ATM515 Aerosol Physics

Lecture 4: Characterization of aerosols
Part II

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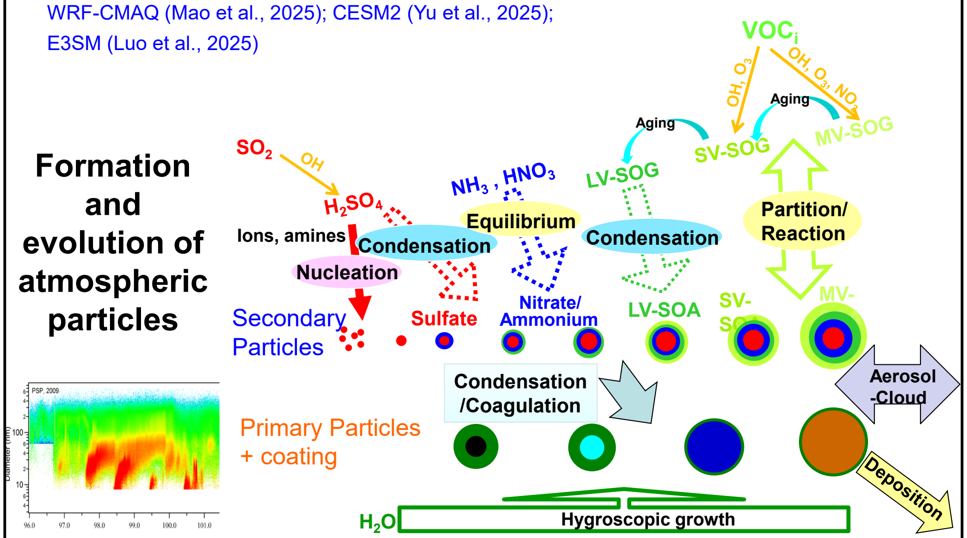
Advanced Particle Microphysics (APM) Model for 3-D models

→GEOS-Chem (Yu and Luo, 2009); WRF-Chem (Luo and Yu, 2011);
NAQPMS (Chen et al., 2017); IAP-AACM (Chen et al., 2021);
WRF-CMAQ (Mao et al., 2025); CESM2 (Yu et al., 2025);
E3SM (Luo et al., 2025)



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The number of bins and size range (dry diameter) for various types of particles are:

Secondary particles (composed of sulphate, nitrate, ammonium, and secondary organic species): 40 bins (0.0012–12 μm)

Sea salt: 20 bins (0.012–12 μm)

Dust: 15 bins (0.03–50 μm)

Black carbon: 15 bins (0.01–1 μm)

Primary organic carbon:15 bins (0.01–1 μm)

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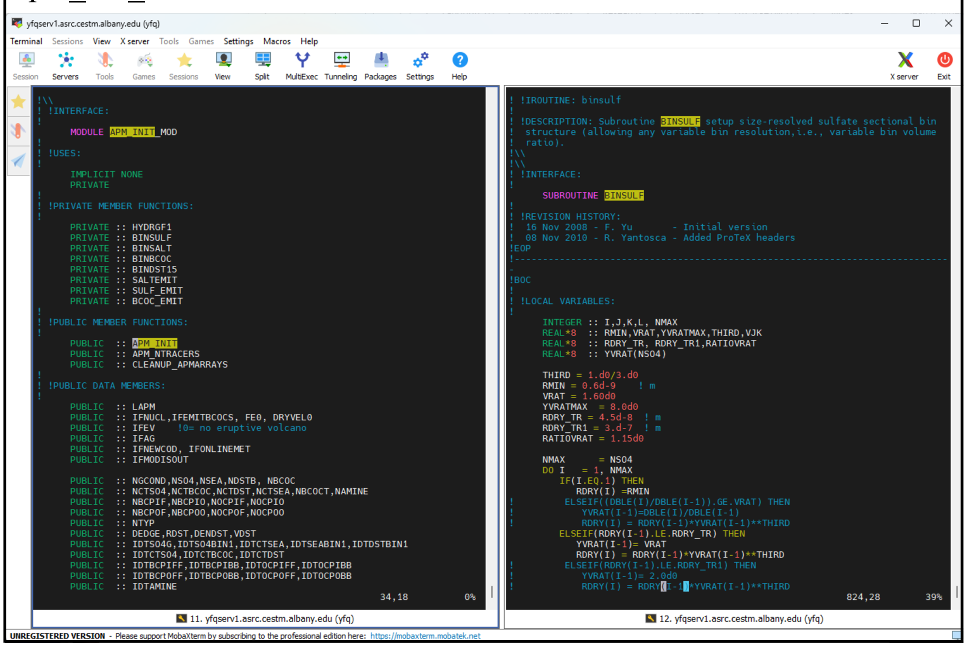
APM sets up bin structures for various type of particles at apm_init_mod.f90



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Parameters often used in characterizing an aerosol size distribution

- MEAN (arithmetic average):

  The sum of all the particles sizes divided by the number of particles

$$\overline{d_p} = \frac{\sum d_p}{N} = \frac{\sum n_i d_{pi}}{\sum n_i} = \int_0^\infty d_p q(d_p) dd_p$$

- MEDIAN:
  - The diameter for which 50% of the total are smaller and 50% are larger; the diameter corresponds to a cumulative fraction of 50%
- MODE:
  - Most frequent size; setting the derivative of the frequency function to 0 and solving for d_p.
  - For a symmetrical distribution, the mean, median and mode have the same value.

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Mean size

The mean particle diameter, $\overline{D}_p$, of the population is

$$\overline{D}_p = \frac{\sum_{k=1}^{M} N_k D_k}{\sum_{k=1}^{M} N_k} = \frac{1}{N}\sum_{k=1}^{M} N_k D_k$$

Degree of the spread

The variance, σ^2, a measure of the spread of the distribution around the mean diameter $\overline{D}_p$, is defined by

$$\sigma^2 = \frac{\sum_{k=1}^{M} N_k (D_k - \overline{D}_p)^2}{\sum_{k=1}^{M} N_k} = \frac{1}{N}\sum_{k=1}^{M} N_k (D_k - \overline{D}_p)^2$$

A value of σ^2 equal to zero would mean that every one of the particles in the distribution has precisely diameter $\overline{D}_p$. An increasing σ^2 indicates that the spread of the distribution around the mean diameter D_p is increasing

$$\sigma^2 = \frac{\int_0^\infty (D_p - \overline{D}_p)^2 n_N(D_p)\, dD_p}{\int_0^\infty n_N(D_p)\, dD_p} = \frac{1}{N}\int_0^\infty (D_p - \overline{D}_p)^2 n_N(D_p)\, dD_p$$

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- GEOMETRIC MEAN:

  the Nth root of the product of N values

$$d_{pg} = \left(d_{p1}^{n_1} d_{p2}^{n_2} d_{p3}^{n_3} \ldots\right)^{1/N} = \left(\prod d_{pi}^{n(d_{pi})}\right)^{1/N}$$

Expressed in terms of $\ln(d_p)$

$$\ln d_{pg} = \frac{\sum n_i \cdot \ln d_{pi}}{N}$$

$n(d_p)$: n as a function of d_p

$$d_{pg} = \exp\left[\frac{\sum n_i \cdot \ln d_{pi}}{N}\right] = \exp\left[\frac{\int n(d_p) \cdot \ln d_p \cdot dd_p}{\int n(d_p) \cdot dd_p}\right]$$

- For a monodisperse aerosol, $\overline{d_p} = d_{pg}$
  otherwise, $\overline{d_p} > d_{pg}$
- Very commonly used because an aerosol system typically covers a wide size range from 0.001 to 1000 μm

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- **Count Mean Diameter**: based on **number** of particles.

$$\overline{d_{pn}} = \frac{\sum d_p}{N} = \frac{\sum n_i d_{pi}}{\sum n_i} = \int_0^\infty d_p n(d_p) dd_p$$

- **Mass Mean Diameter**: based on **mass** of particles.

$$\overline{d_{pm}} = \frac{\sum m_i d_{pi}}{\sum m_i} = \int_0^\infty d_p m(d_p) dd_p$$

Conversion

$$m = \rho_p \cdot n \cdot \upsilon_p = \rho_p \cdot n \cdot \frac{\pi}{6} d_p^3 = k_1 \cdot n \cdot d_p^3$$

Q: In addition to the representative size, what other aerosol property can we use to present the aerosol size distribution in a concise way?

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Size distribution based on different independent variables

$$n_N(D_p) = \frac{dN}{dD_p} \quad n_N^e(\ln D_p) = \frac{dN}{d\ln D_p} \quad n_N^\circ(\log D_p) = \frac{dN}{d\log D_p}$$

$$n_S(D_p) = \frac{dS}{dD_p} \quad n_S^e(\ln D_p) = \frac{dS}{d\ln D_p} \quad n_S^\circ(\log D_p) = \frac{dS}{d\log D_p}$$

$$n_V(D_p) = \frac{dV}{dD_p} \quad n_V^e(\ln D_p) = \frac{dV}{d\ln D_p} \quad n_V^\circ(\log D_p) = \frac{dV}{d\log D_p}$$

$$n_N(D_p)\, dD_p = \text{the number of particles per } cm^3 \text{ of air having diameters in the range } D_p \text{ to } D_p + dD_p$$

$$n_N^e(\ln D_p)\, d\ln D_p = \text{number of particles per } cm^3 \text{ of air in the size range } \ln D_p \text{ to } \ln D_p + d\ln D_p$$

n^o(logDp): Aerosol distribution as a functions of the base 10 logarithm logDp is more widely used in the field.

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Moments of the PSD

- Definition: The quantity proportional to particle size raised to a power; an integral aerosol property

$$M_n = \sum n_i(d_{pi}) \cdot d_{pi}^n = \int_0^\infty n(d_p) \cdot d_p^n \, dd_p$$

$n(d_p)$: n as a function of d_p

Q: What is M_o?

$$M_o = \sum n_i(d_{pi}) = \int_0^\infty n(d_p)\, dd_p$$

Q: What is M_1?
Q: What is M_1/M_0?
Q: What is M_2/M_0? M_3/M_0?
Q: Which is larger? M_1/M_0? $(M_2/M_0)^{1/2}$? $(M_3/M_0)^{1/3}$?

Zeroth moment M0: total concentration;
1st moment M1: M1/M0: number average particle diameter
2nd moment M2 is proportional to total surface area A (M2 = A/pi), $(M2/M0)^{1/2}$ = surface area mean diameter
3rd moment M3 is proportional to total volume V (M3 = 6V/pi): $(M3/M0)^{1/3}$ = volume mean diameter

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Normal Distribution

The normal distribution for a quantity u defined from $-\infty < u < \infty$ is given by

$$n(u) = \frac{N}{(2\pi)^{1/2}\sigma_u} \exp\left(-\frac{(u-\overline{u})^2}{2\sigma_u^2}\right)$$

where $\overline{u}$ is the mean of the distribution, σ_u^2 is the variance, and

$$N = \int_{-\infty}^{\infty} n(u)\, du$$

The normal distribution has the characteristic bell shape, with a maximum at $\overline{u}$. The standard deviation, σ_u, quantifies the width of the distribution, and 68% of the area below the curve is in the range $\overline{u} \pm \sigma_u$.

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Log-Normal Distribution

$u = \ln D_p$

$$n_N^e(\ln D_p) = \frac{dN}{d\ln D_p} = \frac{N_t}{(2\pi)^{1/2}\ln\sigma_g}\exp\left(-\frac{(\ln D_p - \ln \bar{D}_{pg})^2}{2\ln^2\sigma_g}\right)$$

$$n_N(D_p) = \frac{dN}{dD_p} = \frac{N_t}{(2\pi)^{1/2} D_p \ln\sigma_g}\exp\left(-\frac{(\ln D_p - \ln \bar{D}_{pg})^2}{2\ln^2\sigma_g}\right)$$

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$$n_N(D_p) = \frac{dN}{dD_p} \quad n_N^e(\ln D_p) = \frac{dN}{d\ln D_p} \quad n_N^{\circ}(\log D_p) = \frac{dN}{d\log D_p}$$

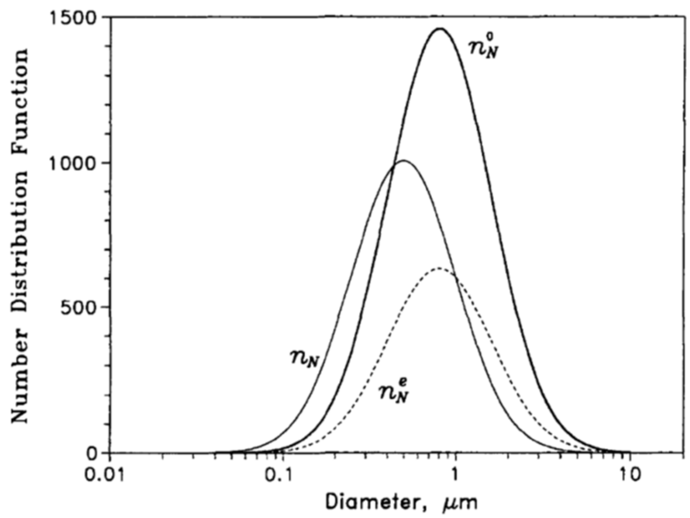

FIGURE 8.7 Aerosol distribution functions, $n_N(D_p)$, $n_N^{\circ}(\log D_p)$ and $n_N^e(\ln D_p)$ for a lognormally distributed aerosol distribution $\bar{D}_{pg} = 0.8$ μm and $\sigma_g = 1.5$ versus $\log D_p$. Even if all three functions describe the same aerosol population, they differ from each other because they use a different independent variable. The aerosol number is the area below the $n_N^{\circ}(\log D_p)$ curve.

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Properties of Log-Normal Distribution

$$n_N(D_p) = \frac{dN}{dD_p} = \frac{N}{(2\pi)^{1/2} D_p \ln\sigma_g} \exp\left(-\frac{(\ln D_p - \ln \overline{D}_{pg})^2}{2\ln^2\sigma_g}\right)$$

$$\boxed{\overline{D}_p = \overline{D}_{pg} \exp\left(\frac{\ln^2\sigma_g}{2}\right)}$$

D_{pg} is the median diameter

$$n_S(D_p) = \frac{\pi D_p^2 N}{(2\pi)^{1/2} D_p \ln\sigma_g} \exp\left(-\frac{(\ln D_p - \ln \overline{D}_{pg})^2}{2\ln^2\sigma_g}\right)$$

$$\boxed{\ln \overline{D}_{pgS} = \ln \overline{D}_{pg} + 2\ln^2\sigma_g}$$

$$n_V(D_p) = \frac{\pi D_p^3 N}{6(2\pi)^{1/2} D_p \ln\sigma_g} \exp\left(-\frac{(\ln D_p - \ln \overline{D}_{pg})^2}{2\ln^2\sigma_g}\right)$$

$$\boxed{\ln \overline{D}_{pgV} = \ln \overline{D}_{pg} + 3\ln^2\sigma_g}$$

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Ambient Aerosol Size Distributions

$$n_N^\circ(\log D_p) = \sum_{i=1}^{n} \frac{N_i}{(2\pi)^{1/2} \log \sigma_i} \exp\left(-\frac{(\log D_p - \log \overline{D}_{pi})^2}{2 \log^2 \sigma_i}\right)$$

How many parameters are needed to describe the full aerosol distribution?

TABLE 8.3 Parameters for Model Aerosol Distributions Expressed as the Sum of Three Lognormal Modes

	Mode I			Mode II			Mode III		
Type	N (cm^{-3})	D_p (µm)	log σ	N (cm^{-3})	D_p (µm)	log σ	N (cm^{-3})	D_p (µm)	log σ
Urban	9.93×10^4	0.013	0.245	1.11×10^3	0.014	0.666	3.64×10^4	0.05	0.337
Marine	133	0.008	0.657	66.6	0.266	0.210	3.1	0.58	0.396
Rural	6650	0.015	0.225	147	0.054	0.557	1990	0.084	0.266
Remote continental	3200	0.02	0.161	2900	0.116	0.217	0.3	1.8	0.380
Free troposphere	129	0.007	0.645	59.7	0.250	0.253	63.5	0.52	0.425
Polar	21.7	0.138	0.245	0.186	0.75	0.300	3×10^{-4}	8.6	0.291
Desert	726	0.002	0.247	114	0.038	0.770	0.178	21.6	0.438

Source: Jaenicke (1993).

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The Power-Law Distribution

$$n_N^\circ(\log D_p) = \frac{C}{(D_p)^\alpha}$$

$$n_V^\circ(\log D_p) = \frac{\pi C}{6} D_p^{3-\alpha}$$

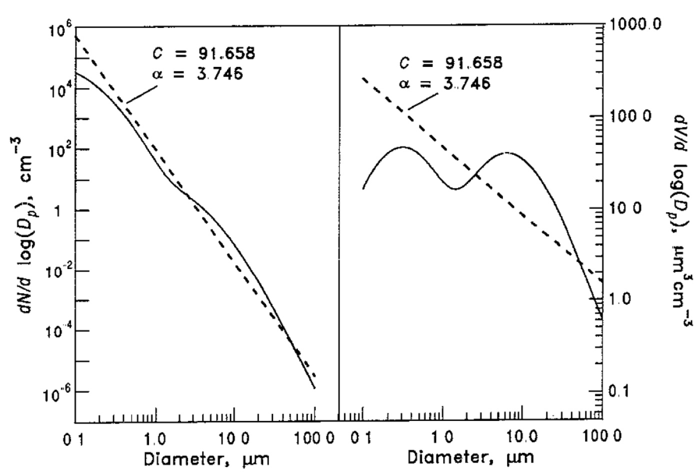

FIGURE 7.10 Fitting of an urban aerosol number distribution with a power-law distribution (left) and comparison of the corresponding volume distributions (right). Even if the power-law distribution appears to match the number distribution, it fails to reproduce the volume distribution.

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Hands-on example

Download the example excel sheet from class website

03-Particle_Size_Distribution_ClassExample.xlsx

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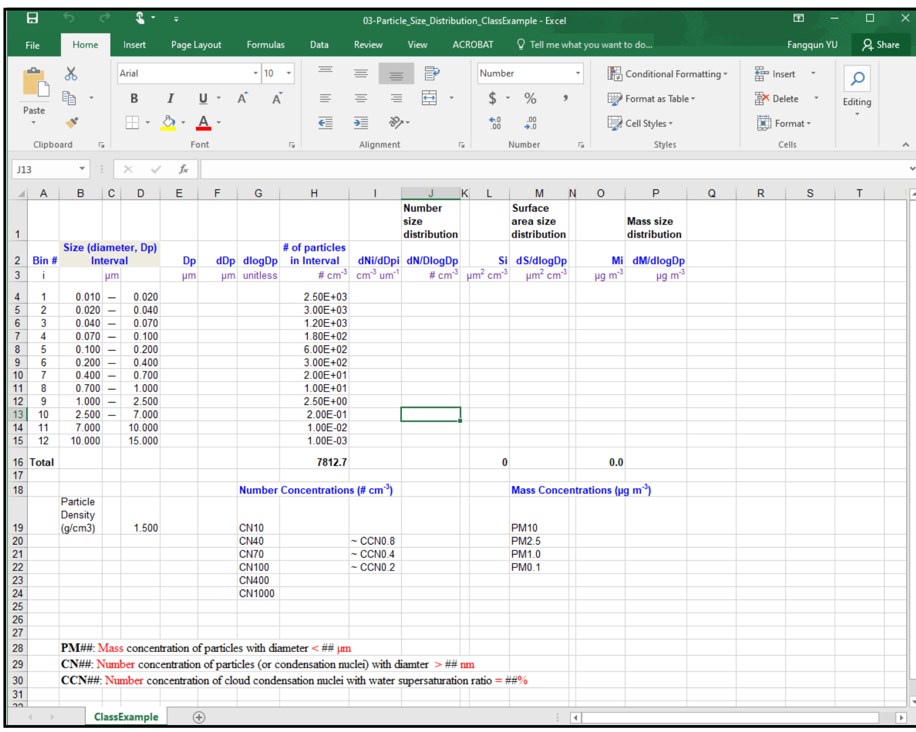

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1										Number size distribution			Surface area size distribution			Mass size distribution
2	Bin #	Size (diameter, Dp) Interval			Dp	dDp	dlogDp	# of particles in Interval	dNi/dDpi	dN/DlogDp		Si	dS/dlogDp		Mi	dM/dlogDp
3	i		μm		μm	μm	unitless	# cm^{-3}	cm^{-3} um^{-1}	# cm^{-3}		$μm^2$ cm^{-3}	$μm^2$ cm^{-3}		μg m^{-3}	μg m^{-3}
4	1	0.010	—	0.020				2.50E+03								
5	2	0.020	—	0.040				3.00E+03								
6	3	0.040	—	0.070				1.20E+03								
7	4	0.070	—	0.100				1.80E+02								
8	5	0.100	—	0.200				6.00E+02								
9	6	0.200	—	0.400				3.00E+02								
10	7	0.400	—	0.700				2.00E+01								
11	8	0.700	—	1.000				1.00E+01								
12	9	1.000	—	2.500				2.50E+00								
13	10	2.500	—	7.000				2.00E-01								
14	11	7.000		10.000				1.00E-02								
15	12	10.000		15.000				1.00E-03								
16	**Total**							**7812.7**				**0**			**0.0**	
17																
18							Number Concentrations (# cm^{-3})						Mass Concentrations (μg m^{-3})			
19		Particle Density (g/cm3)		1.500			CN10						PM10			
20							CN40		~ CCN0.8				PM2.5			
21							CN70		~ CCN0.4				PM1.0			
22							CN100		~ CCN0.2				PM0.1			
23							CN400									
24							CN1000									

PM##: Mass concentration of particles with diameter < ## μm

CN##: Number concentration of particles (or condensation nuclei) with diamter > ## nm

CCN##: Number concentration of cloud condensation nuclei with water supersaturation ratio = ##%

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