Overhead Slides for

Chapter 14

of

Fundamentals of Atmospheric Modeling

by

Mark Z. Jacobson

Department of
Civil & Environmental Engineering
Stanford University
Stanford, CA 94305-4020

January 30, 2002

Gas, Aerosol, Cloud Drop, and Raindrop Sizes

Table 14.1.

	Diameter (µm)	Number Concentration (molec. or partic. cm^{-3})	Mass Concentration (µg m^{-3})
Gas molecules	0.0005	2.45×10^{19}	1.2×10^{9}
Small aerosols	< 0.2	$10^{3} - 10^{6}$	< 1
Medium aerosols	0.2 - 1.0	$1 - 10^{4}$	< 250
Large aerosols	1.0 - 100	< 1 - 10	< 250
Fog drops	10 - 20	1 - 500	$10^{4} - 5 \times 10^{5}$
Average cloud drops	10 - 200	< 10 - 1000	$< 10^{5} - 5 \times 10^{6}$
Large cloud drops	200	< 1 - 10	$< 10^{5} - 5 \times 10^{6}$
Drizzle	400	0.1	$10^{5} - 5 \times 10^{6}$
Small raindrops	1000	0.01	$10^{5} - 5 \times 10^{6}$
Medium raindrops	2000	0.001	$10^{5} - 5 \times 10^{6}$
Large raindrops	8000	< 0.001	$10^{5} - 5 \times 10^{6}$

Particles and Size Distributions

Particle

Agglomerations of molecules in the liquid and / or solid phases, suspended in air

Includes aerosols, fog drops, cloud drops, and raindrops

Example 14.1. - Idealized particle size distribution

10,000 particles of radius between 0.05 and 0.5 μm
100 particles of radius between 0.5 and 5.0 μm
10 particles of radius between 5.0 and 50 μm

Example 14.2. Number of size bins needs to be limited

10^5 grid cells

100 size bins

100 components per size bin

--> 10^9 words = 8 gigabytes to store concentration

Volume Ratio Size Structure

Volume of particles in one size bin

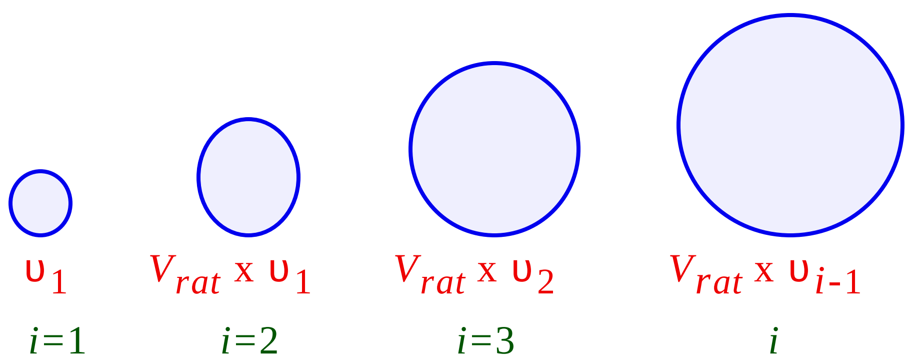
$$\upsilon_i = V_{rat}\upsilon_{i-1} \qquad (14.1)$$

$$\upsilon_i = \upsilon_1 V_{rat}^{i-1} \qquad (14.2)$$

Volume-diameter relationship for spherical particles

$$\upsilon_i = \pi d_i^3 / 6$$

Fig. 14.1. Variation in particle sizes with the volume ratio size structure.



Volume Ratio Size Structure

Volume ratio of adjacent size bins

$$V_{rat} = \left(\frac{\upsilon_{N_B}}{\upsilon_1}\right)^{1/(N_B-1)} = \left(\frac{d_{N_B}}{d_1}\right)^{3/(N_B-1)} \qquad (14.3)$$

Example 14.3.

	d_1	= 0.01 μm
	d_{N_B}	= 1000 μm
	N_B	= 30 size bins
--->	V_{rat}	= 3.29

Number of size bins

$$N_B = 1 + \frac{\ln\left[\left(d_{N_B}/d_1\right)^3\right]}{\ln V_{rat}} \qquad (14.4)$$

Example 14.4.

	d_1	= 0.01 μm
	d_{N_B}	= 1000 μm
	V_{rat}	= 4,
--->	N_B	= 26 size bins
	V_{rat}	= 2,
--->	N_B	= 51 size bins

Volume Ratio Size Structure

Average volume in a size bin

$$\upsilon_i = \frac{1}{2}\left(\upsilon_{i,hi} + \upsilon_{i,lo}\right) \qquad (14.5)$$

Relationship between high- and low-edge volume

$$\upsilon_{i,hi} = V_{rat}\upsilon_{i,lo} \qquad (14.6)$$

Substitute (14.6) into (14.5) --> low edge volume

$$\upsilon_{i,lo} = \frac{2\upsilon_i}{1+V_{rat}} \qquad (14.7)$$

Volume width of a size bin

$$\Delta\upsilon_i = \upsilon_{i,hi} - \upsilon_{i,lo} = \frac{2\upsilon_{i+1}}{1+V_{rat}} - \frac{2\upsilon_i}{1+V_{rat}} = \frac{2\upsilon_i\left(V_{rat}-1\right)}{1+V_{rat}} \qquad (14.8)$$

Diameter width of a size bin

$$\Delta d_i = d_{i,hi} - d_{i,lo} = \left(\frac{6}{\pi}\right)^{1/3}\left(\upsilon_{i,hi}^{1/3} - \upsilon_{i,lo}^{1/3}\right) = d_i 2^{1/3}\frac{V_{rat}^{1/3}-1}{\left(1+V_{rat}\right)^{1/3}}$$

(14.9)

Particle Concentrations

Number concentration in a size bin

$$n_i = \frac{v_i}{\upsilon_i} \qquad (14.10)$$

Number concentration in a size distribution

$$N_D = \sum_{i=1}^{N_B} n_i \qquad (14.11)$$

Volume concentration in a size bin

$$v_i = \sum_{q=1}^{N_V} v_{q,i} \qquad (14.12)$$

Surface area concentration in a size bin

$$a_i = n_i 4\pi r_i^2 = n_i \pi d_i^2 \qquad (14.13)$$

Particle Concentrations

Mass concentration in a size bin

$$\boldsymbol{m}_i = \sum_{q=1}^{N_V} \boldsymbol{m}_{q,i} = c_m \sum_{q=1}^{N_V} \rho_q v_{q,i} = c_m \rho_{p,i} \sum_{q=1}^{N_V} v_{q,i} = c_m \rho_{p,i} v_i$$

(14.14)

Volume-averaged mass density (g cm^{-3}) of particle of size *i*

$$\rho_{p,i} = \frac{\sum_{q=1}^{N_V} \left(v_{i,q} \rho_q \right)}{\sum_{q=1}^{N_V} v_{i,q}} \qquad (14.15)$$

Example 14.5.

	$\boldsymbol{m}_{q,i}$	= 3.0 μg m^{-3} for water
	$\boldsymbol{m}_{q,i}$	= 2.0 μg m^{-3} for sulfate
	d_i	= 0.5 μm
	ρ_q	= 1.0 g cm^{-3} for water
	ρ_q	= 1.83 g cm^{-3} for sulfate
--->	$v_{q,i}$	= 3 x 10^{-12} cm^3 cm^{-3} for water
--->	$v_{q,i}$	= 1.09 x 10^{-12} cm^3 cm^{-3} for sulfate
--->	$\boldsymbol{m}_i$	= 5.0 μg m^{-3}
--->	v_i	= 4.09 x 10^{-12} cm^3 cm^{-3}
--->	υ_i	= 6.54 x 10^{-14} cm^3
--->	n_i	= 62.5 partic. cm^{-3}
--->	a_i	= 4.8 x 10^{-7} cm^2 cm^{-3}

Lognormal Distribution

Bell-curve distribution on a log scale

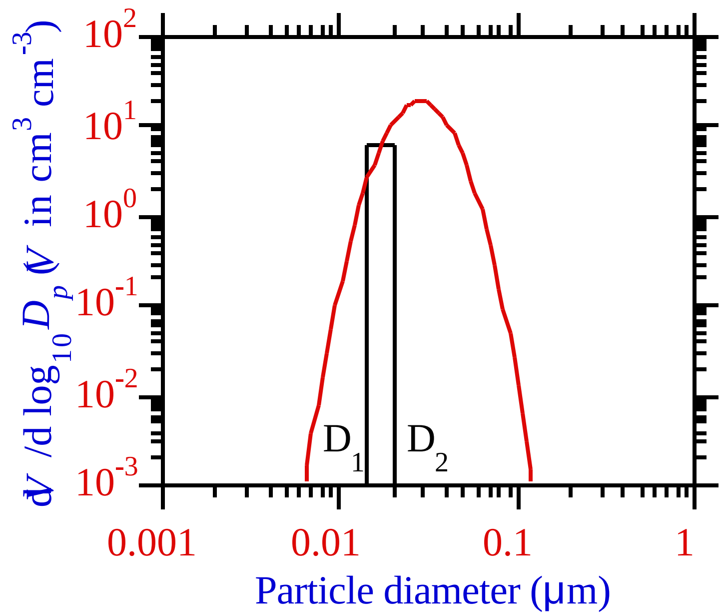
Geometric mean diameter

50% of area under a lognormal curve lies below it

Geometric standard deviation

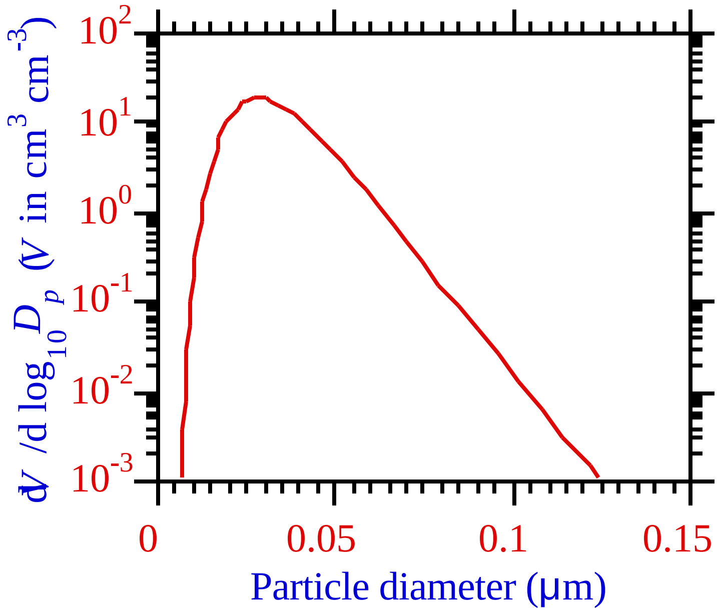
68% of area under a lognormal curve lies between +/1 one geometric standard deviation around the mean diameter

Fig. 14.2 a. A lognormal particle volume distribution.



Lognormal Distribution

Fig. 14.2 b. The lognormal curve drawn on a linear scale.



Lognormal Parameters From Data

Hering low-pressure impactor -- 7 size regimes

0.05	- 0.075 µm	0.5	- 1.0 µm
0.075	- 0.12 µm	1.0	- 2.0 µm
0.12	- 0.26 µm	2.0	- 4.0 µm
0.26	- 0.5 µm		

Natural log of geometric mean mass diameter

$$\ln \bar{D}_M = \frac{1}{M_L} \sum_{j=1}^{7} \left(\boldsymbol{m}_j \ln d_j \right) \qquad (14.16)$$

Total mass concentration of particles (µg m^{-3})

$$M_L = \sum_{j=1}^{7} \boldsymbol{m}_j$$

Natural log of geometric mean volume diameter

$$\ln \bar{D}_V = \frac{1}{V_L} \sum_{j=1}^{7} \left(v_j \ln d_j \right) \qquad (14.17)$$

Total volume concentration of particles (cm^3 cm^{-3})

$$V_L = \sum_{j=1}^{7} v_j \qquad v_j = \frac{\boldsymbol{m}_j}{c_m \rho_j}$$

Lognormal Parameters From Data

Natural log of geometric mean area diameter

$$\ln \bar{D}_A = \frac{1}{A_L} \sum_{j=1}^{7} \left(a_j \ln d_j \right) \qquad (14.18)$$

Total area concentration of particles (cm^2 cm^{-3})

$$A_L = \sum_{j=1}^{7} a_j \qquad\qquad a_j = \frac{3m_j}{c_m \rho_j r_j}$$

Natural log of geometric mean number diameter

$$\ln \bar{D}_N = \frac{1}{N_L} \sum_{j=1}^{7} \left(n_j \ln d_j \right) \qquad (14.19)$$

Total number concentration of particles (partic. cm^{-3})

$$N_L = \sum_{j=1}^{7} n_j \qquad\qquad n_j = \frac{m_j}{c_m \rho_j \upsilon_j}$$

Natural log of geometric standard deviation

$$\ln \sigma_g = \sqrt{\frac{1}{M_L} \sum_{j=1}^{7} \left(m_j \ln^2 \frac{d_j}{\bar{D}_M} \right)} = \sqrt{\frac{1}{V_L} \sum_{j=1}^{7} \left(v_j \ln^2 \frac{d_j}{\bar{D}_V} \right)}$$

$$= \sqrt{\frac{1}{A_L} \sum_{j=1}^{7} \left(a_j \ln^2 \frac{d_j}{\bar{D}_A} \right)} = \sqrt{\frac{1}{N_L} \sum_{j=1}^{7} \left(n_j \ln^2 \frac{d_j}{\bar{D}_N} \right)} \qquad (14.20)$$

Redistribute Mass, etc. With Lognormal Parameters

Redistribute mass concentration in model size bin

$$\boldsymbol{m}_i = \frac{\mathrm{M}_L \Delta d_i}{d_i \sqrt{2\pi} \ln \sigma_g} \exp\left[-\frac{\ln^2\left(d_i / \bar{D}_M\right)}{2 \ln^2 \sigma_g}\right] \qquad (14.21)$$

Redistribute volume concentration

$$v_i = \frac{\mathrm{V}_L \Delta d_i}{d_i \sqrt{2\pi} \ln \sigma_g} \exp\left[-\frac{\ln^2\left(d_i / \bar{D}_V\right)}{2 \ln^2 \sigma_g}\right] \qquad (14.22)$$

Redistribute area concentration

$$a_i = \frac{\mathrm{A}_L \Delta d_i}{d_i \sqrt{2\pi} \ln \sigma_g} \exp\left[-\frac{\ln^2\left(d_i / \bar{D}_A\right)}{2 \ln^2 \sigma_g}\right] \qquad (14.23)$$

Redistribute number concentration

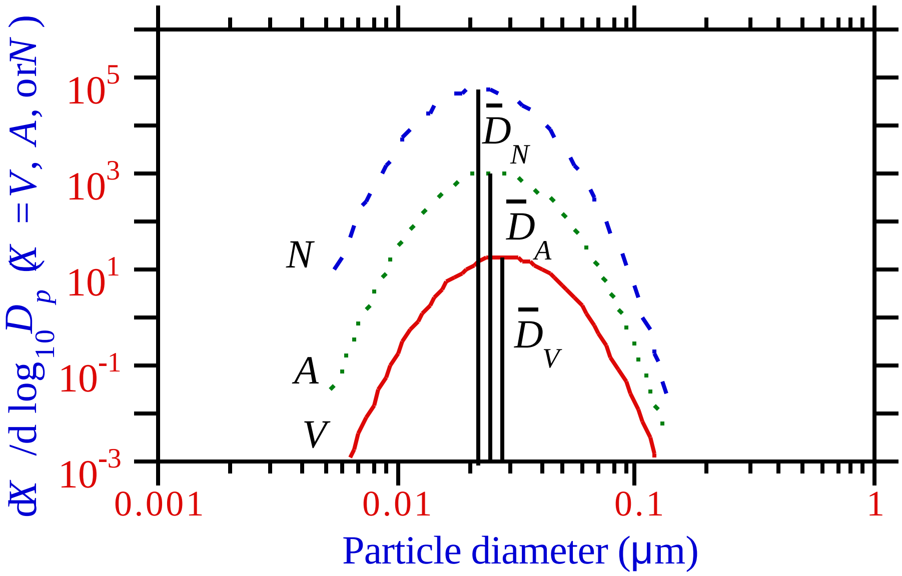
$$n_i = \frac{\mathrm{N}_L \Delta d_i}{d_i \sqrt{2\pi} \ln \sigma_g} \exp\left[-\frac{\ln^2\left(d_i / \bar{D}_N\right)}{2 \ln^2 \sigma_g}\right] \qquad (14.24)$$

Exact volume concentration in a mode

$$V_L = \int_0^\infty v_d \, \mathrm{d}d = \frac{\pi}{6} \int_0^\infty n_d d^3 \, \mathrm{d}d = \frac{\pi}{6} \bar{D}_N^3 \exp\left(\frac{9}{2} \ln^2 \sigma_g\right) \mathrm{N}_L \qquad (14.25)$$

Lognormal Modes

Fig. 14.3. Number (partic. cm^{-3}), area (cm^2 cm^{-3}), and volume (cm^3 cm^{-3}) concentrations for a lognormal distribution.



Lognormal Parameters for Continental Particles

Table 14.2.

(Whitby, 1978)

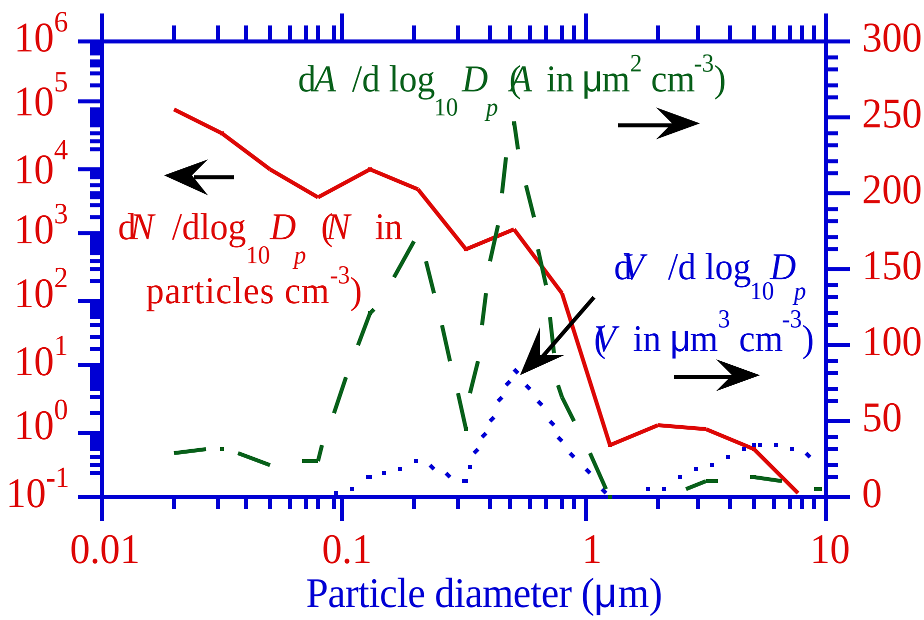
	<---------------------- Mode ------------------->		
Parameter	Nuclei	Accumulation	Coarse
σ_g	1.7	2.03	2.15
Number (partic. cm^{-3})	7.7×10^4	1.3×10^4	4.2
$\bar{D}_N$ (µm)	0.013	0.069	0.97
Surface (μm^2 cm^{-3})	74	535	41
$\bar{D}_A$ (µm)	0.023	0.19	3.1
Volume (μm^3 cm^{-3})	0.33	22	29
$\bar{D}_V$ (µm)	0.031	0.31	5.7

Quadramodal Size Distribution

Quadramodal lognormal distribution

Mode	Diameter Range or Peak (μm)
Nucleation	< 0.1
Accumulation	0.1 - 2
submode 1	~ 0.2
submode 2	~ 0.5 - 0.7
Coarse	> 2

Fig. 14.4. Size distribution at Claremont, California, on the morning of August 27, 1987.



Marshall-Palmer Distribution

Raindrop number concentration between d_i and $d_i + \Delta d_i$

$$n_i = \Delta d_i n_0 e^{-\lambda_r d_i} \qquad (14.30)$$

$\Delta d_i n_0$ = value of n_i at $d_i = 0$

n_0 = 8.0 x 10^{-6} partic. cm^{-3} μm^{-1}

λ_r = $4.1 \times 10^{-3} R^{-0.21}$ μm^{-1}

R = rainfall rate (1 - 25 mm hr^{-1})

Total number concentration and liquid water content

$$n_T = n_0 / \lambda_r \qquad w_L = 10^{-6} \rho_w \pi n_0 / \lambda_r^4$$

Example 14.6.

	R	= 5 mm hr^{-1}
	d_i	= 1.0 mm
	$d_i + \Delta d_i$	= 2.0 mm
--->	n_i	= 0.00043 partic. cm^{-3}
--->	n_T	= 0.0027 partic. cm^{-3}
--->	w_L	= 0.34 g m^{-3}

Modified Gamma Distribution

Number concentration of drops (partic. cm^{-3}) in size bin *i*

$$n_i = \Delta d_i A_g r_i^{\alpha_g} \exp\left[-\frac{\alpha_g}{\gamma_g}\left(\frac{r_i}{r_{c,g}}\right)^{\gamma_g}\right] \qquad (14.31)$$

Table 14.3. Modified gamma size distribution parameters.

Cloud Type	A_g	α_g	γ_g	r_{cg} (μm)	Liquid Water Content (g m^{-3})	Number Conc. (partic. cm^{-3})
Stratocumulus base	0.2823	5.0	1.19	5.33	0.141	100
Stratocumulus top	0.19779	2.0	2.46	10.19	0.796	100
Stratus base	0.97923	5.0	1.05	4.70	0.114	100
Stratus top	0.38180	3.0	1.3	6.75	0.379	100
Nimbostratus base	0.08061	5.0	1.24	6.41	0.235	100
Nimbostratus top	1.0969	1.0	2.41	9.67	1.034	100
Cumulus congestus	0.5481	4.0	1.0	6.0	0.297	100
Light rain	4.97x10^{-8}	2.0	0.5	70.0	1.17	0.01

Example 14.7.

Find number concentration of droplets between 14 and 16 μm in diameter at base of a stratus cloud.

---> r_{cg} = 7.5 μm

---> Δd_i = 2 μm ---> n_i = 19.46 partic. cm^{-3}

Full-Stationary Size Structure

Average volume in size bin (υ_i) stays constant. When growth occurs, n_i changes.

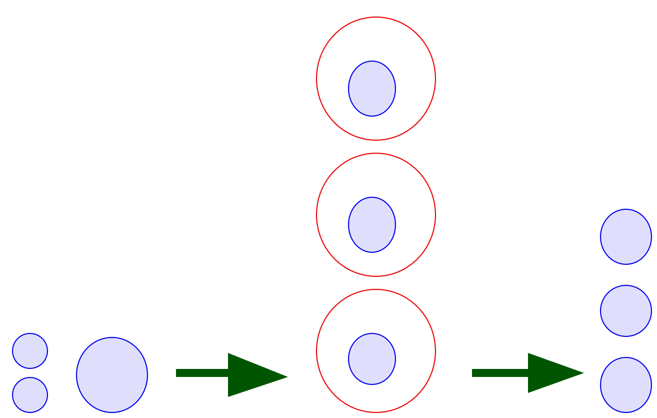
Advantages:

- Covers wide range in diameter space with few bins
- Nucleation, emissions, transport treated realistically

Disadvantages:

- When growth occurs, information about the original composition of the growing particle is lost.
- Growth leads to numerical diffusion

Fig. 14.5. Demonstration of a problem with the full-stationary size bin structure.



Full-Moving Structure

Number concentration (n_i) of particles in a size bin does not change during growth; instead, volume (υ_i) changes

Advantages:

- Core volume preserved during growth
- No numerical diffusion during growth

Disadvantages:

- Nucleation, emissions, transport treated unrealistically.
- Reordering of size bins required for coagulation

Fig. 14.6. Preservation of aerosol material upon growth and evaporation in a moving structure.

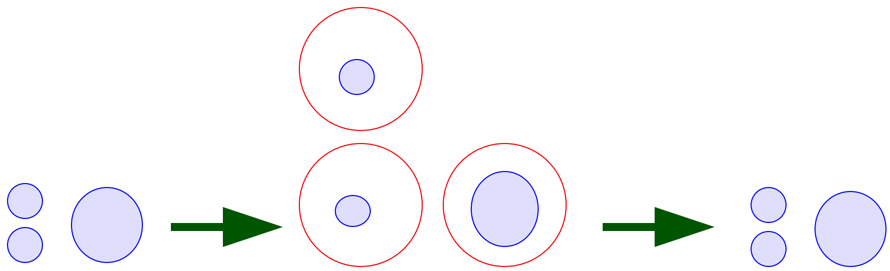
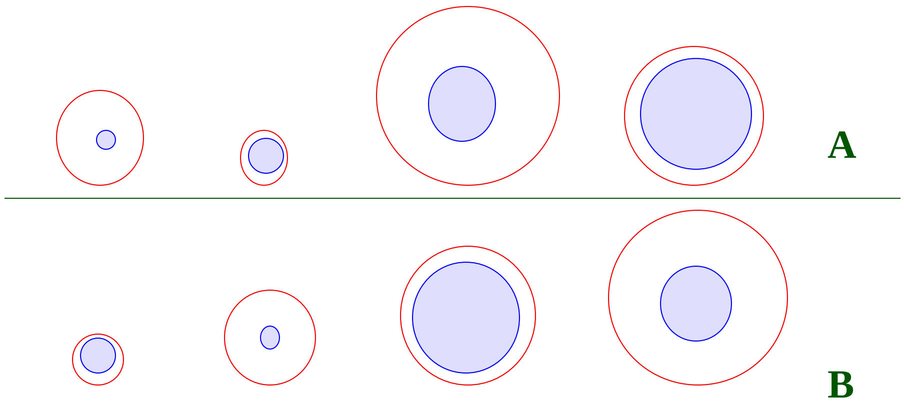


Fig. 14.7. Particle size bin reordering for coagulation



Quasistationary Structure

Same as full-stationary structure, except particle volumes fluctuate during growth. Adjusted particle volumes are fit back onto a stationary grid.

Advantages and disadvantages:

- Same as for full stationary structure

Example:

- After growth, particles in bin *i* have volume υ_i', where $\upsilon_j \le \upsilon_i' < \upsilon_k$

- Partition *i* particles between bins *j* and *k*,

Conserve particle number concentration

$$n_i = n_j + n_k$$

Conserve particle volume concentration

$$n_i \upsilon_i' = n_j \upsilon_j + n_k \upsilon_k$$

Solution to this set of two equations and two unknowns

$$n_j = n_i \frac{\upsilon_k - \upsilon_i'}{\upsilon_k - \upsilon_j} \qquad n_k = n_i \frac{\upsilon_i' - \upsilon_j}{\upsilon_k - \upsilon_j} \qquad (14.32)$$

Moving-Center Structure

Particle volume (υ_i) is varies between $\upsilon_{i,hi}$ and $\upsilon_{i,lo}$ during growth, but $\upsilon_{i,hi}$, $\upsilon_{i,lo}$, and $d\upsilon_i$ remain fixed.

Advantages:

- Covers wide range in diameter space with few bins
- Little numerical diffusion during growth
- Nucleation, emissions, transport treated realistically.

Disadvantages:

- When growth occurs, information about the original composition of the growing particle is lost.

Fig. 14.8. Comparison of moving-center, full-moving, and quasi stationary size structure after growth of water onto aerosols to form cloud-sized drops.