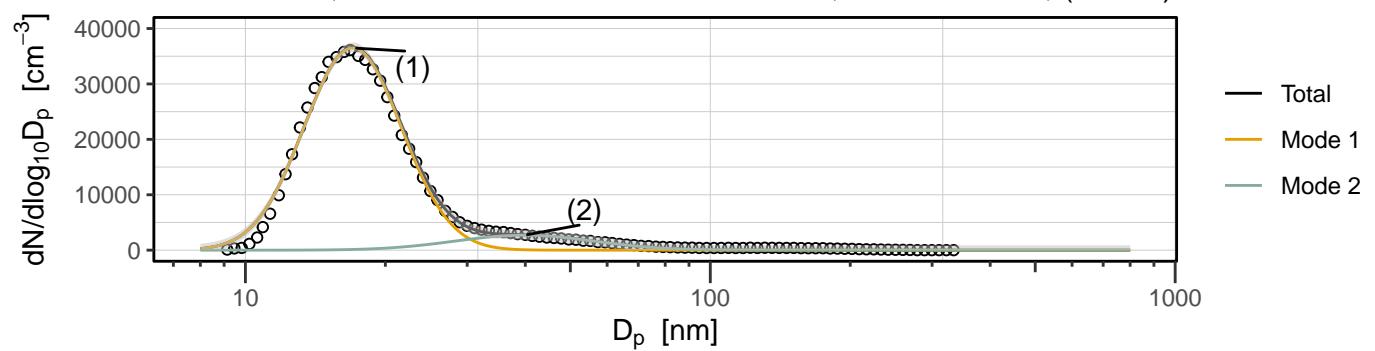
Pass: TRUE, Concentration RMSE: 684.64 n/cc, NRMSE: 0.04, (n = 12)



```
##  
## $`2022-03-23 17:00:00`
```

2022-03-23 16:33:41 – 2022-03-23 17:28:41

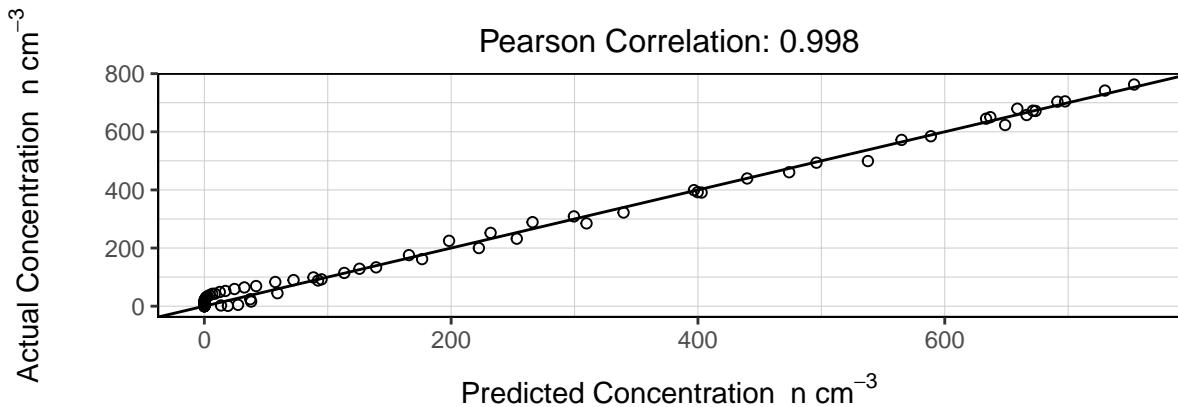
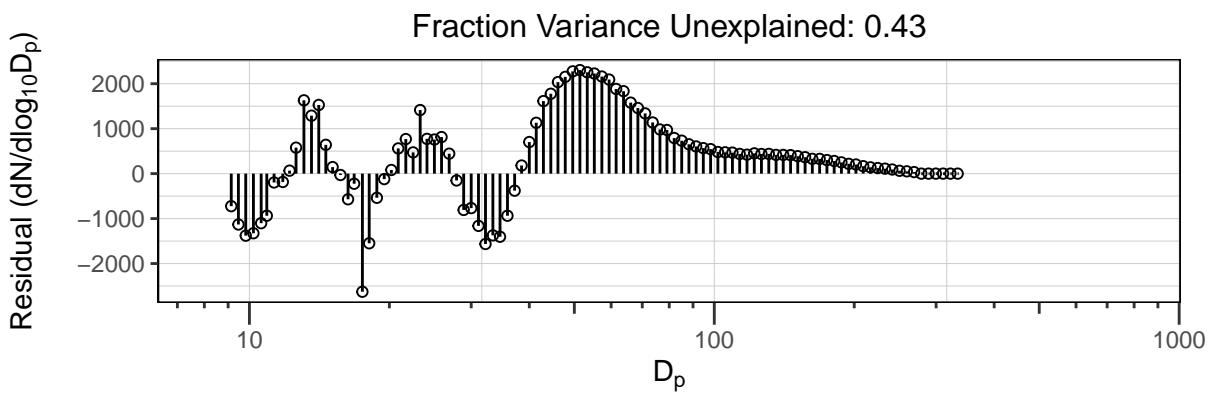
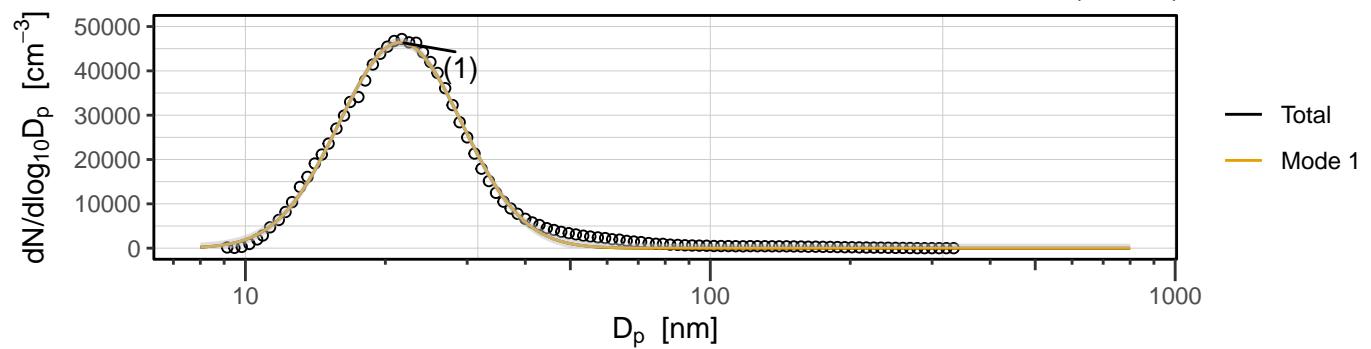
Pass: TRUE, Concentration RMSE: 864.42 n/cc, NRMSE: 0.02, (n = 12)



```
##  
## $`2022-03-23 18:00:00`
```

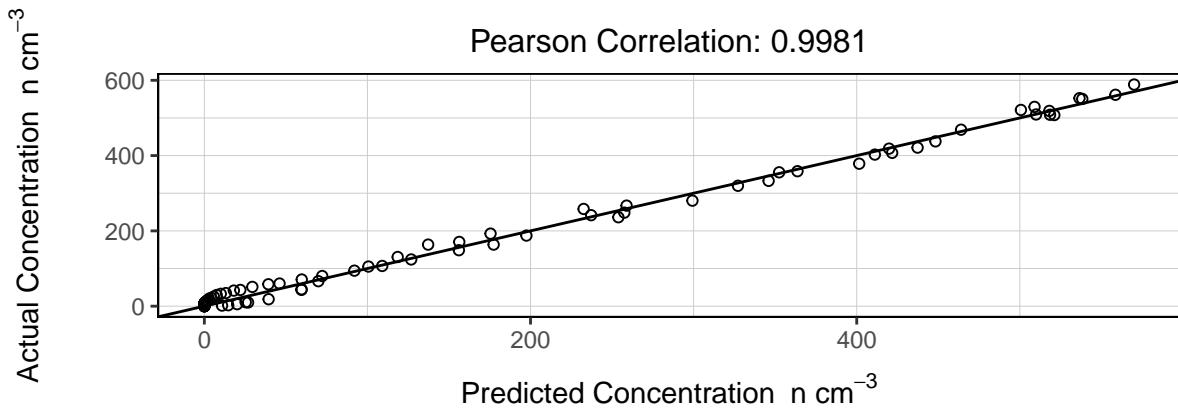
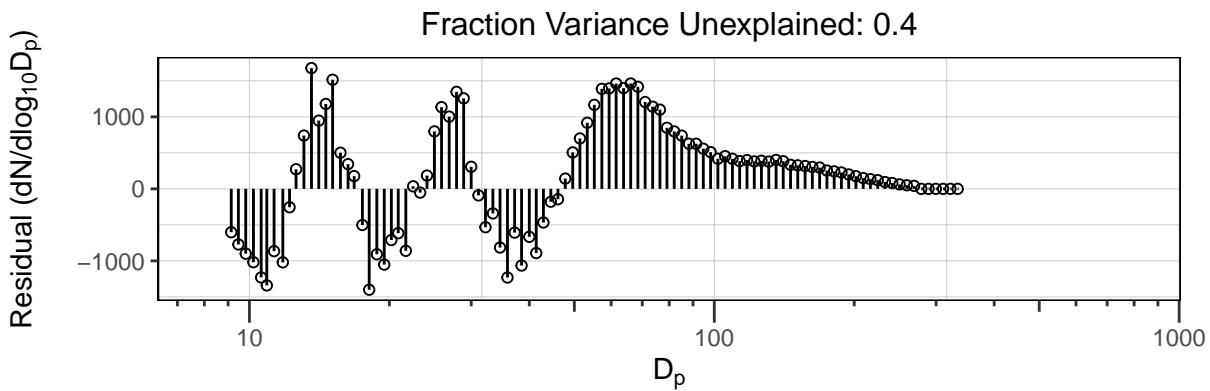
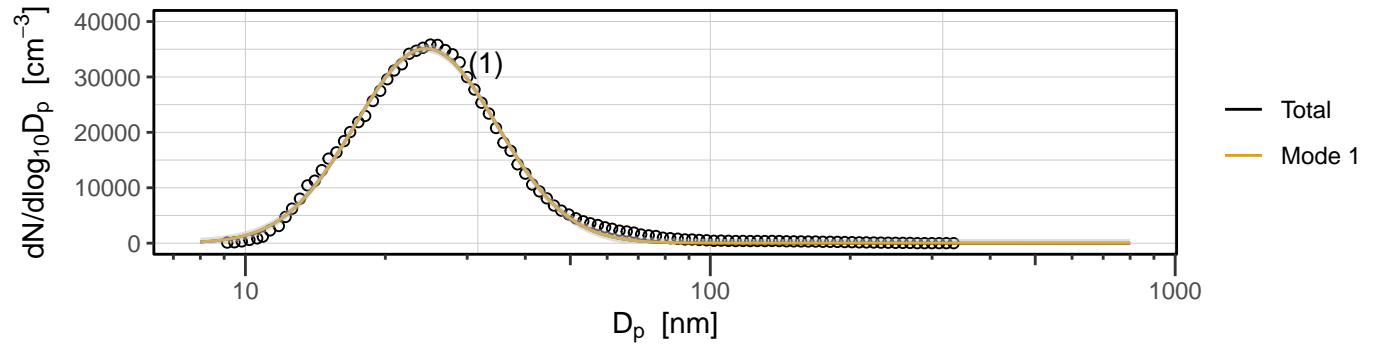
2022-03-23 17:33:41 – 2022-03-23 18:28:40

Pass: TRUE, Concentration RMSE: 1035.04 n/cc, NRMSE: 0.02, (n = 12)



```
##  
## $`2022-03-23 19:00:00`
```

2022-03-23 18:33:40 – 2022-03-23 18:58:41  
 Pass: TRUE, Concentration RMSE: 764.08 n/cc, NRMSE: 0.02, (n = 6)



Note - for higher resolution scans, the variation within the scan may be too high to capture. The following is an example.

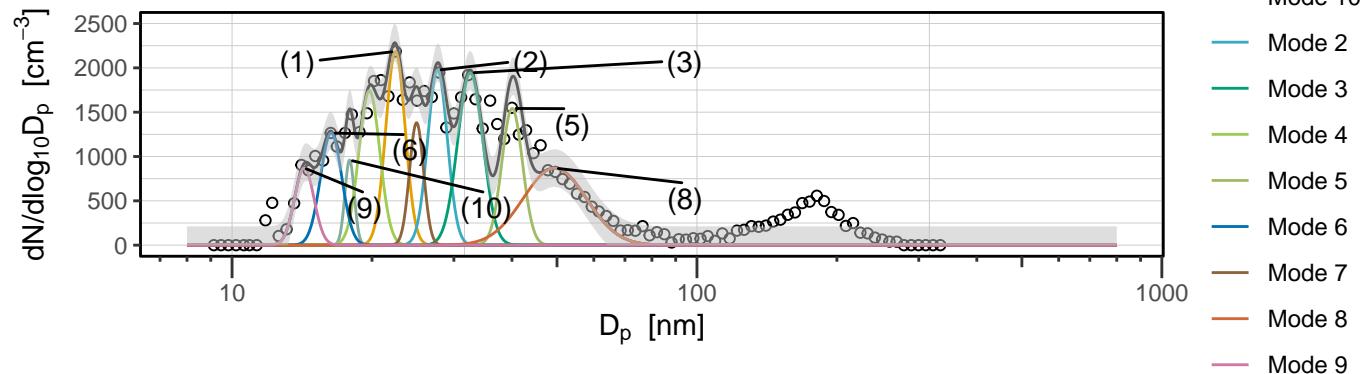
```
## $`2022-03-23 14:05:00`  

## Warning: ggrepel: 2 unlabeled data points (too many overlaps). Consider  

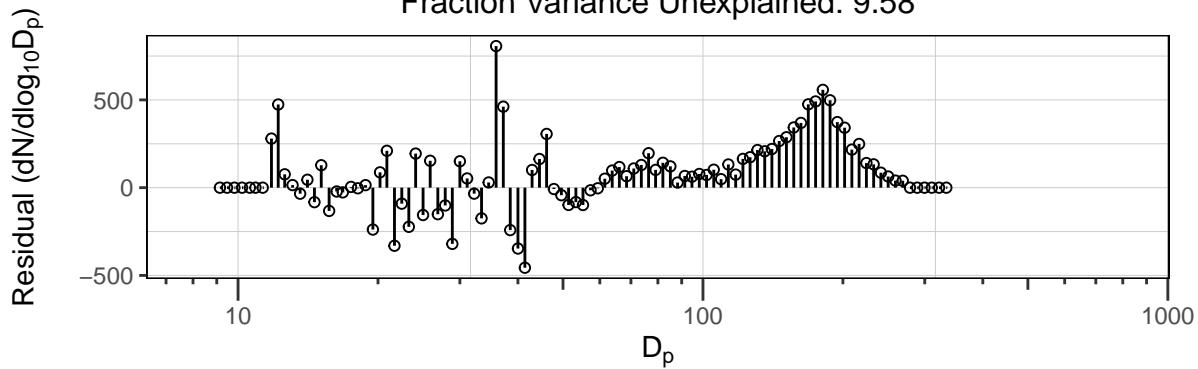
## increasing max.overlaps
```

2022-03-23 14:03:40 – 2022-03-23 14:03:40

Pass: FALSE, Concentration RMSE: 212.49 n/cc, NRMSE: 0.1, (n = 1)



Fraction Variance Unexplained: 9.58



Pearson Correlation: 0.9633

