

# ENVE 576

## Indoor Air Pollution

Fall 2017

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**September 26, 2017**

Particulate matter: physics, size distributions, respiratory deposition

Built  
Environment  
Research  
@ IIT



*Advancing energy, environmental, and  
sustainability research within the built environment*

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**Built Environment Research Group**  
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# Schedule updates

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- HW #2 is due today
  - Emissions models and sorption dynamics
- HW #3 will be assigned today
  - Reactive deposition and aerosol calculations

# Project topics

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- Topic selection suggestions
  - Your interest is the most important factor
    - Don't shy away from big issues
  - Approach from a fundamental perspective
    - Think about Sources and Losses, Exposures and Doses
  - Consider data availability
  - Considerably more than glorified HW problem
  - Do a preliminary literature search to focus your efforts

# Topic justification due

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- Less than 1/2 page (a few sentences is fine)
- Describe topic in enough detail that I can provide feedback
- Include references to show that there is enough to get started on your project
- **Due October 3<sup>rd</sup> to me via email**
- Criteria
  - Importance
  - Creativity
  - Justification
  - Reasonable scope

# Lab instrumentation: T/RH and power/energy



Temperature/RH



Data logging

Temperature



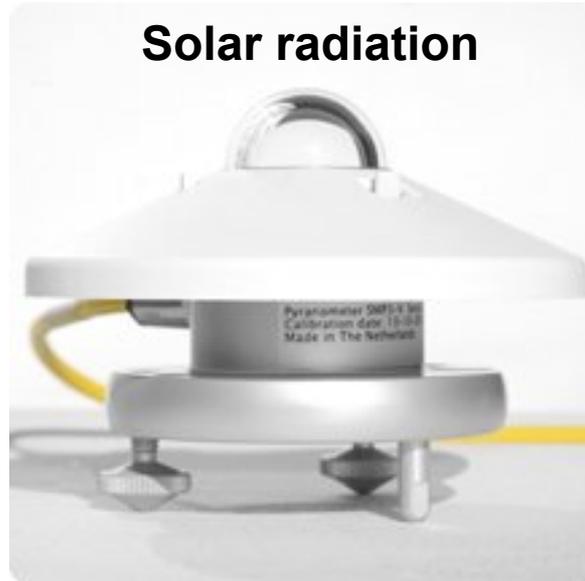
Heat flux



IR camera



Solar radiation



Electric power



# Lab instrumentation: HVAC diagnostics



**Blower door  
(envelope leakage)**

**Duct blaster  
(duct leakage  
and airflow)**



**Pressure**



**TrueFlow  
(HVAC airflow rates)**



# Lab instrumentation: Air quality (mostly PM)



**NanoScan SMPS**  
10 to 500 nm



**Optical particle sizer**  
0.3 to 10  $\mu\text{m}$



**CO<sub>2</sub>**  
(for AER)  
**CO**



**DustTrak**  
PM<sub>2.5</sub>/PM<sub>10</sub>



**CPC**  
< 1  $\mu\text{m}$



**CPC respirator fit tester**  
< 1  $\mu\text{m}$



**Also BC, O<sub>3</sub>, NO<sub>2</sub>**  
**and TVOC**

# Lab instrumentation: Air quality

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- Cheaper instruments



**Foobot IAQ monitor**



**Dylos particle counter**

# Lab facilities

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# Final project topics

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Name	Project topic
Cheng, Cheng	
Duan, Haoran	
Horin, Brett Andrew	
Jittasirinuwat, Vitoon	
Killarney, Sean Joseph	
Kotur, Ajay Ashok	
Li, Jiabin	
Moitra, Kshetij	
Sun, Liuyang	
Zhu, Tianxing	
Ali, Asra Fatima	
Kang, Hyerim	
Manikonda, Anusha	
Wright, Eric	

**Remember:**

- Teams of up to 2
- Project topic justification due October 3<sup>rd</sup>

# Tips on introduction and literature review

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- Objectives
  - Grab reader and pull them into your story
  - Cite all relevant references
  - Establish gaps in existing research
  - Define parameters and make case for their importance
  - Organize and lay out rest of paper
- Start with a interesting fact about your topic
  - No need to be alarmist or over-the-top
  - Use a short sentence
  - Layer on more complicated ideas
- Conduct a comprehensive literature review
  - Use [Web of Science](#) and [Google Scholar](#) to find other sources
- Don't need to cite all details about previous work
  - Just the central idea and most impactful previous findings

# Tips on introduction and literature review

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- Challenge is striking balance between accurately representing work of others and not going into too much detail
- Cite and define key parameters and emphasize why they are important
- After reading introduction, the reader should know the direction of the rest of the paper
- Keep it short (~3 paragraphs)
  - General motivation and importance
  - Previous work
  - Gaps in literature
  - Organizing principle of paper
  - Define and justify important parameters

# Tips on introduction and literature review

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- Avoid passive voice, be active
- It is acceptable to use “I” or “we”
- Vary your language:
  - Smith et al. (1972) measured ...
  - Zhao and Stephens (2015) investigated...
  - Several studies report differences between... (Katz, 2004; Kinney et al., 2000; Allen and Collins, 1999)
- Follow the format for citations and references
- A good literature review:
  - Summarizes all important articles in the field
  - Cites high quality references
    - Also refers to lower quality references *if necessary*
  - States what is novel about the paper
    - Mentions what is missing in the literature
    - Does not denigrate others

# Rest of your paper

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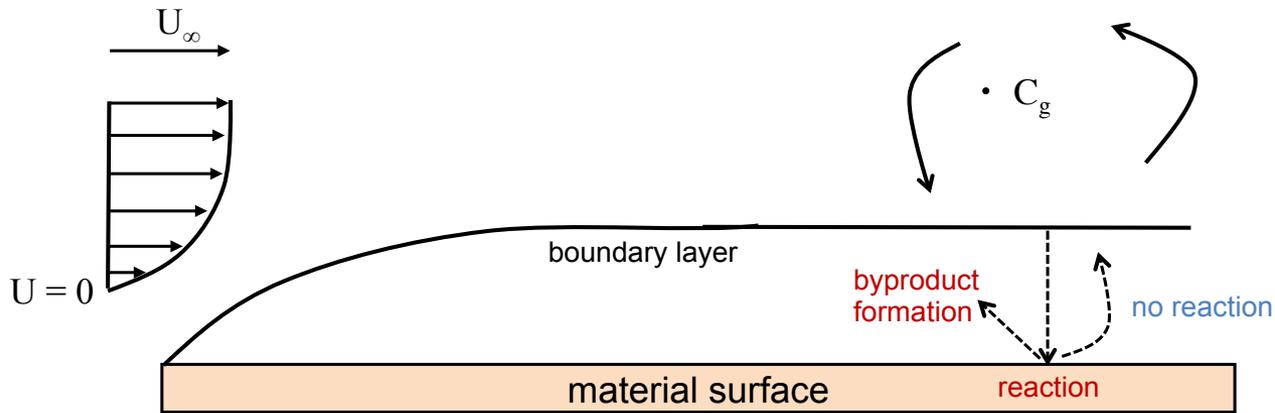
- Literature review is a key component
- So is the remaining methodology, results, discussion and conclusion
  - When in doubt, follow examples of previously published papers
    - e.g., just about anything from our suggested readings list
- Measurements are **not** required
  - No additional points for measurement vs. modeling study

# Review from last time

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- Last time we covered:
  - Reactions of gas-phase compounds
    - Heterogeneous (reactive deposition)
    - Homogeneous (gas-phase chemistry)
- Today we will begin ~3 weeks of lectures on particulate matter
  - Starting with:
    - Single particle physics
    - Particle size distributions
    - Respiratory deposition

# Reactive deposition: summary



- For reactive gas-phase pollutants, we will have an additional loss rate to account for reactive losses to material surfaces

$$\frac{dC}{dt} = P\lambda C_{out} + \frac{E}{V} - \lambda C - \frac{v_d A}{V} C \quad k_{dep} = \frac{v_d A}{V}$$

$$v_d = \frac{v_s v_t}{v_s + v_t}$$

$$\frac{1}{v_d} = \frac{1}{v_t} + \frac{1}{v_s} = \frac{1}{v_t} + \frac{4}{\gamma \langle v \rangle}$$

$v_s$  = surface-limited deposition velocity (m/hr)

$v_t$  = transport-limited deposition velocity (m/hr)

$\gamma$  = reaction probability (-)

$\langle v \rangle$  = Boltzmann velocity (m/hr)

# Reactive deposition: byproduct formation

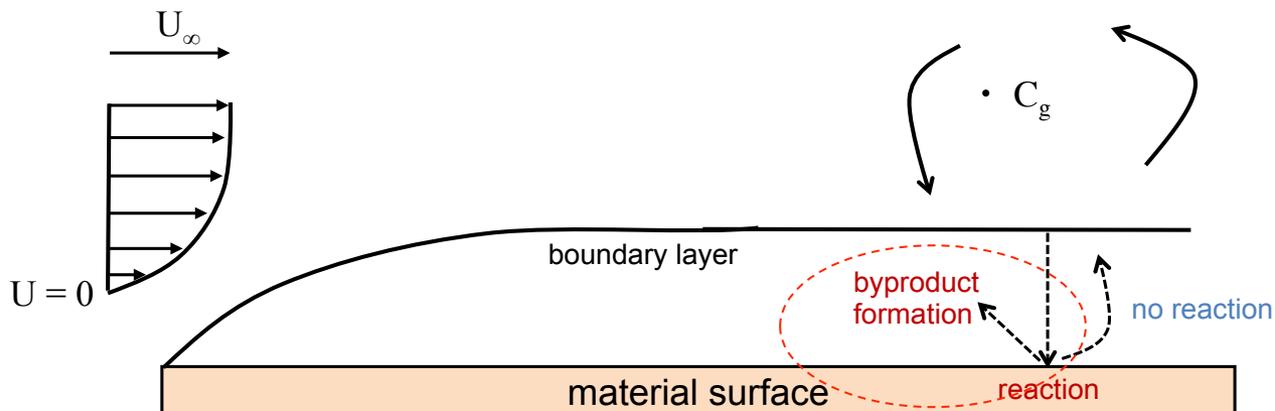
- Reactive deposition to surfaces removes indoor pollutants
  - Can also generate others in the form of reaction by-products

$$R_{byproduct} = (v_d AC) Y_i f_{conversion}$$

$R_{byproduct,i}$  = by-product  $i$  production rate (moles/hr)

$Y_i$  = molar yield of  $i$  (moles  $i$  per moles of gas consumed)

$f_{conversion}$  = conversion factor (e.g.,  $\frac{10^{-6}}{MW}$  to convert from  $\frac{\mu\text{g}}{\text{m}^3}$  to  $\frac{\text{moles}}{\text{hour}}$ )



# Byproduct formation: mass balance

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- Mass balance on reactive pollutant (e.g., ozone)

$$\frac{dC}{dt} = P\lambda C_{O_3,out} - \lambda C_{O_3} - \frac{v_d A}{V} C_{O_3}$$

- Mass balance on byproduct  $i$

$$\frac{dC_i}{dt} = P\lambda C_{i,out} - \lambda C_i + Y_i \frac{v_{d,O_3} A}{V} f_{conversion} C_{O_3}$$

Tracking two species, need two mass balances...

# Homogeneous chemistry

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- Homogeneous reactions also occur in indoor environments
  - Gas  $i$  + Gas  $j$   $\rightarrow$  Byproduct  $k$

$$R_{\text{homogeneous}} = -k_{ij}C_iC_jV$$

$R_{\text{homogeneous}}$  = loss rate due to homogeneous reactions between  $i$  and  $j$   
(moles/hr or  $\mu\text{g/hr}$ )

$k_{ij}$  = reaction rate constant ( $\text{ppb}^{-1} \text{hr}^{-1}$ )

$k_{ij}C_j$  = reaction rate (1/hr)

- Need at least 3 mass balances
  - Two reactants + product(s)  $R_{\text{byproduct},k} = (k_{ij}C_iC_j)Y_k f_{\text{conversion}}$
- For a reaction to be relevant indoors, it must occur on a relevant time scale
  - $k_jC_j$  (1/hr) needs to be on the same order as  $\lambda$  (1/hr)
    - Reaction must be reasonably fast

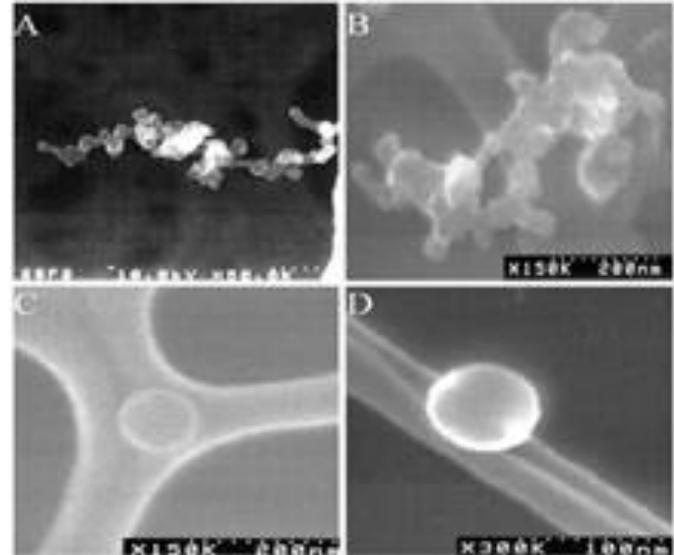
# **PARTICULATE MATTER**

Overview, physics, size distributions, respiratory deposition

# Particulate matter (PM)

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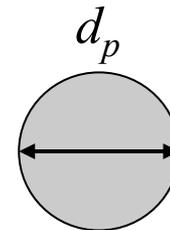
- Particulate matter (PM) is its own class of pollutant
  - PM consists of a mixture of solid particles and liquid droplets suspended in air
  - Primary emissions are emitted directly by sources
    - Outdoors: Industry, construction, roads, smokestacks, fires, vehicles
    - Indoors: Smoking, cooking, resuspension of dust, transport from outdoors
  - Secondary emissions are formed in atmospheric reactions and some indoor reactions
- Health effects
  - Respiratory, cardiovascular, others
- Visibility effects outdoors



# Particle sizes

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- Usually referring to a characteristic dimension
  - Diameter for sphere
  - Diameter for fibers (e.g. asbestos)
  - Equivalent diameter for non-spherical
- Micrometer ( $\mu\text{m}$ )
  - $1 \mu\text{m} = 10^{-6} \text{ m}$
- Nanometer (nm)
  - $1 \text{ nm} = 10^{-9} \text{ m}$
- We usually treat particles as spherical:
  - Or 'equivalent' spheres



$$V = \frac{\pi}{6} d_p^3$$

# Particle sizes

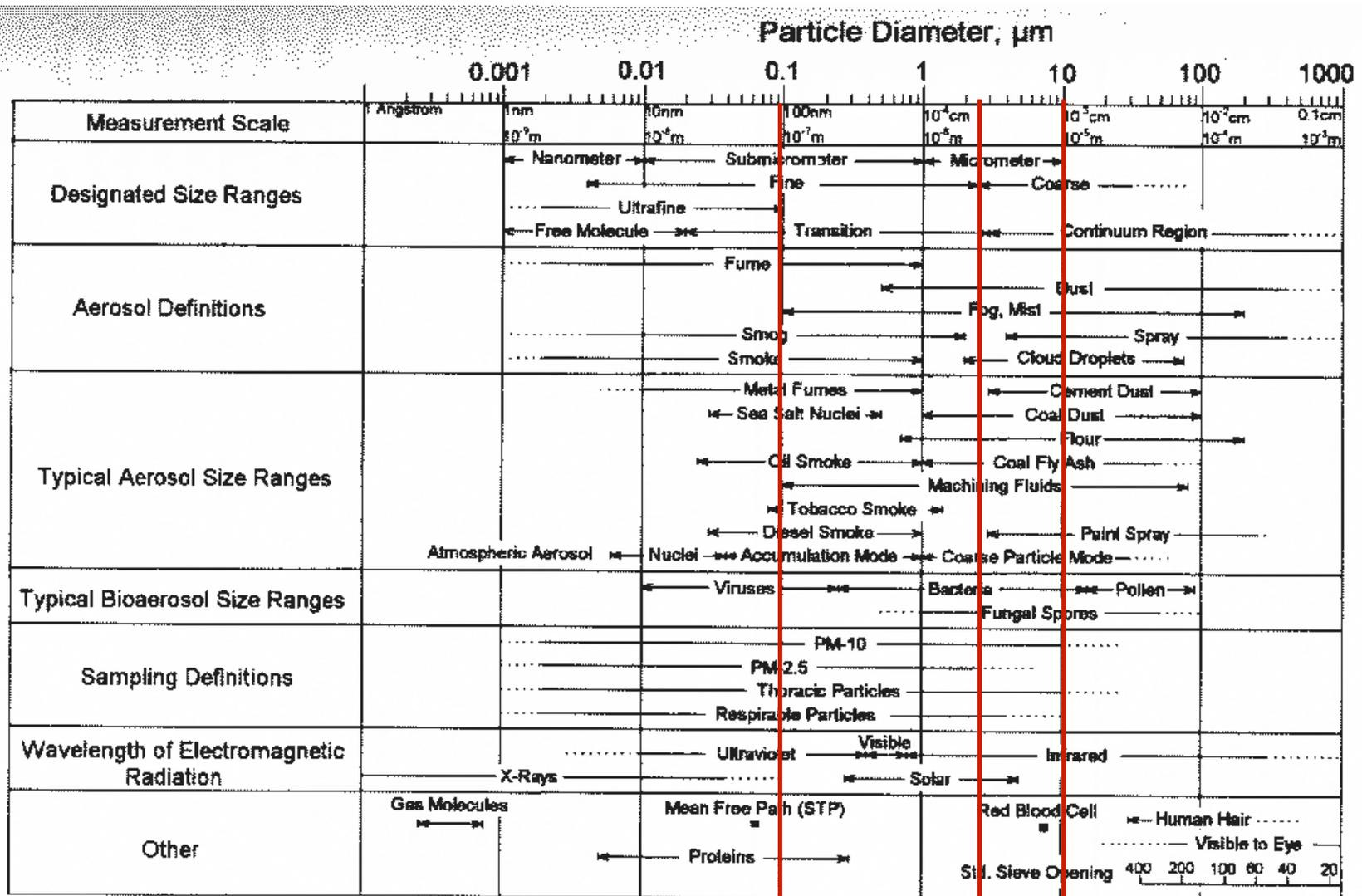
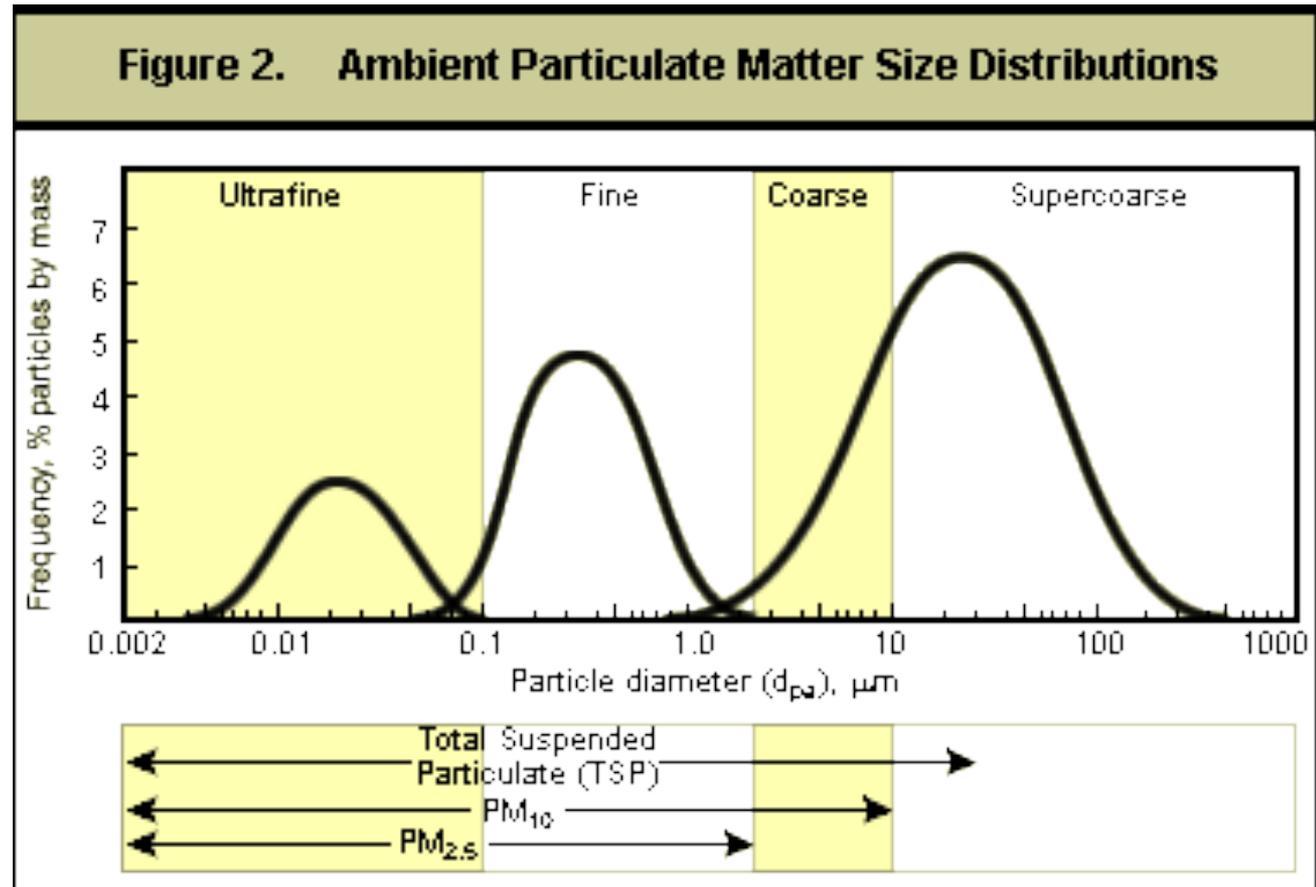


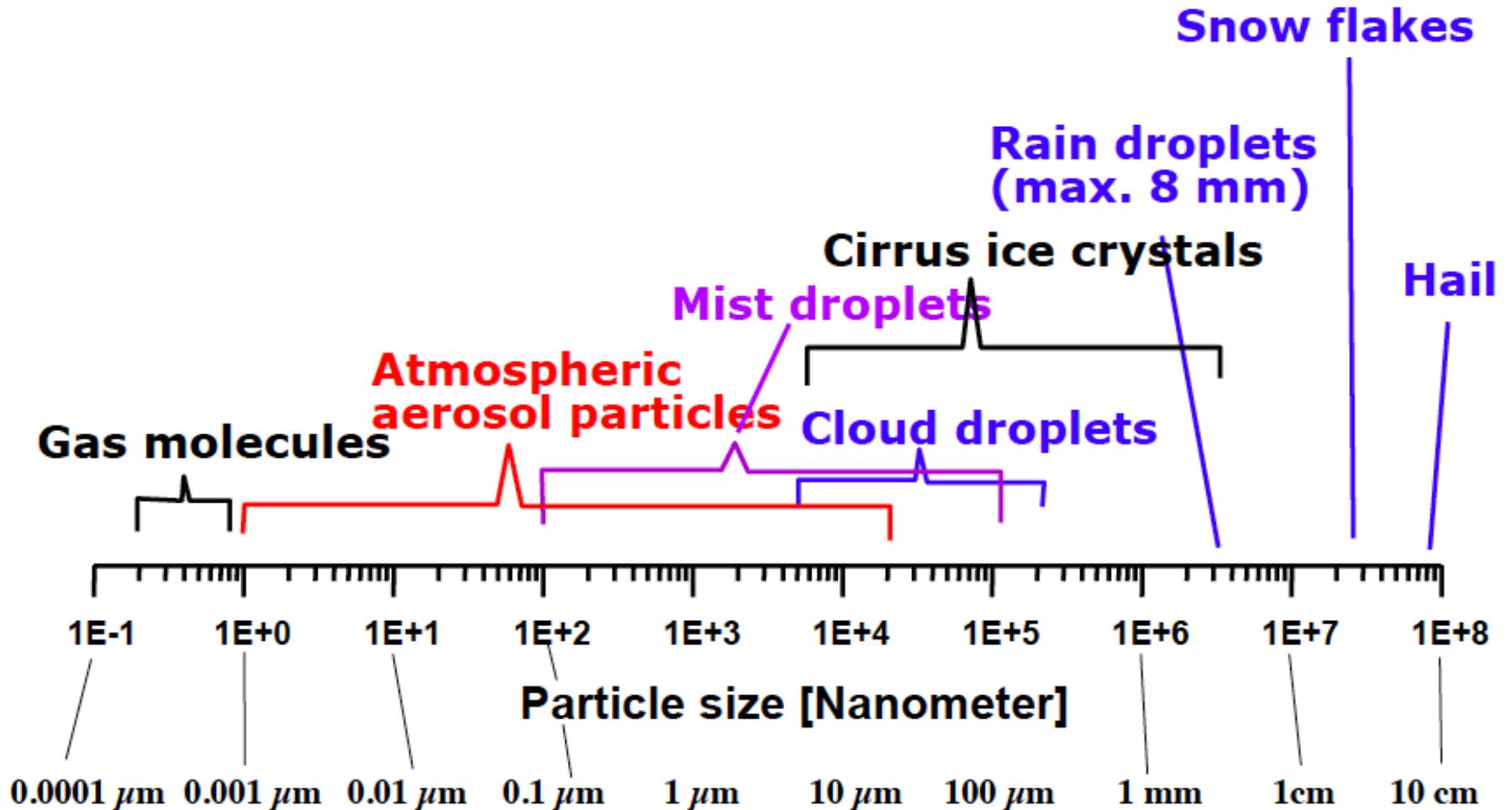
FIGURE 1.6 Particle size ranges and definitions for aerosols.

# How are particle concentrations reported?

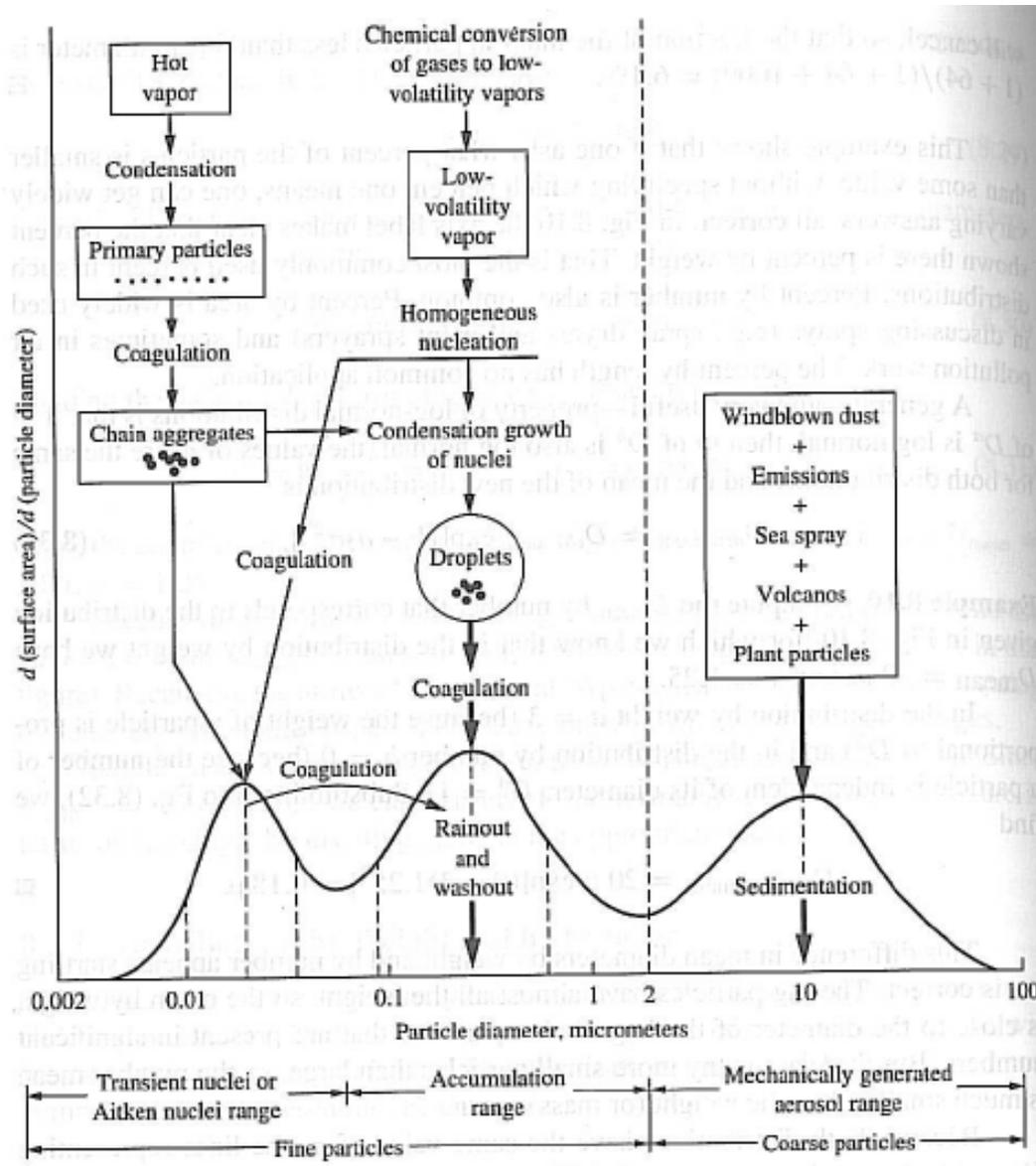
- Number
  - #/cm<sup>3</sup>
  - UFP <100 nm
- Surface area
  - cm<sup>2</sup>/cm<sup>3</sup>
- Volume
  - m<sup>3</sup>/m<sup>3</sup>
- Mass
  - μg/m<sup>3</sup>
  - PM<sub>2.5</sub>
  - PM<sub>10</sub>
  - PM<sub>2.5-10</sub>
  - TSP
  - RSP



# Particle sizes



# Particle formation mechanisms, surface area, and size



# **PARTICLE MOTION**

What affects the movement of particles?

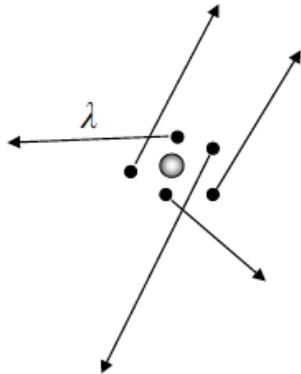
# Particle motion in gases: Size regime

- Continuum regime and free molecular regime
  - Behavior of a particle in a gas is characterized by the ratio of the mean free path of the gas molecules to the diameter of the particle
  - Ratio is called the Knudsen number ( $Kn$ ):

$$Kn = \frac{2\lambda}{d_p}$$

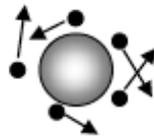
$d_p$  = particle diameter ( $\mu\text{m}$ )

$\lambda$  = mean free path of air ( $0.066 \mu\text{m}$  @ STP)



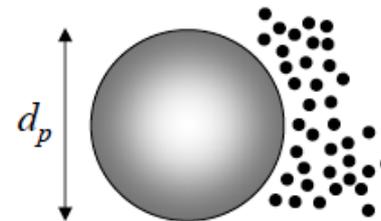
Free molecular regime  
 $Kn \rightarrow \infty$

$$d_p < \sim 10 \text{ nm}$$



Transition regime  
 $Kn \approx 1$

$$10 \text{ nm} < d_p < 1 \mu\text{m}$$



Continuum regime  
 $Kn \ll 1$

$$d_p > \sim 1 \mu\text{m}$$

# Particle motion in gases: Flow regime

- Reynolds number:

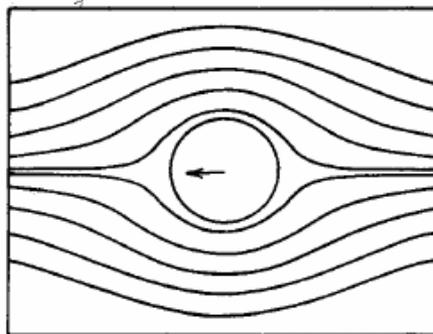
- Re is the ratio of inertial forces to frictional forces for fluid flow through a pipe or around an obstacle
- For flow around a particle:

$$\text{Re} = \frac{\rho_{air} V d_p}{\mu}$$

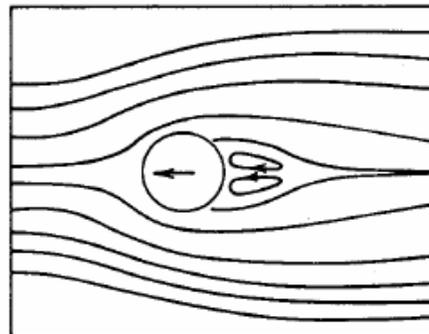
$\rho_{air}$  = air density (kg/m<sup>3</sup>)  
 $V$  = relative velocity between particle and air (m/s)  
 $\mu$  = dynamic viscosity of air ( $1.8 \times 10^{-5}$  kg/(m-s) at STP)

- For flow around a particle:

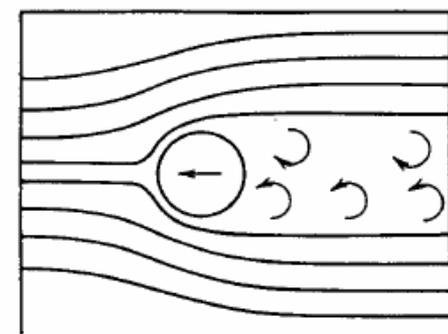
- Re < 1: laminar flow (frictional forces dominate)
- Re > 1: turbulent flow (inertial forces dominate)



Re = 0.1 (a)



Re = 2 (b)



Re = 250 (c)

Hinds 1999

# Particle motion in gases: Drag forces (large $d_p$ )

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- Newton's resistance law

- Newton derived an equation for the force resisting the motion of a sphere passing through a gas:

$$F_D = C_D \frac{\pi}{8} \rho_{air} d_p^2 V^2$$

$F_D = \text{drag force (kg-m/s}^2\text{)}$   
 $C_D = \text{drag coefficient (-)}$

- Assumes only inertia of air is important (not friction forces)
- Therefore, this assumption is only valid for high Re ( $Re > 1000$ )
- For smaller Re, the molecular viscous (friction) forces have to be considered
  - Under laminar flow conditions ( $Re < 1$ ), viscous forces dominate and inertial forces can be neglected
  - In this case, we use **Stokes' Law**

# Particle motion in gases: Drag forces (small $d_p$ )

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- Stokes' law states that:

$$F_D = 3\pi\mu Vd_p$$

$V$  = particle velocity (m/s)

- Valid for laminar flow around a solid sphere

- Comparing Newton's and Stokes' laws:

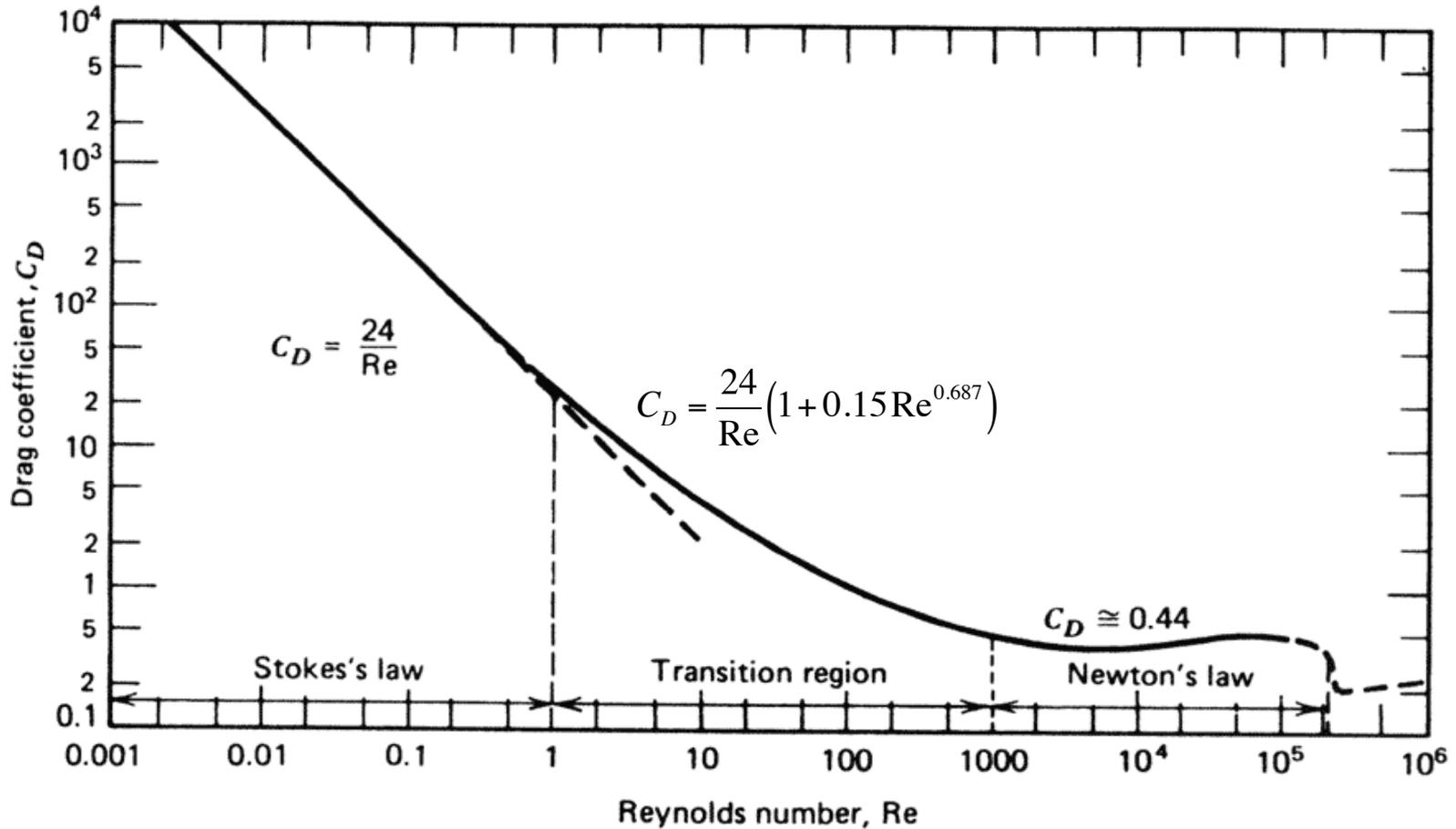
$$F_D = C_D \frac{\pi}{8} \rho_{air} d_p^2 V^2 = 3\pi\mu Vd_p$$

$$C_D = \frac{24\mu}{\rho_{air} Vd_p} = \frac{24}{Re}$$

- Therefore, in the Stokes' regime ( $Re < 1$ ) the drag coefficient is  $24/Re$

# Particle motion in gases

- Drag coefficient,  $C_D$ :



**FIGURE 3.1** Drag coefficient versus Reynolds number for spheres.

# Particle motion in gases: Typical $Re$ values

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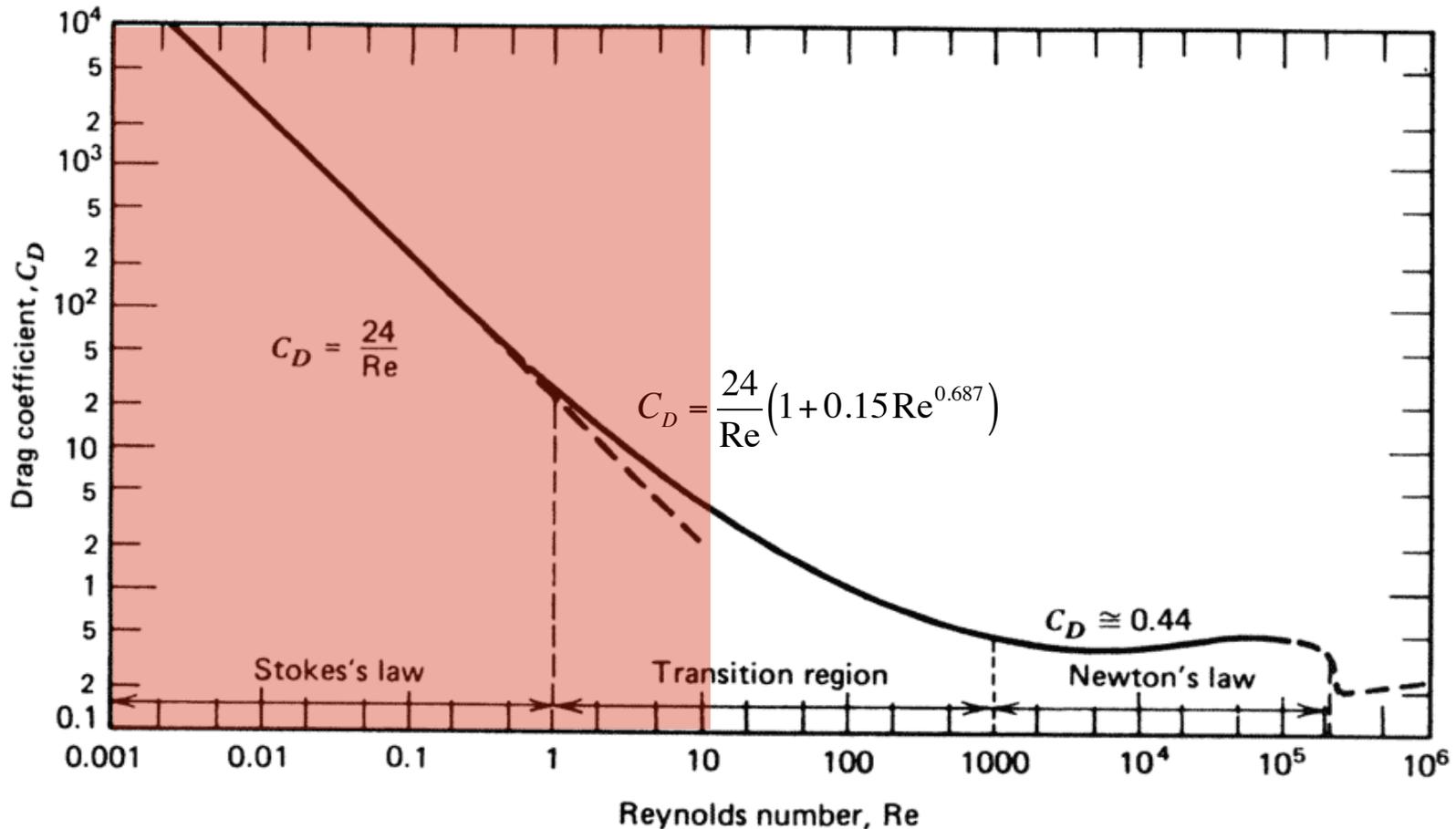
- $Re$  for various particle diameters at STP:
  - Reynolds numbers for particles in air falling at their terminal settling velocities at 298 K

Diameter ( $\mu\text{m}$ )	$Re$
0.1	$7 \times 10^{-9}$
1	$2.8 \times 10^{-6}$
10	$2.5 \times 10^{-3}$
20	0.02
60	0.4
100	2
300	20

- Almost all atmospheric aerosols are in the Stokes' regime and Stokes' law can be applied (i.e.,  $d_p < \sim 80 \mu\text{m}$ )

# Particle motion in gases: Stokes' regime

- Drag coefficient,  $C_D$ :



**FIGURE 3.1** Drag coefficient versus Reynolds number for spheres.

# Particle motion in gases: Newton's and Stokes' Laws

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- When a particle is released into the air, it quickly reaches its **“terminal settling velocity,”**  $V_{TS}$ 
  - $V_{TS}$  is a condition of constant velocity wherein the drag force of the air on the particle  $F_D$  is exactly equal but opposite to the force of gravity  $F_G$

$$F_G = mg = \frac{\pi}{6} \rho_p d_p^3 g \qquad F_D = 3\pi\mu V d_p$$

$$\frac{\pi}{6} \rho_p d_p^3 g = 3\pi\mu V d_p$$

$$V_{TS} = \frac{\rho_p d_p^2 g}{18\mu}$$

# Particle motion in gases

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- In the derivation of Stokes' law, it is assumed that the relative velocity of the gas (air) at the surface of the particle is zero
- This doesn't hold for small particles whose size approaches the mean free path of air ( $Kn \leq 1$ )
  - Particles less than about 1  $\mu\text{m}$
- Stokes' law has to be corrected for “slip” conditions:
  - Cunningham slip correction factor,  $C_C$ :

$$F_D = \frac{3\pi\mu V d_p}{C_C}$$

$$C_C = 1 + \frac{\lambda}{d_p} \left( 2.34 + 1.05e^{-0.39\frac{d_p}{\lambda}} \right)$$

Based on  $Kn \rightarrow$  lets you use Stokes' law for all regimes

# Particle motion in gases: $V_{TS}$ with slip correction

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$$F_G = mg = \frac{\pi}{6} \rho_p d_p^3 g \quad F_D = \frac{3\pi\mu V d_p}{C_C}$$

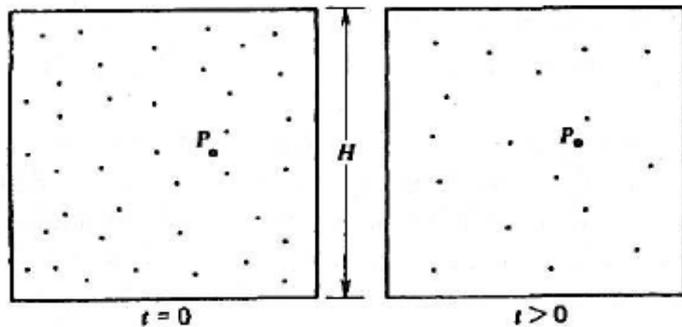
$$\frac{\pi}{6} \rho_p d_p^3 g = \frac{3\pi\mu V d_p}{C_C}$$

$$V_{TS} = \frac{\rho_p d_p^2 g C_C}{18\mu}$$

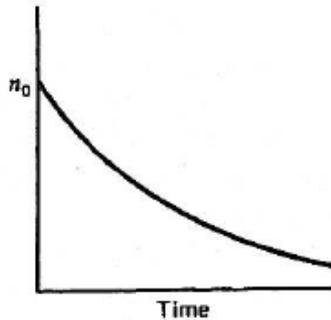
For  $Re < 1$ , which is true for most  $d_p < 100 \mu\text{m}$

# Particle motion in gases

- Terminal settling velocity for particles at STP
- What can we use  $V_{TS}$  for?
- Imagine “stirred settling”

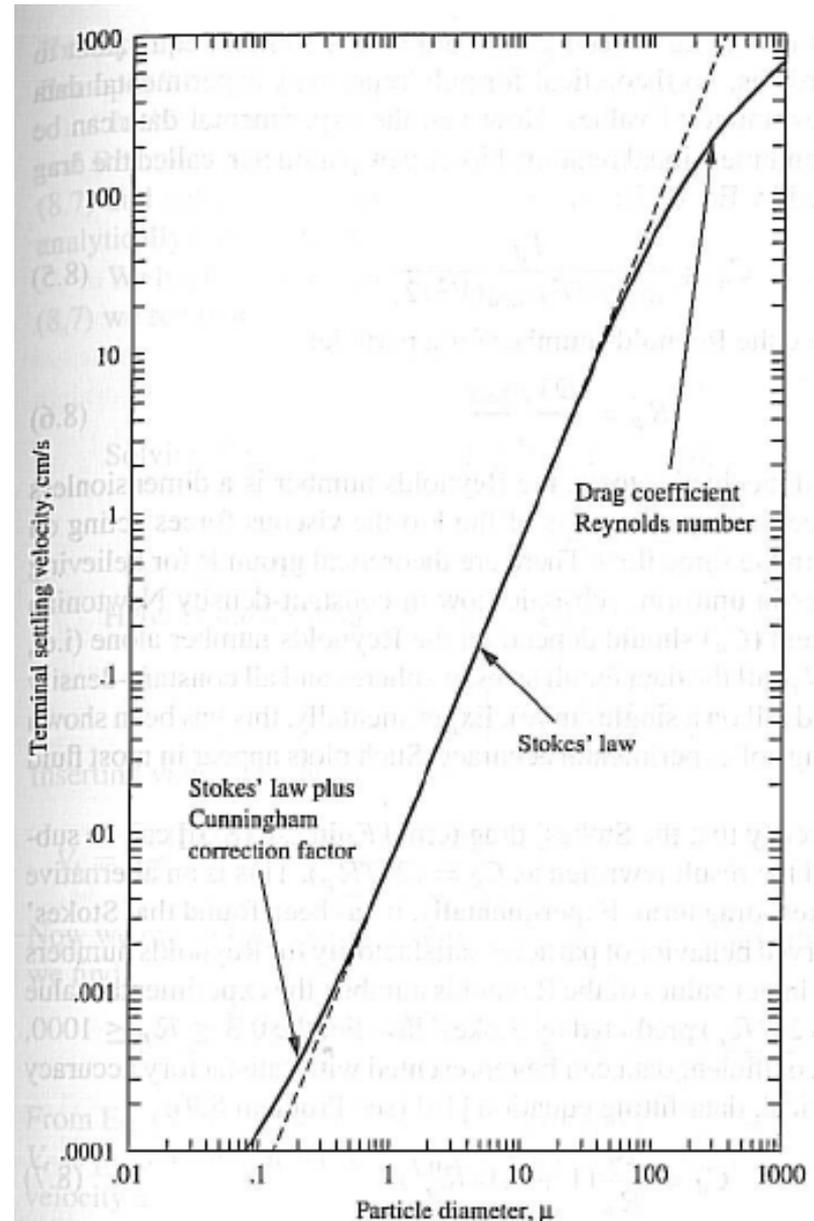


Concentration at P



$$N(t) = N_{t=0} e^{-\frac{V_{TS}t}{H}}$$

Larger particles settle out of the air faster



# Particle motion in gases

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- A couple of other important particle properties also exist
  - Equivalent diameters
  - Aerodynamic diameters
  - Stokes diameters

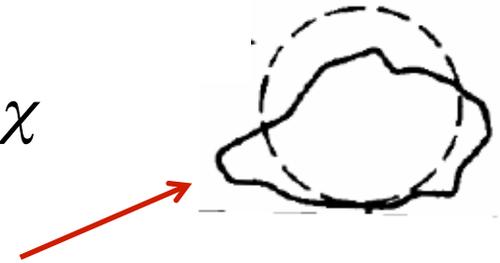
# Non-spherical particles: equivalent diameters

- Many aerosol particles are not spherical
  - For example, soot particles, mineral dust, sea salt
- We can account for the effect of shape on particle motion by introducing a **dynamic shape factor**,  $\chi$ :

Shape	Dynamic Shape Factor, <sup>a</sup> $\chi$		
	Axial Ratio		
	2	5	10
<i>Geometric Shapes</i>			
Sphere	1.00		
Cube <sup>b</sup>	1.08		
Cylinder <sup>b</sup>			
Vertical axis	1.01	1.06	1.20
Horizontal axis	1.14	1.34	1.58
Orientation averaged	1.09	1.23	1.43
Straight chain <sup>c</sup>	1.10	1.35	1.68
Compact cluster			
Three spheres	1.15		
Four spheres	1.17		
<i>Dusts</i>			
Bituminous coal <sup>d</sup>	1.05–1.11		
Quartz <sup>d</sup>	1.36		
Sand <sup>d</sup>	1.57		
Talc <sup>e</sup>	1.88		

$$V_{TS} = \frac{\rho_p g C_C d_e^2}{18\mu\chi}$$

$$F_D = \frac{3\pi\mu V d_e}{C_C} \chi$$



$d_e$  = volume equivalent diameter, or the diameter of a sphere having the same volume and density as the nonspherical particle

$\chi$  = ratio of the actual resisting force of the nonspherical particle to the resisting force a sphere of the same volume and density would have

# Aerodynamic and Stokes diameters

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Two other equivalent diameters are commonly used:

- The **aerodynamic diameter** ( $d_a$ ) is the diameter of a spherical particle having the density of water (1 g/cm<sup>3</sup>) and having the same settling velocity as the particle in question
- The **Stokes diameter** ( $d_s$ ) is the diameter of a spherical particle having the same density and settling velocity as the particle in question

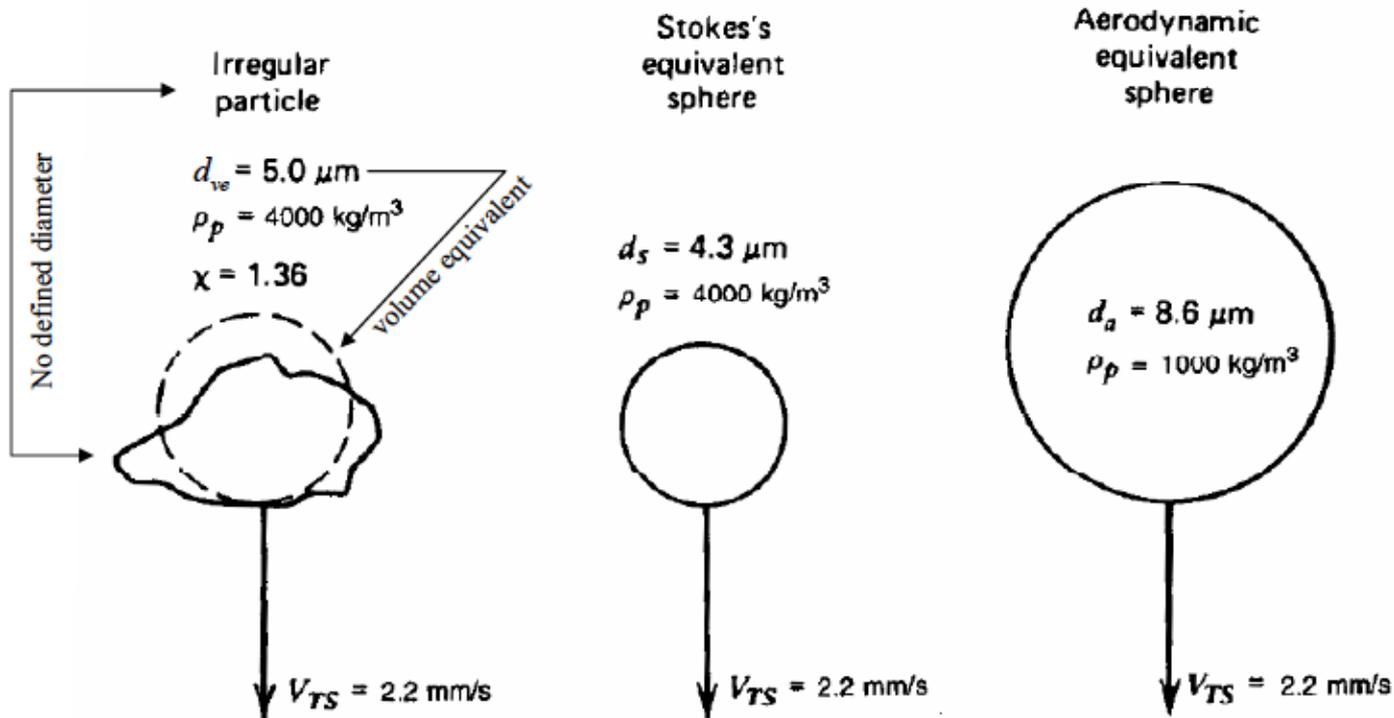
$$V_{TS} = \frac{\rho_p g C_C(d_e) d_e^2}{18\mu\chi} = \frac{\rho_0 g C_C(d_a) d_a^2}{18\mu} = \frac{\rho_p g C_C(d_s) d_s^2}{18\mu}$$

- Note that  $C_C$  has to be calculated as a function of the diameter you're using

# Aerodynamic and Stokes diameters

- For particles with  $d_p > 1 \mu\text{m}$  we can assume  $C_C = 1$ :

$$\frac{\rho_p d_{ve}^2}{\chi} = \rho_p d_S^2 = \rho_0 d_a^2$$



Non-spherical particle and its equivalent diameters

# Other forces

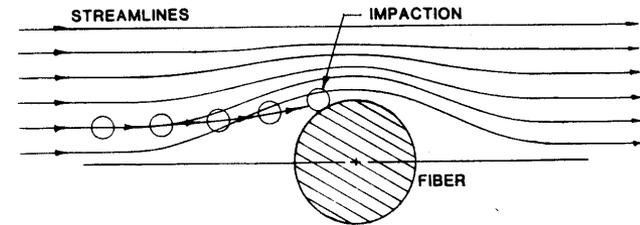
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- Other forces governing particle motion
  - Gravity (already covered)
  - Inertial impaction
  - Brownian diffusion
  - Electrophoretic
  - Thermophoretic
- We don't have time to cover these in full detail
  - But I will provide basic concepts and equations so we can understand what forces act to remove particles of various  $d_p$  from air

# Other important forces

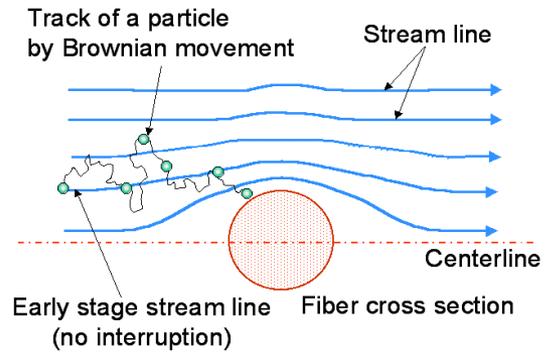
- **Inertial impaction**

- Inertial transfer of particles onto surfaces
- Important for larger particles: scales with  $d_p^2$



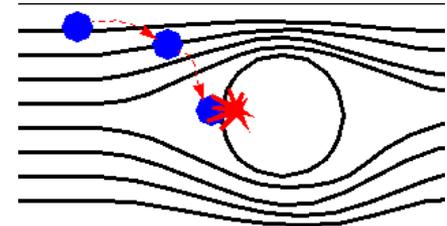
- **Brownian diffusion**

- Movement by random molecular motion across a concentration gradient
- Important for smaller particles: scales with  $1/d_p$



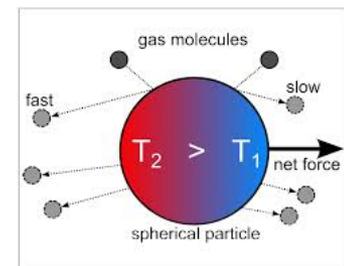
- **Electrophoretic/electrostatic forces**

- Particles can and do acquire charges and can be attracted to oppositely charged surfaces
- Important for smaller particles: scales with  $1/d_p$



- **Thermophoretic forces**

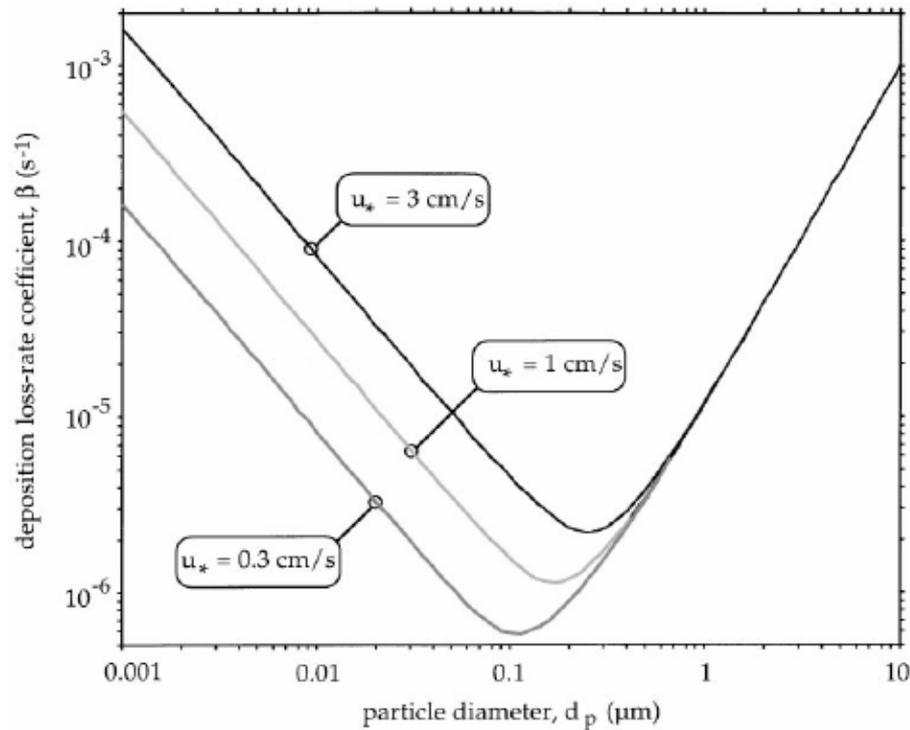
- Particle movement driven by a temperature gradient
- Weak function of  $d_p$  (but nearly constant for all  $d_p$ )



# All forces combine to impact particle **deposition**

- More on this later, but these effects combine to influence particle deposition rates and rate constants

– Particle deposition rate coefficient onto surfaces (1/hr):  $k_{dep} = \frac{v_d A}{V}$



\*Note that ‘friction velocity’ is a function of the ratio of shear stress at a surface to air density

Fig. 5. Particle deposition loss-rate coefficient,  $\beta$ , for typical room dimensions (3 m high  $\times$  4 m  $\times$  5 m) according to the current model. Friction velocities of 0.3–3  $\text{cm s}^{-1}$  approximately span the range expected for mechanically ventilated indoor spaces. Predictions assume air pressure is 1 atm, temperature is 293 K and particle density is  $1.0 \text{ g cm}^{-3}$ .

# **PARTICLE SIZE DISTRIBUTIONS**

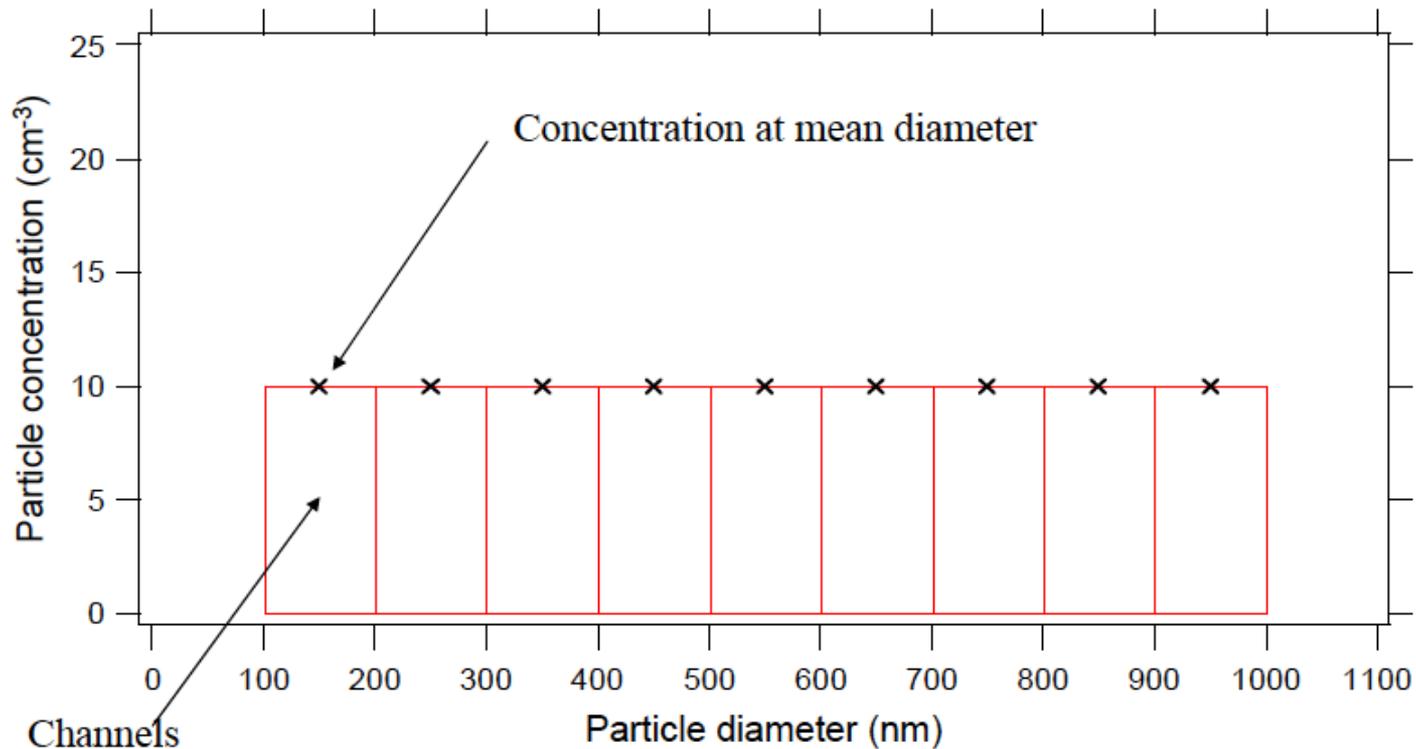
# Size distributions

---

- A **monodisperse** aerosol (i.e., all particles have the same size) does not exist in the ambient atmosphere
  - Not indoors or outdoors
- What we have are **polydispersed** aerosols
  - So we need to describe the sizes of aerosol particles with a particle size distribution (PSD), which gives the concentration of particles as a function of particle diameter
  - Practically, a number concentration is determined between ranges of particle sizes: e.g., in the range  $d_{p2} - d_{p1}$  or  $\Delta d_p$  or  $dd_p$ 
    - Number of particles with diameters between  $d_{p2}$  and  $d_{p1}$

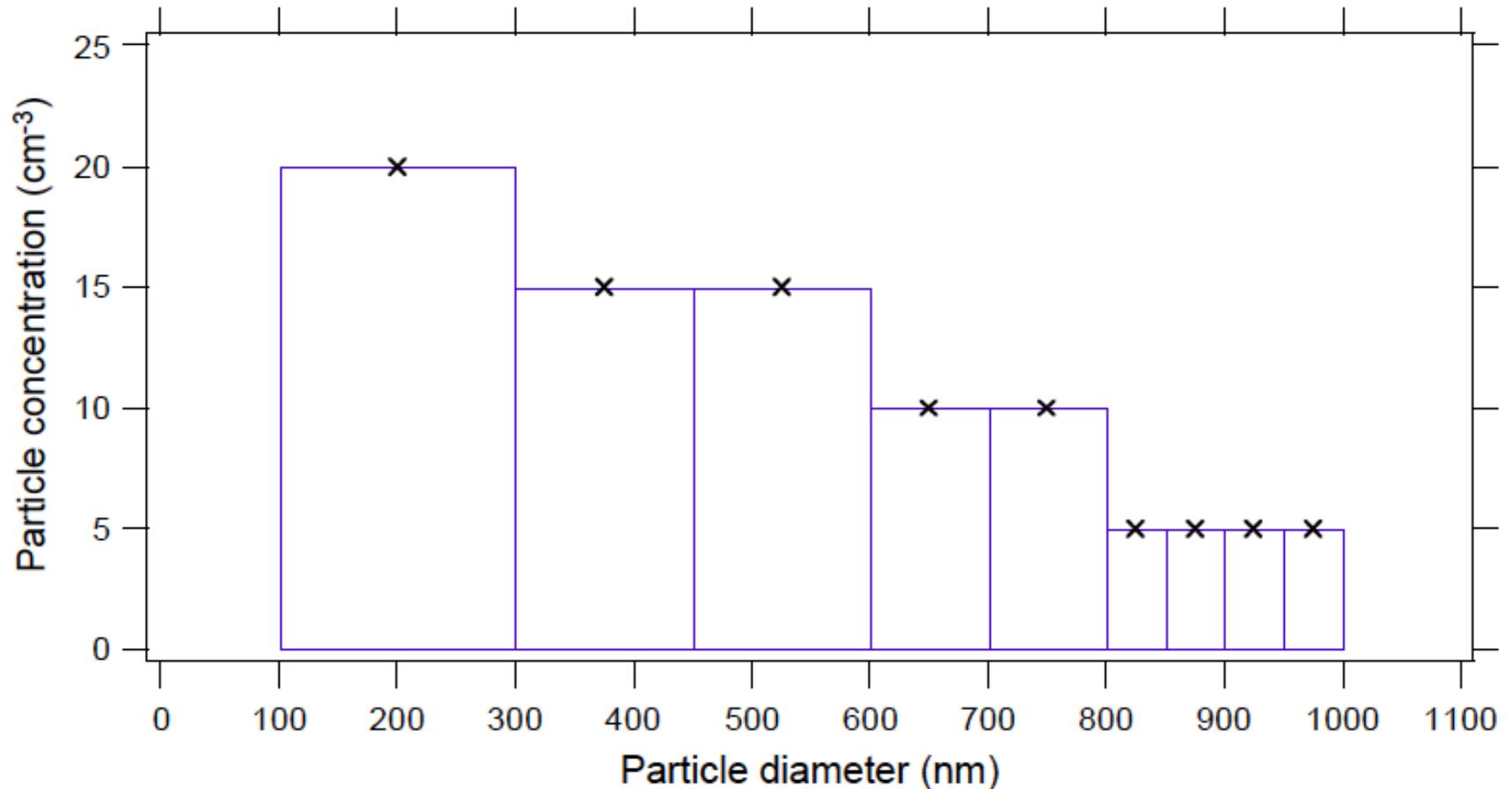
# Size distributions

- Example instrument: 9 size channels, width of 100 nm each, each with 10 particles per  $\text{cm}^3$
- We consider the measured concentration as  $dN$  in each channel



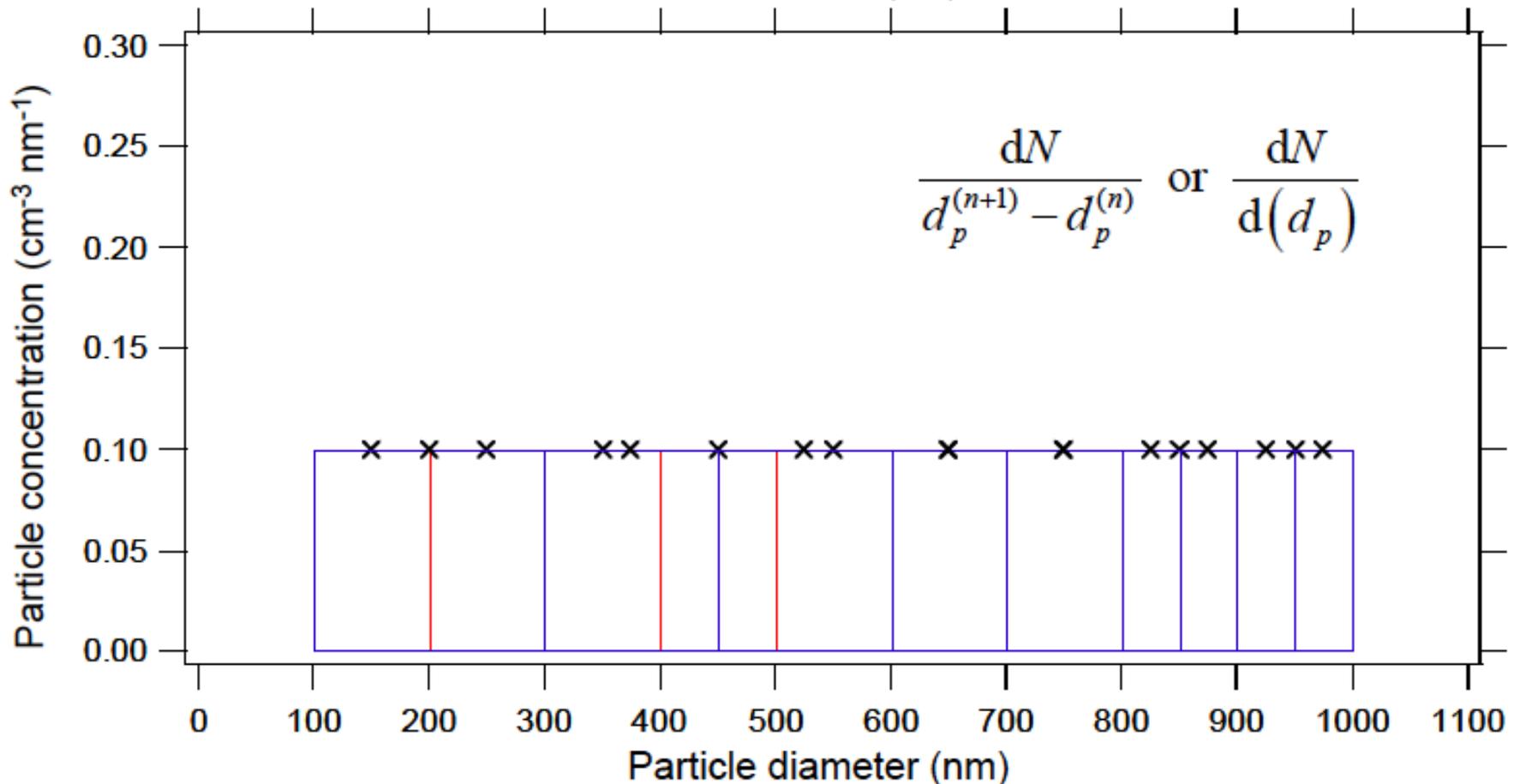
# Size distributions

- If we use a different instrument with different channel widths, the shape of the distribution changes:



# Size distributions

- To avoid this sizing effect, we divide the measured concentrations (dN) by the width of the size channels

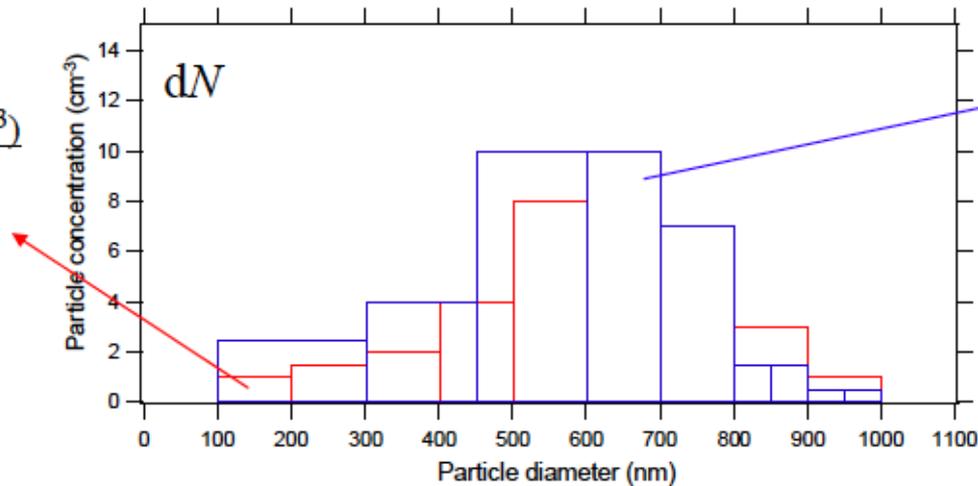


# Size distributions

- Similar example but for a more realistic size distribution

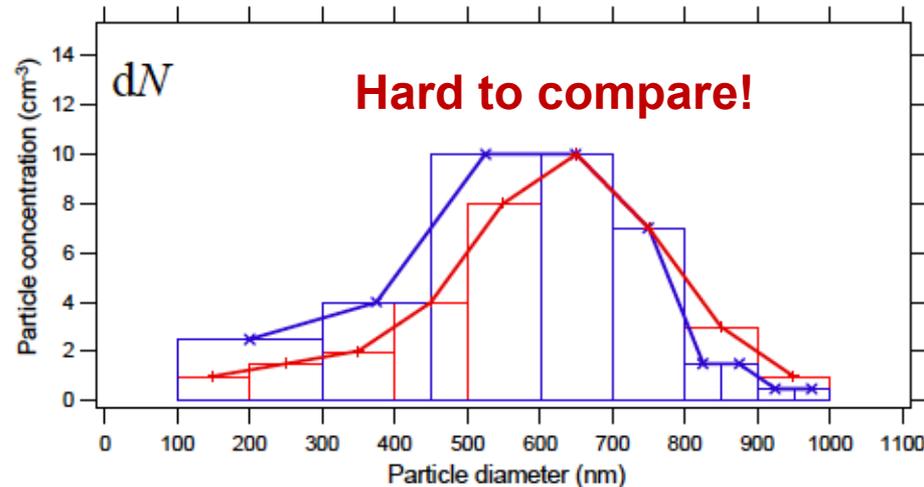
"Instrument 1"

Channel	N (cm <sup>-3</sup> )
100-200	1
200-300	1.5
300-400	2
400-500	4
500-600	8
600-700	10
700-800	7
800-900	3
900-1000	1



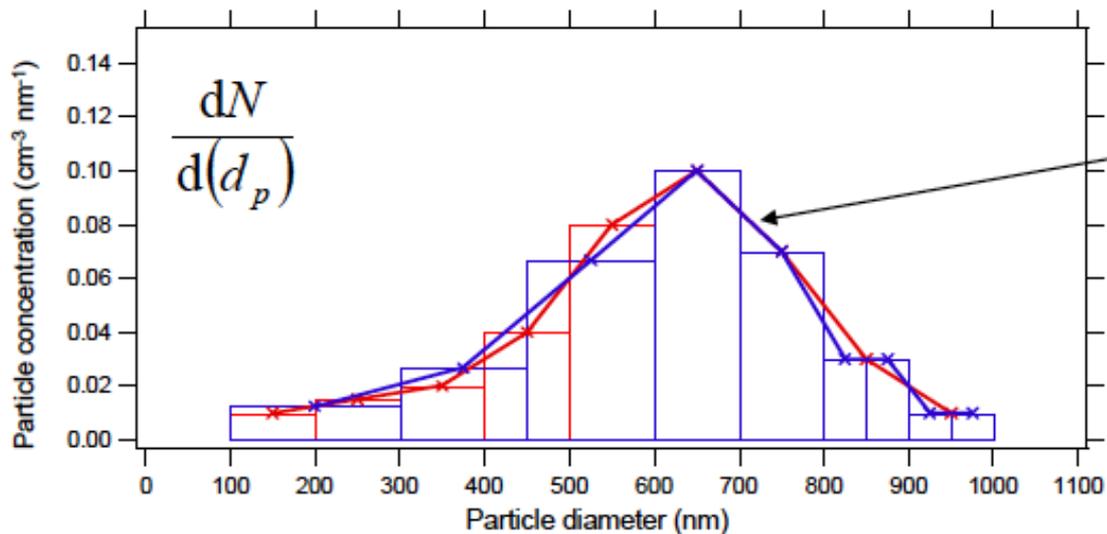
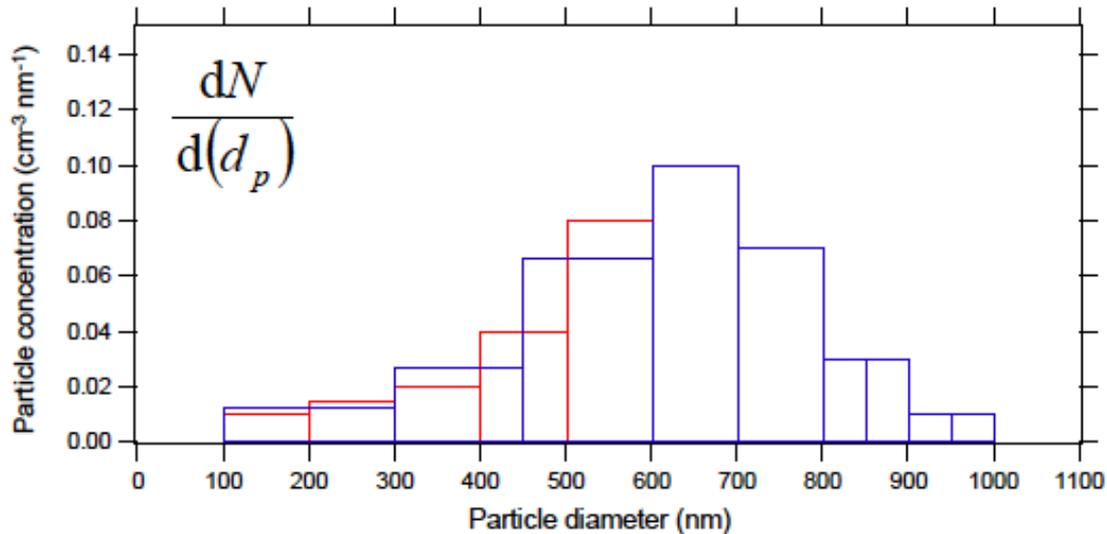
"Instrument 2"

Channel	N (cm <sup>-3</sup> )
100-300	2.5
300-450	4
450-600	10
600-700	10
700-800	7
800-850	1.5
850-900	1.5
900-950	0.5
950-1000	0.5



# Size distributions

- Divide by the channel widths... (better)

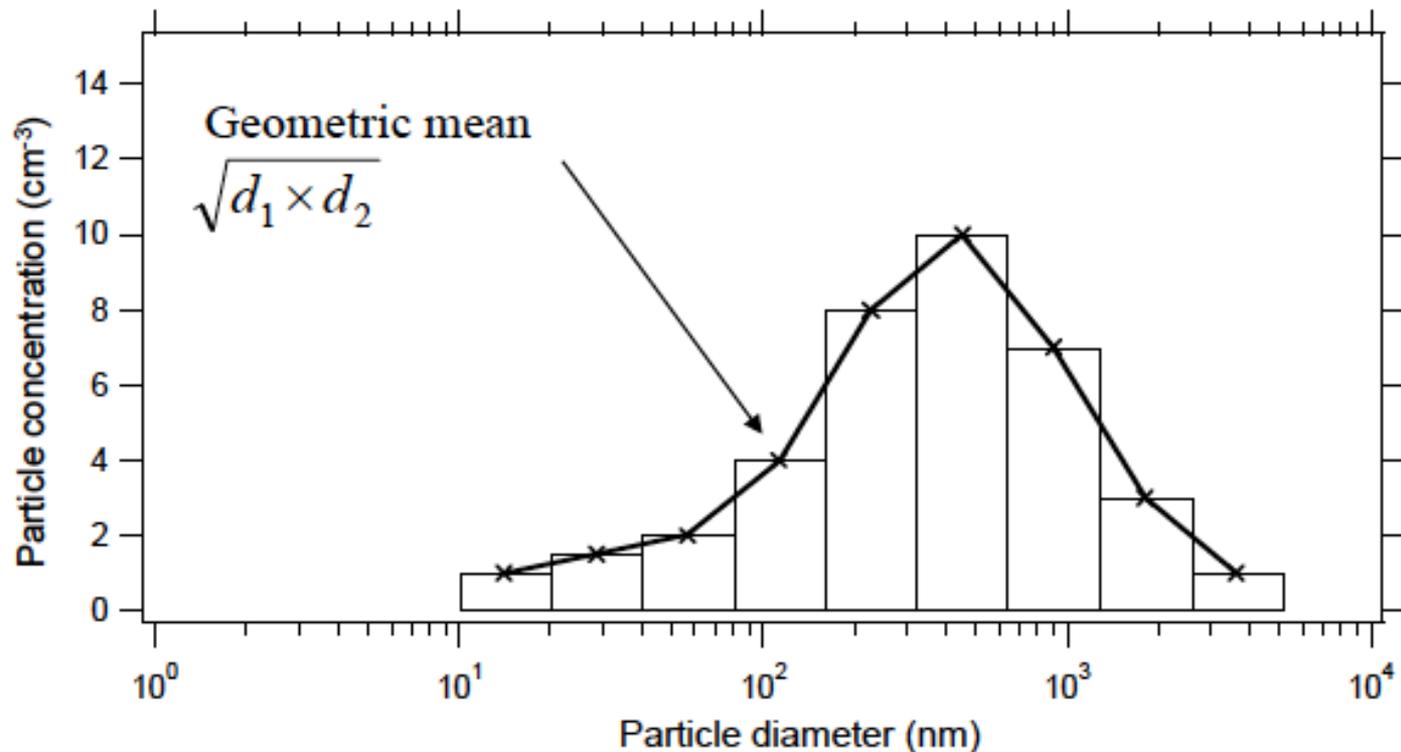


Almost the same distribution despite different measurement channels for the two instruments

# Size distributions

- Since the size range of aerosol particles typically ranges over **several orders of magnitude**, we commonly use log scales for the x-axis ( $d_p$ ) and refer to particle size bins by their geometric mean diameter

Channel	N (cm <sup>-3</sup> )
10-20	1
20-40	1.5
40-80	2
80-160	4
160-320	8
320-640	10
640-1280	7
1280-2560	3
2560-5120	1

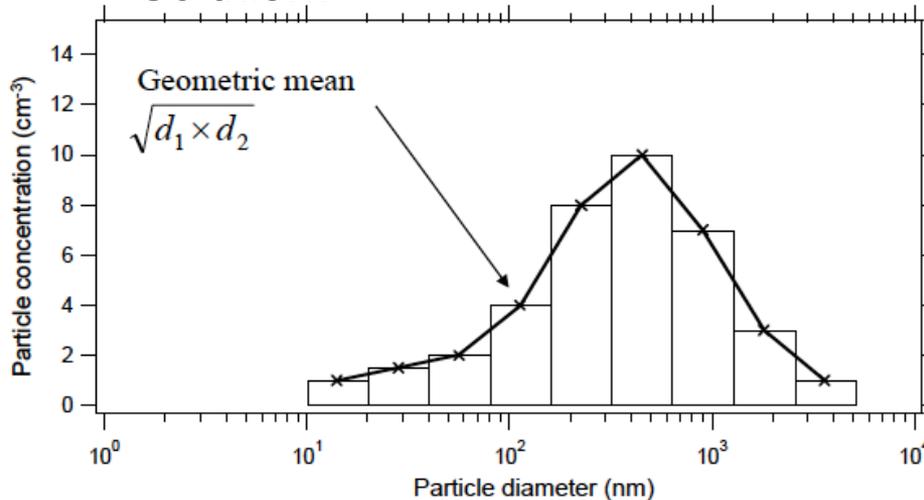


# Size distributions

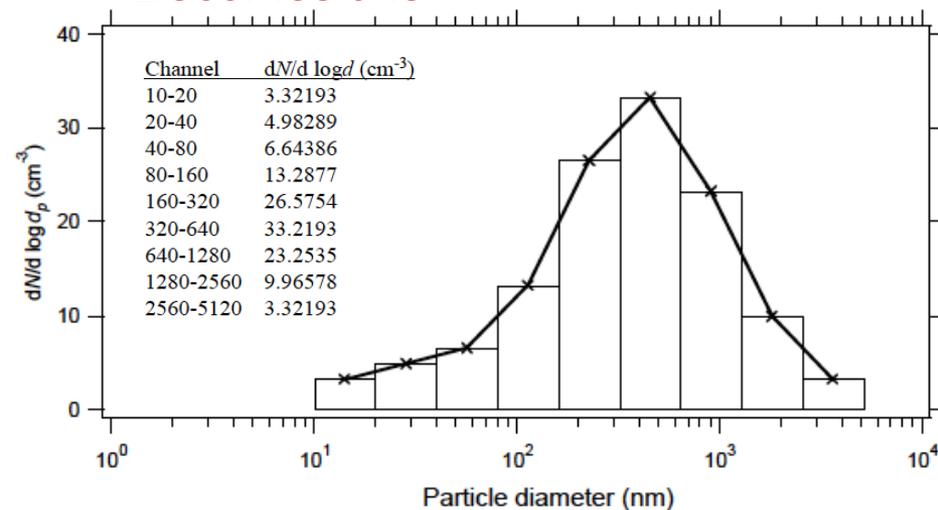
- For log scales we need to account for the channel width differently:

$$\frac{dN}{d \log d_p} = \frac{dN}{\log(d_{p,upperbound}) - \log(d_{p,lowerbound})}$$

So this...



Becomes this...



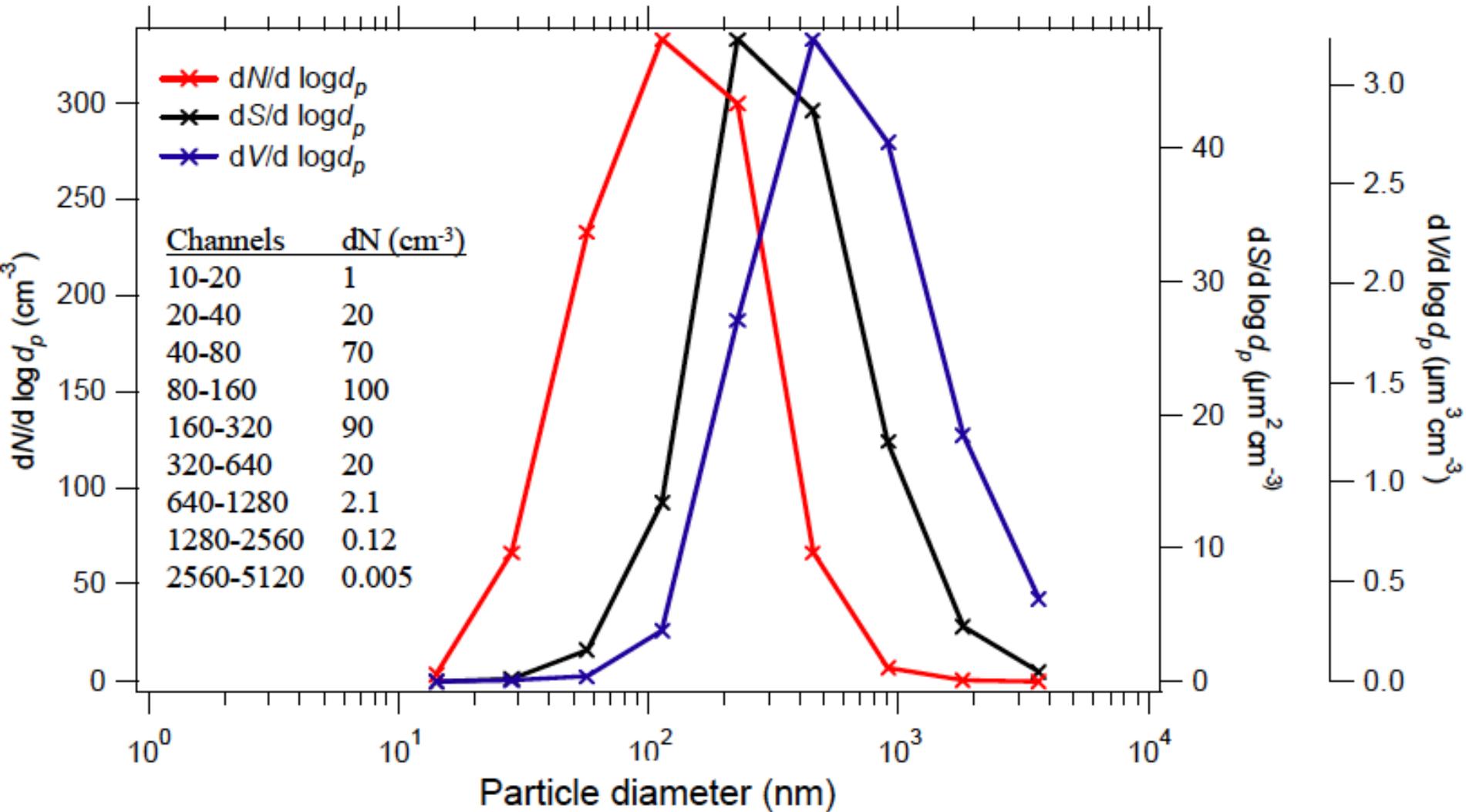
We have transformed  $dN$  into  $dN/d \log d_p$ ,  
but the graphs **scale similarly**

# Number, surface area, volume, and mass distributions

---

- Assuming spherical particles, the number concentration for each particle diameter can be converted to surface and volume concentrations:
- Surface area ( $\mu\text{m}^2$  per  $\text{cm}^3$ ):  $dS = \pi d_p^2 dN$
- Volume ( $\mu\text{m}^3$  per  $\text{cm}^3$ ):  $dV = \frac{\pi}{6} d_p^3 dN$
- If we know particle density
  - We can estimate the mass distribution ( $\mu\text{g}$  per  $\text{cm}^3$ ):  $dM = \rho_p \frac{\pi}{6} d_p^3 dN$

# Number, surface area, volume, and mass distributions



# Describing distributions mathematically

---

- Let  $n(D_p)$  = size distribution function ( $\mu\text{m}^{-1} \text{cm}^{-3}$ )
- Let  $dN = n(D_p)dD_p$  = number of particles per unit volume of air having diameters in the range  $D_p$  to  $(D_p + dD_p)$
- Total number of particles per unit volume of air is:

$$N = \int_0^{\infty} n(D_p)dD_p \quad [\#/ \text{cm}^3]$$

# Describing distributions mathematically

---

- Because particle diameters in an aerosol often vary over several orders of magnitude, it is usually most convenient to express the size distribution in terms of the logarithm of the particle diameter
  - Either  $\ln(D_p)$  or  $\log(D_p)$
- Define:  $dN = n(\log D_p) d\log D_p$ 
  - Where  $dN$  = the number of particles per  $\text{cm}^3$  of air in the size range of  $\log D_p$  to  $\log D_p + d\log D_p$
  - Note:  $n(\log D_p) \neq n(D_p)$

# Describing distributions mathematically

---

- Total number of particles is therefore:

$$N = \int_{-\infty}^{\infty} n(\log D_p) d\log D_p \quad [\text{cm}^{-3}]$$

- Normalized size distribution function with respect to  $\log D_p$ :

$$\tilde{n}(\log D_p) = \frac{n(\log D_p)}{N} \quad [\text{dimensionless}]$$

- Generic log-normal distributions:

- If quantity  $u$  is log-normally distributed, the probability density function for  $u$  obeys a Gaussian distribution:

$$n(u) = \frac{N}{\sigma_u \sqrt{2\pi}} \exp\left[-\frac{(u - \bar{u})^2}{2\sigma_u^2}\right] \quad \begin{array}{l} \bar{u} = \text{mean} \\ \sigma^2 = \text{variance} \\ \sigma = \text{std dev} \end{array}$$

# Describing distributions mathematically

---

- For our purposes, replace  $\bar{u}$  with the arithmetic mean of  $\ln D_p$ , which is defined as the geometric mean diameter  $D_g$ :

$$\ln D_g = \frac{\sum n_i \ln D_{p,i}}{N}$$

- And the standard deviation,  $\sigma$ , is replaced by the standard deviation of the logarithms, called the geometric standard deviation,  $\sigma_g$ :

$$\ln \sigma_g = \left[ \frac{\sum n_i (\ln D_i - \ln D_g)^2}{N - 1} \right]^{1/2}$$

# Describing distributions mathematically

---

- The size distribution function,  $n(D_p)$ , can now be described following a log-normal distribution:

$$n(D_p) = \frac{N}{D_p \times (\ln \sigma_g) \sqrt{2\pi}} \exp \left[ \frac{-\left(\ln D_p - \ln D_g\right)^2}{2(\ln \sigma_g)^2} \right]$$

- Where the aerosol can be described with only 3 parameters:

$N$ : Total particle number concentration

$\sigma_g$ : Geometric standard deviation

$\bar{d}_g$ : Geometric mean diameter

$d_g$  is in units of  $\mu\text{m}$

$\ln(d_g)$  or  $\log(d_g)$  is dimensionless

$\sigma_g$  is dimensionless with a value greater than or equal to 1.0

# Describing distributions mathematically

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- Then, the cumulative distribution of an aerosol can then be characterized as follows:

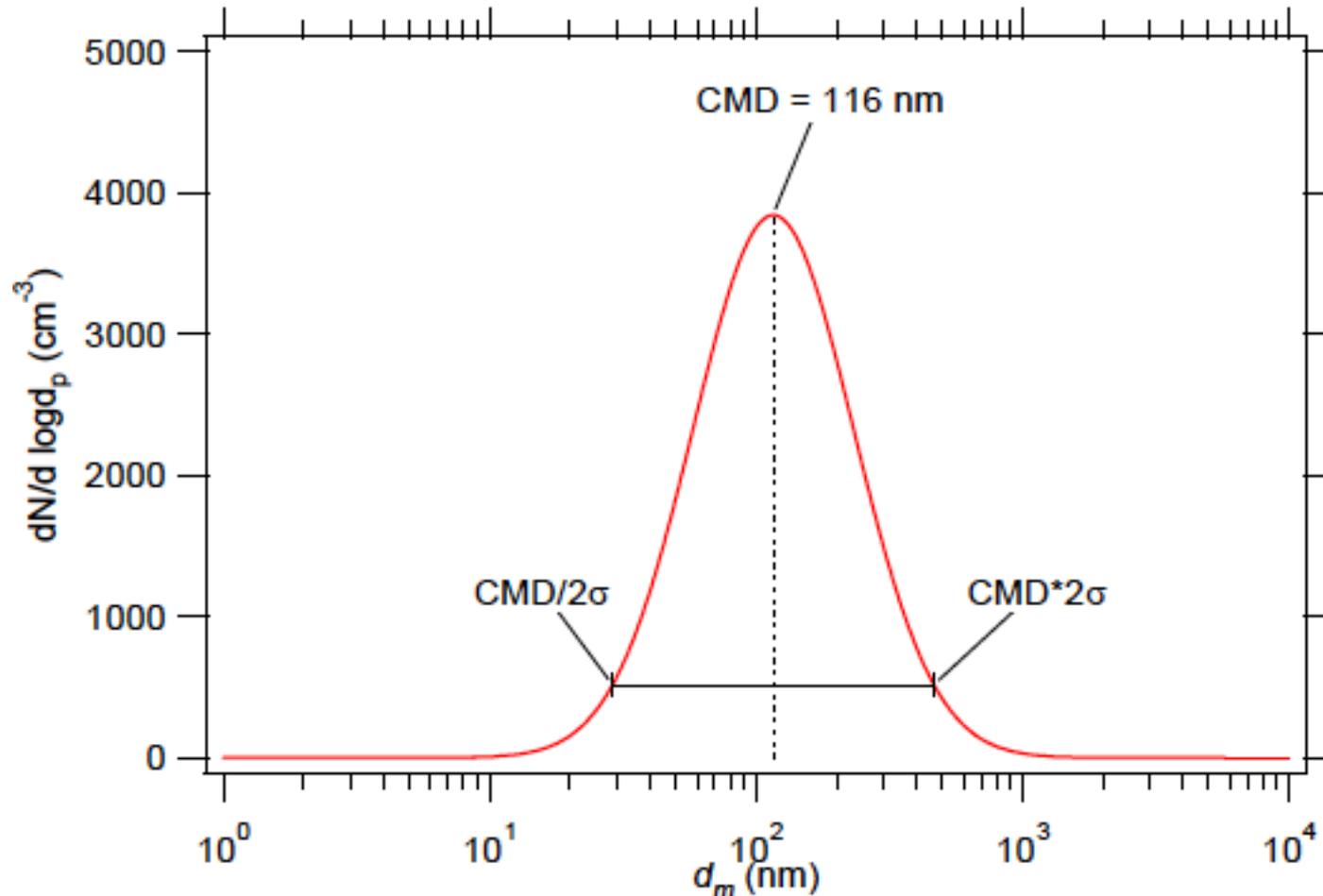
$$F(D_p) = \frac{N}{2} + \frac{N}{2} \operatorname{erf} \left[ \frac{\ln \left( \frac{D_p}{D_g} \right)}{\ln \sigma_g \times \sqrt{2}} \right]$$

$F(D_p)$  is in units of  $\#/cm^3$

- If a lognormal distribution based on number, then  $D_g$  is known as the count mean diameter (CMD), or the particle size for which half the total number of particles is larger and half is smaller
  - Mass median diameter (MMD) if distribution is based on mass

# Lognormal distribution

- 95% of particles are in a size range given by:  $e^{\ln \bar{d}_g \pm 2 \ln \sigma_g}$



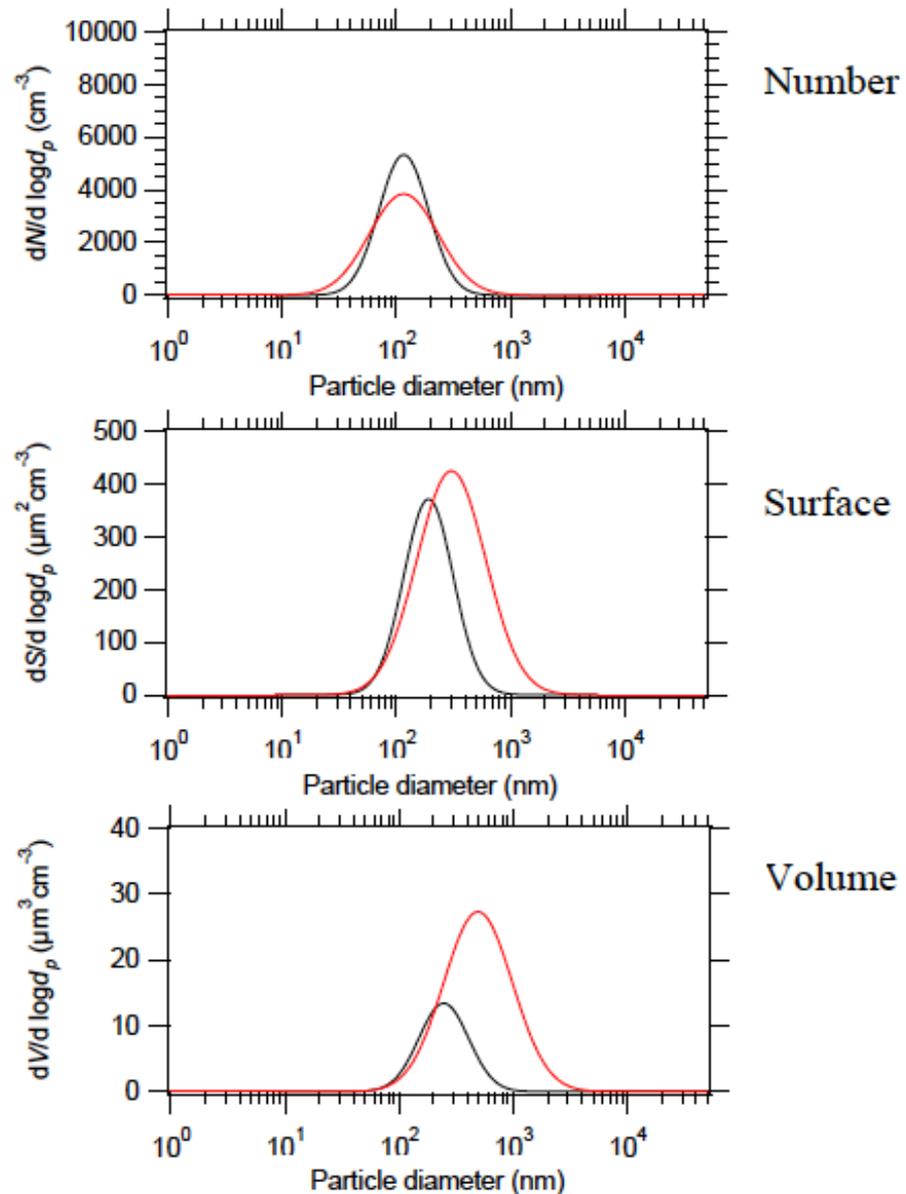
# Lognormal distribution: dN, dS, and dV

- Example distribution for one 'mode':

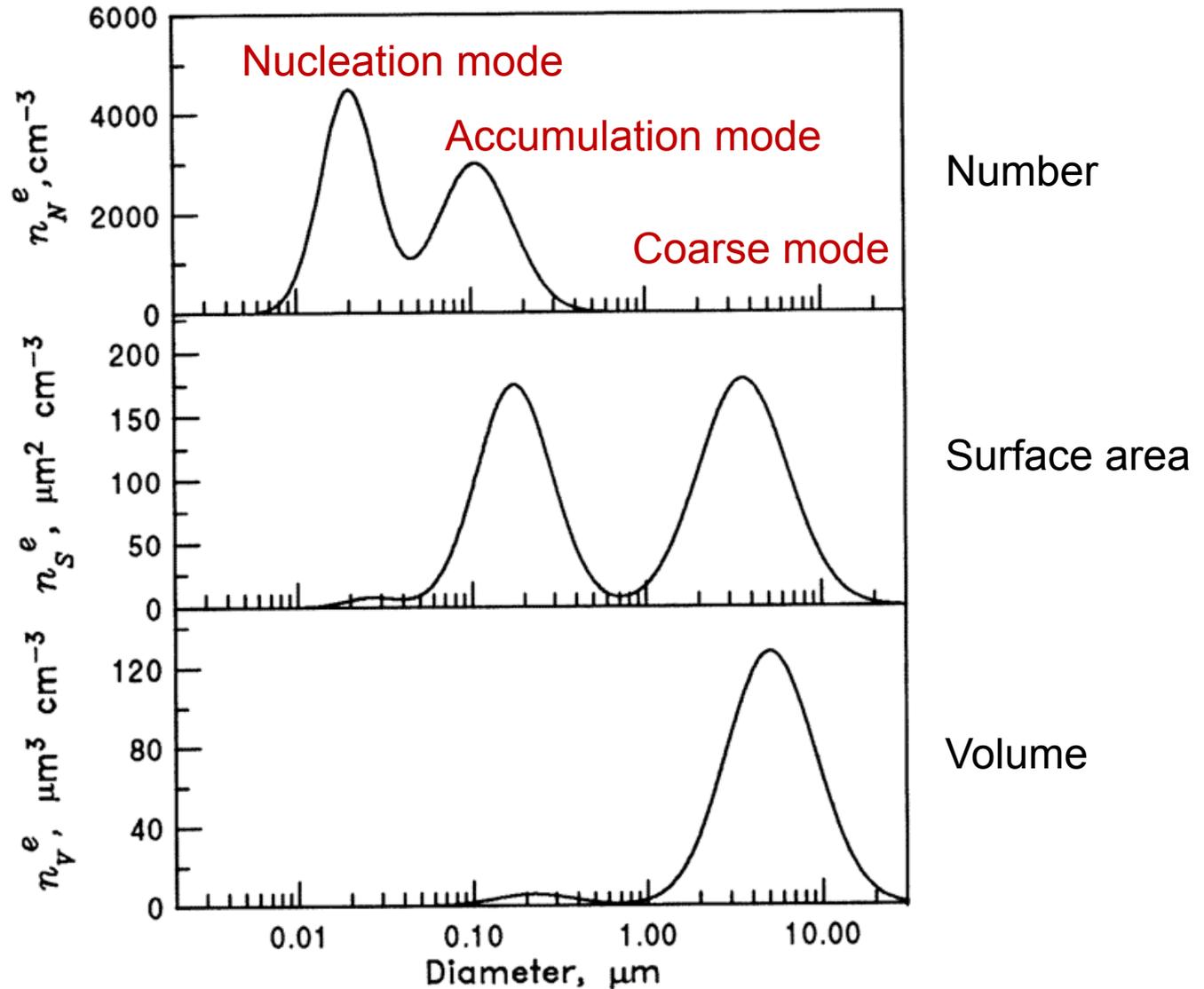
$$N = 2900 \text{ cm}^{-3}$$

~~$$\sigma_g = 1.65$$~~ 
$$\sigma_g = 2.0$$

$$\bar{d}_g = 116 \text{ nm}$$



# Typical aerosol distributions include multiple 'modes'



# Lognormal distributions: Summing across modes

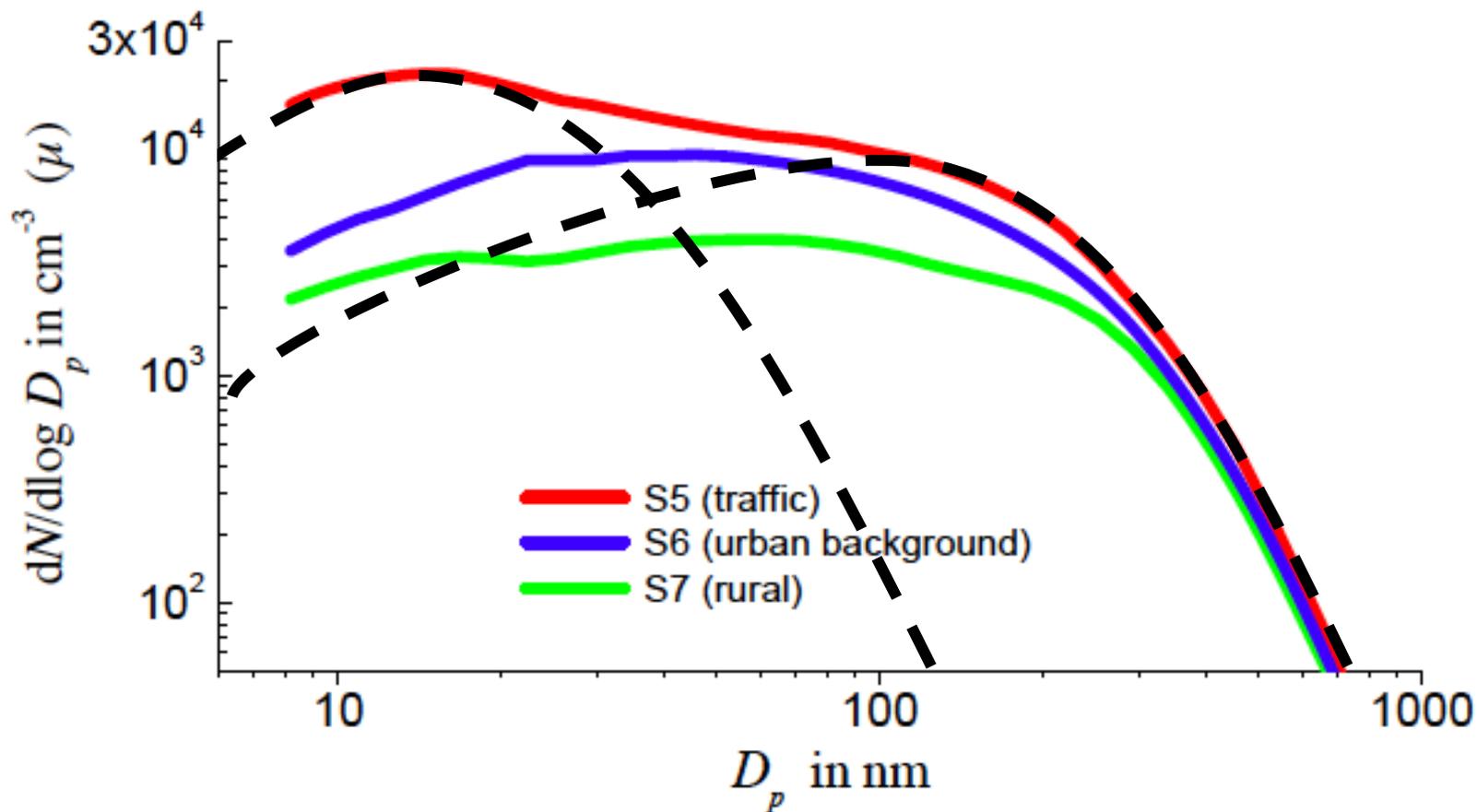
$$\frac{dN}{d \log d_p} = \sum_{i=1}^n \frac{N_i}{\sqrt{2\pi \log \sigma_i}} e^{-\left(\frac{(\log d_p - \log \bar{d}_{g,i})^2}{2(\log \sigma_i)^2}\right)}$$

Type	Mode I			Mode II			Mode III		
	$N$ ( $\text{cm}^{-3}$ )	$D_p$ ( $\mu\text{m}$ )	$\log \sigma$	$N$ ( $\text{cm}^{-3}$ )	$D_p$ ( $\mu\text{m}$ )	$\log \sigma$	$N$ ( $\text{cm}^{-3}$ )	$D_p$ ( $\mu\text{m}$ )	$\log \sigma$
Urban	$9.93 \times 10^4$	0.013	0.245	$1.11 \times 10^3$	0.014	0.666	$3.64 \times 10^4$	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	$3 \times 10^{-4}$	8.6	0.291
Desert	726	0.002	0.247	114	0.038	0.770	0.178	21.6	0.438

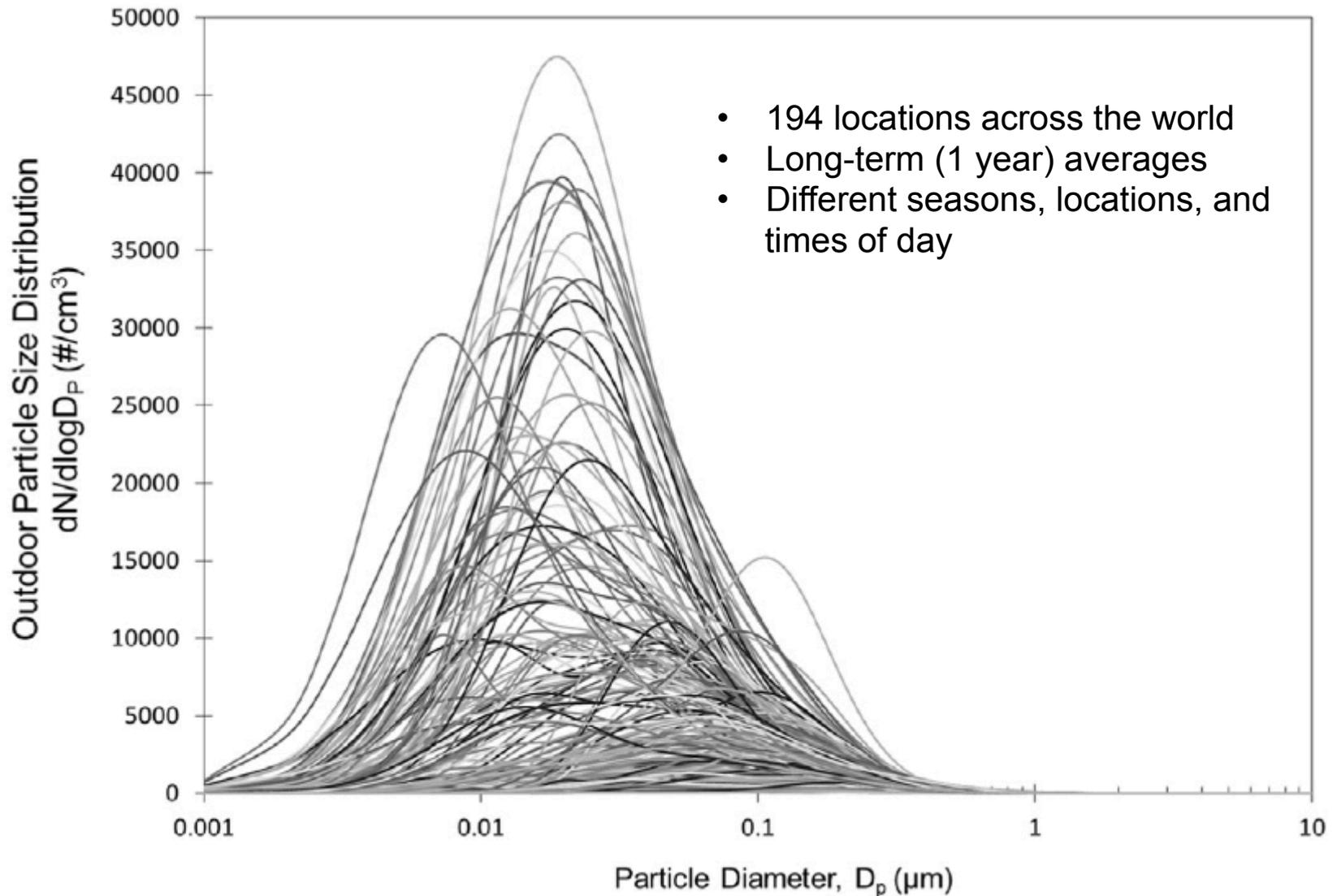
Source: Jaenicke (1993).

# Typical outdoor PSDs

- Submicron particles outdoors in 3 locations in Germany



# Typical outdoor PSDs



# Riley et al 2002 particle size distributions

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- See Excel sheet

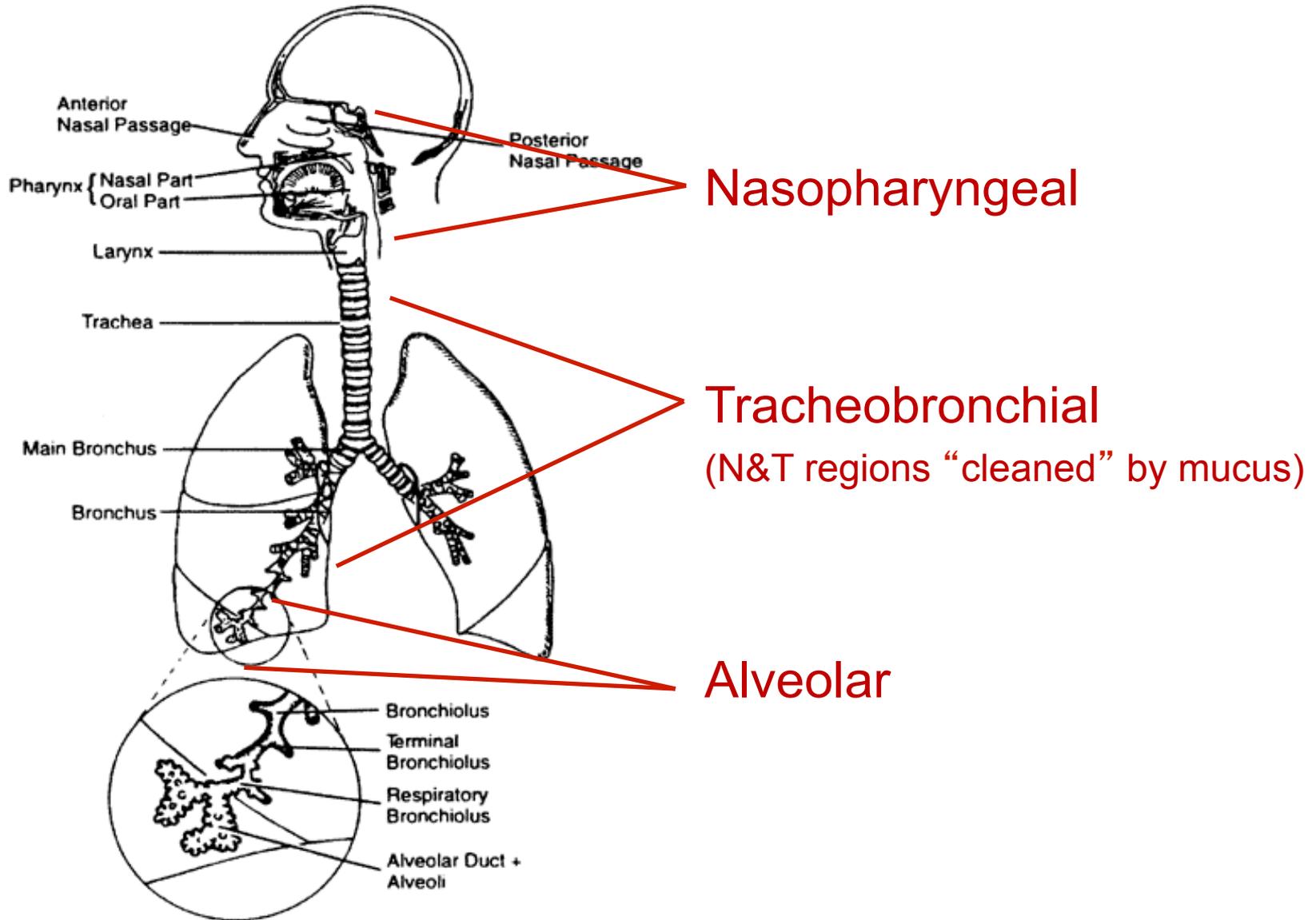
# **RESPIRATORY DEPOSITION**

# Why are we so concerned about particle size?

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- One reason is because particles of different sizes deposit in different areas of our respiratory system with different efficiencies
- Humans breathe 10-25 m<sup>3</sup>/day
  - ~0.5 L/breath at rest
  - ~12 breaths/minute at rest
- Surface area of lung devoted to gas exchange is ~75 m<sup>2</sup>
  - 1/2 area of singles tennis court in alveolar region
- Velocities range from cm/s to mm/s

# Human respiratory system



# Lung parameters

**TABLE 11.1 Characteristics of Selected Regions of the Lung<sup>a</sup>**

Airway	Generation	Number per Generation	Diameter (mm)	Length (mm)	Total Cross Section (cm <sup>2</sup> )	Velocity <sup>a</sup> (mm/s)	Residence Time <sup>b</sup> (ms)
Trachea	0	1	18	120	2.5	3900	30
Main bronchus	1	2	12	48	2.3	4300	11
Lobar bronchus	2	4	8.3	19	2.1	4600	4.1
Segmental bronchus	4	16	4.5	13	2.5	3900	3.2
Bronchi with cartilage in wall	8	260	1.9	6.4	6.9	1400	4.4
Terminal bronchus	11	2000	1.1	3.9	20	520	7.4
Bronchioles with muscles in wall	14	16,000	0.74	2.3	69	140	16
Terminal bronchiole	16	66,000	0.60	1.6	180	54	31
Respiratory bronchiole	18	$0.26 \times 10^6$	0.50	1.2	530	19	60
Alveolar duct	21	$2 \times 10^6$	0.43	0.7	3200	3.2	210
Alveolar sac	23	$8 \times 10^6$	0.41	0.5	72,000	0.9	550
Alveoli		$300 \times 10^6$	0.28	0.2			

<sup>a</sup>Based on Weibel's model A; regular dichotomy average adult lung with volume.  $0.0048 \text{ m}^3$  [ $4800 \text{ cm}^3$ ] at about three-fourths maximal inflation. Table adapted from Lippmann (1995).

<sup>b</sup>At a flow rate of  $3.6 \text{ m}^3/\text{hr}$  [ $1.0 \text{ L/s}$ ].

Note: based on steady flow

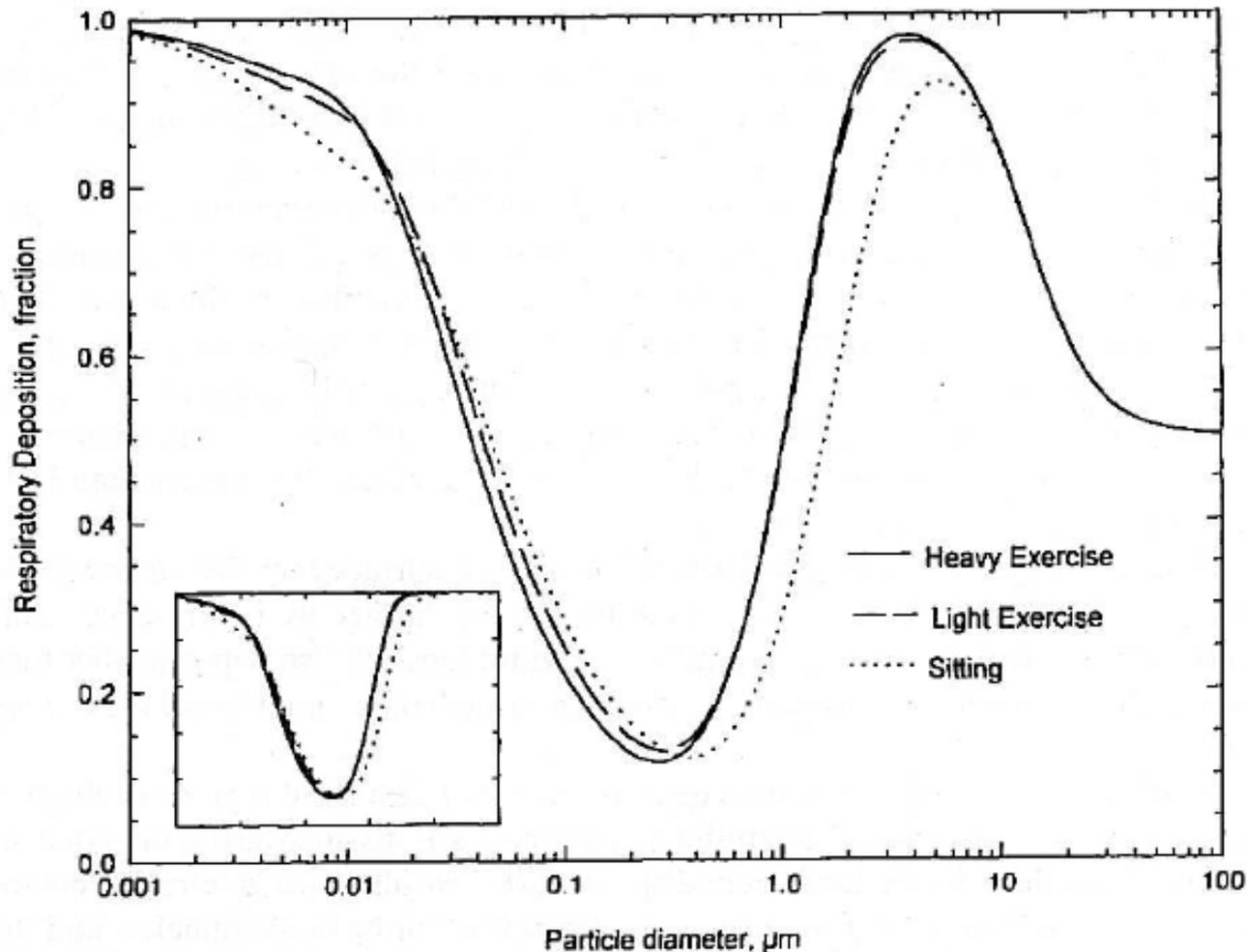
# Particle deposition in lungs

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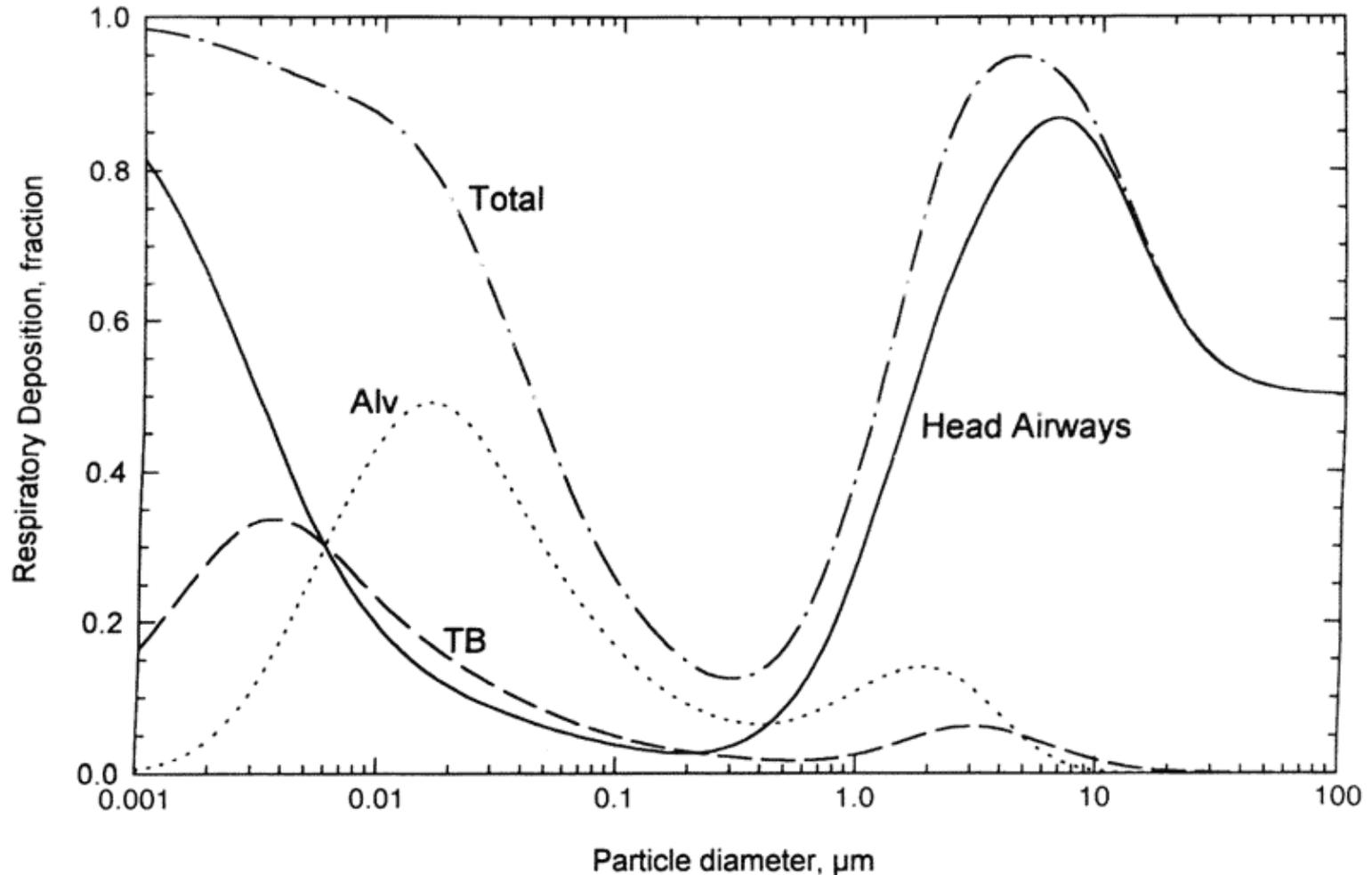
- Similar to other systems
  - Diffusion, settling, impaction are primary
  - Can neglect minor electrostatic forces
- Challenges
  - Flow field is developing and unsteady
  - Particles are growing (humidification)

# Total respiratory deposition

- Based on ICRP model, average for males/females
  - ICRP = International Commission on Radiological Protection



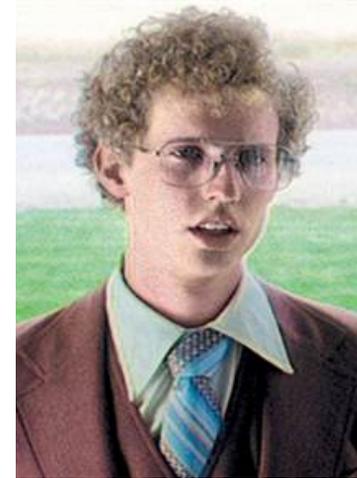
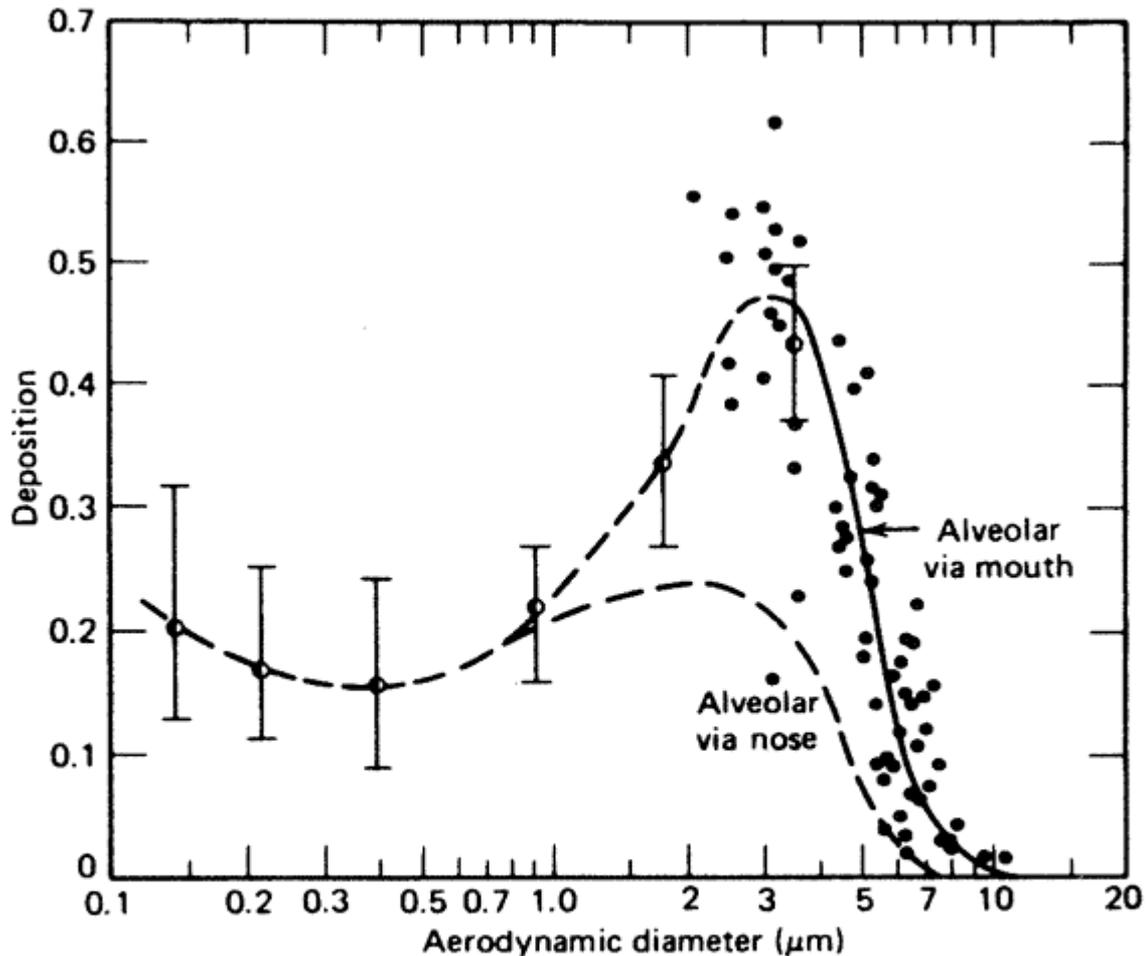
# Respiratory deposition by region



**FIGURE 11.3** Predicted total and regional deposition for light exercise (nose breathing) based on ICRP deposition model. Average data for males and females.

# Alveolar deposition by breathing type

Depends on whether you're a nose breather or a mouth breather



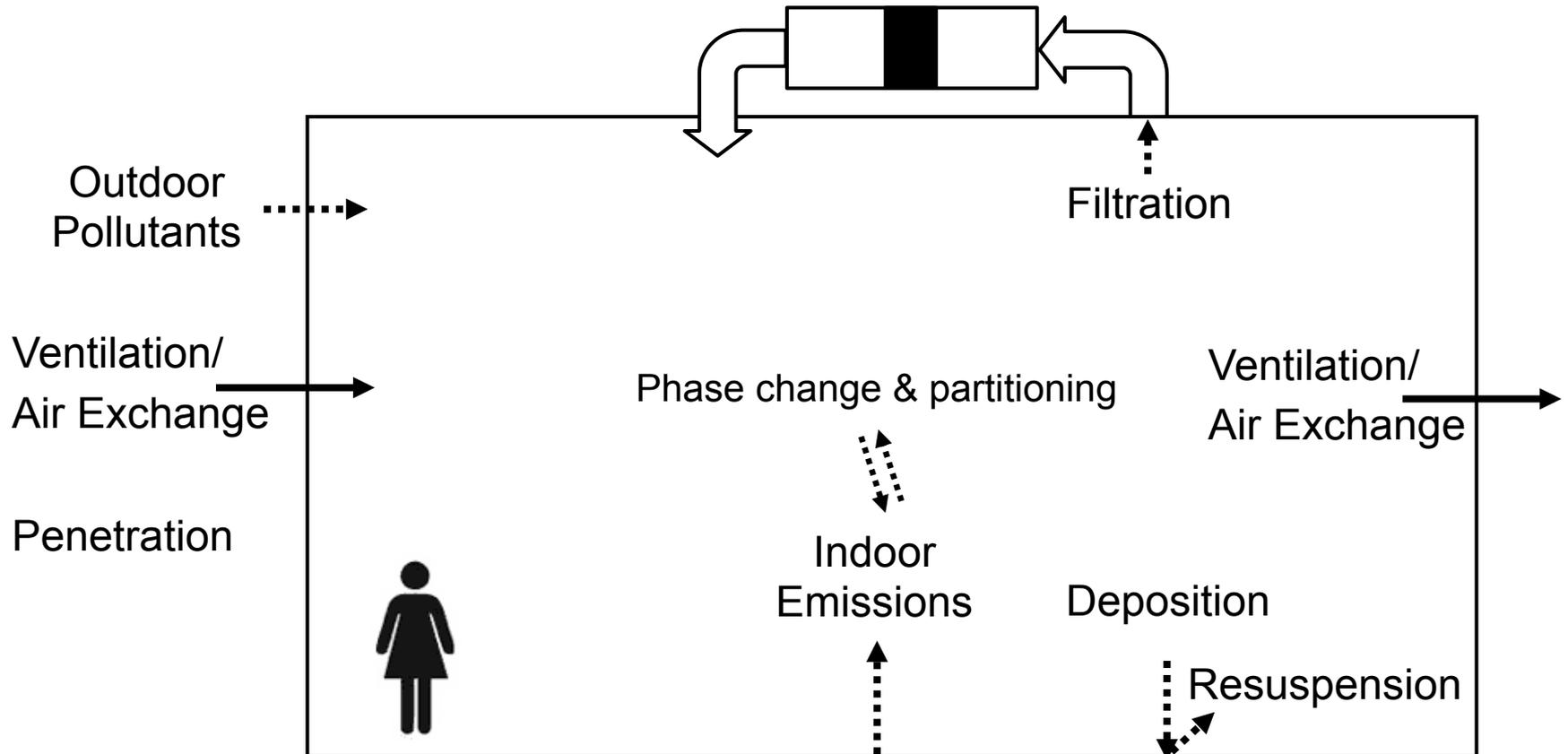
**FIGURE 11.4** Experimental data for deposition in the alveolar region. Deposition is expressed as a fraction of mouthpiece inhalation versus aerodynamic diameter (geometric diameter used below  $0.5 \mu\text{m}$ ). Reprinted with permission from Lippmann (1977).

# So what?

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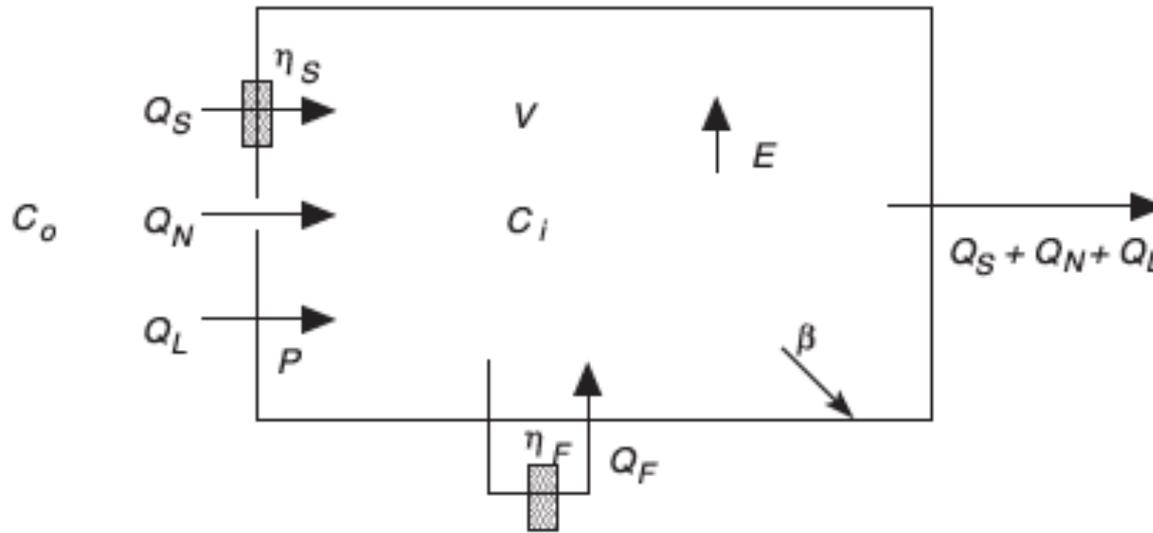
- We now understand more about particle sizes
  - And how different size particles deposit in different regions of our respiratory system
- We can examine different sources to determine their sizes
  - e.g., ETS or cooking particles
- And we can examine what particles will deposit in lungs?
  - And in which region?
- Helps elucidate health effects that may be observed

# Mass (or number) balance approach for particles



# Mass (or number) balance approach for particles

- Basic mass/number balance on particles of diameter  $i$ :



$$V \frac{dC_i}{dt} = E_i + C_{out,i} [Q_{vent} (1 - \eta_{vent,i}) + Q_{nat} + Q_{inf} P_i] - C_i [Q_{vent} + Q_{nat} + Q_{inf} + v_{d,i} A + Q_{filt} \eta_{filt,i}]$$

$$\frac{dC_i}{dt} = \frac{E_i}{V} + C_{out,i} [\lambda_{vent} (1 - \eta_{vent,i}) + \lambda_{nat} + \lambda_{inf} P_i] - C_i [\lambda_{vent} + \lambda_{nat} + \lambda_{inf} + k_{dep,i} + \lambda_{filt} \eta_{filt,i}]$$

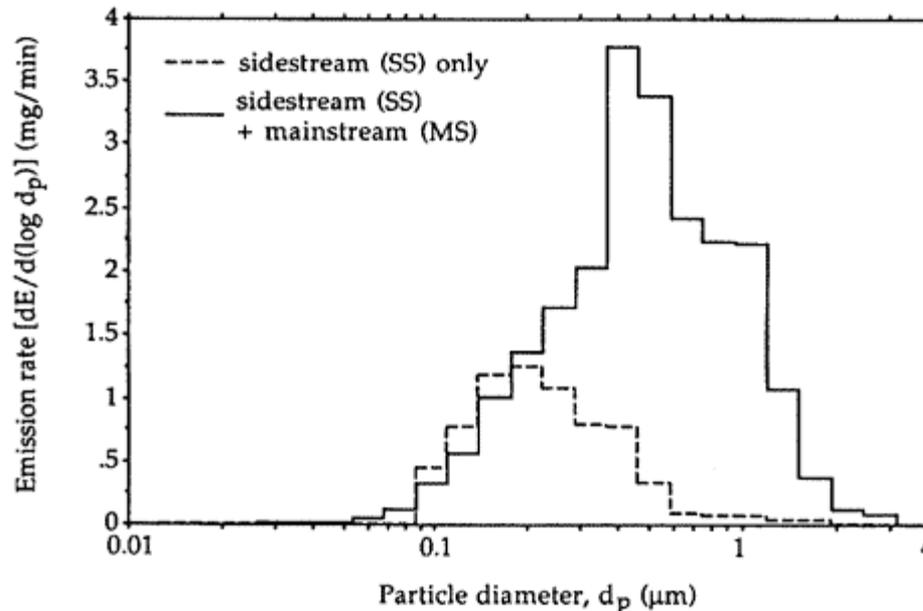
Which parameters vary by particle size?

# ETS lung penetration example

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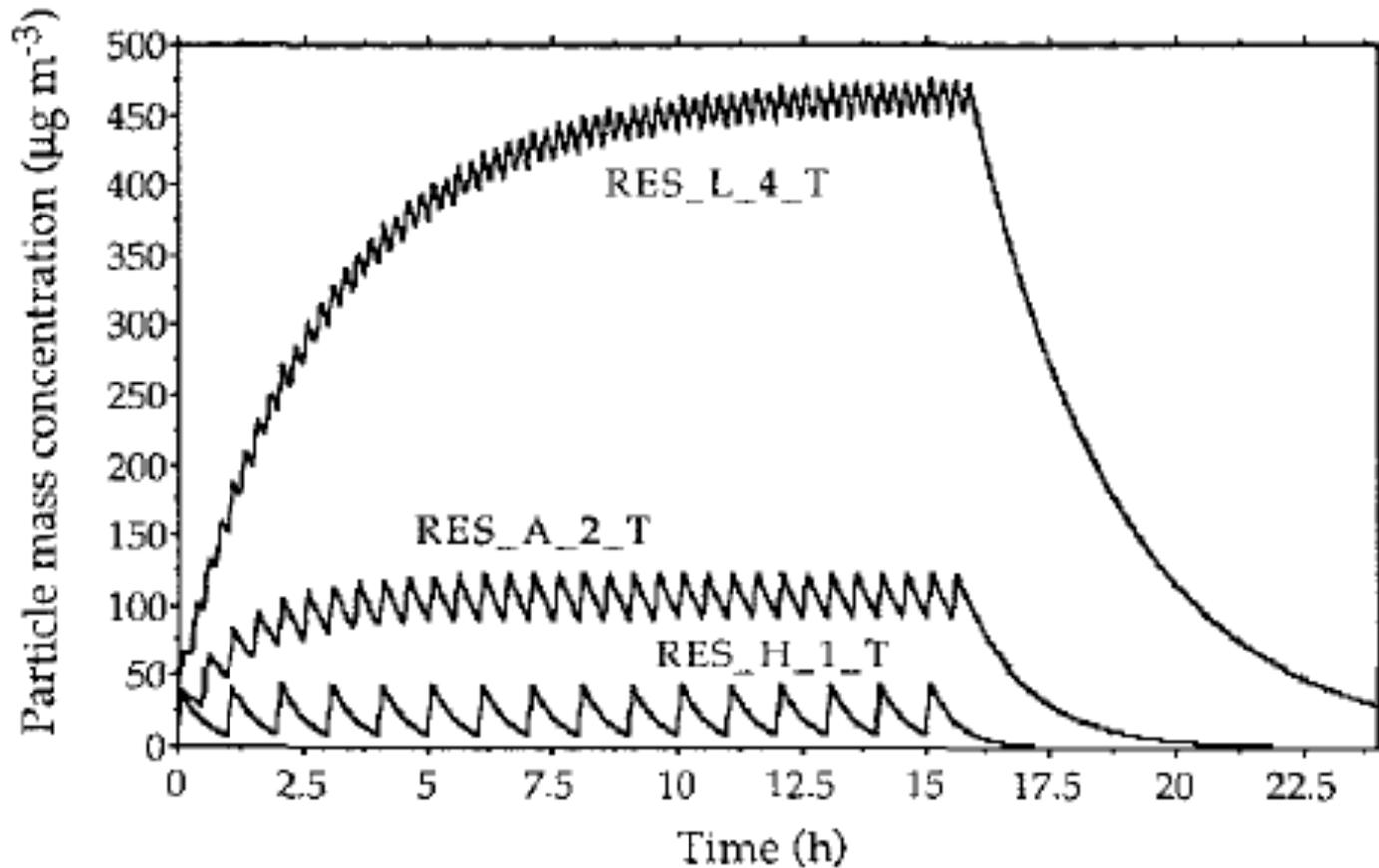
- Nazaroff, W. W., Hung, W. Y., Sasse, A. and Gadgil, A. J., 1993. Predicting regional lung deposition of environmental tobacco-smoke particles. *Aerosol Science and Technology* **19**, 243-254.
- Modeling exercise
  - Examine emissions from ETS
  - Used lung deposition model to examine where ETS particles end up
- Dynamic model
  - Assumed uniform cigarette smoking rate for first 16 hours of a day
  - Followed by 8 non-smoking hours
  - Varied smoking activity, age of exposed individuals

# Emissions from ETS



**FIGURE 1.** Effective particle emission rate from a burning cigarette as a function of particle diameter. The form of the figure is such that the area under a curve between two particle sizes is proportional to the mass emission rate of all particles within those size limits. These experiments were reported by Sextro et al. (1991). The emission profiles are based on a presumed particle density of  $1.4 \text{ g cm}^{-3}$ .

# Indoor concentration profiles from ETS



*Simulation designations*

RES\_H\_1\_S

RES\_A\_2\_S

RES\_L\_4\_S

RES\_H\_1\_T

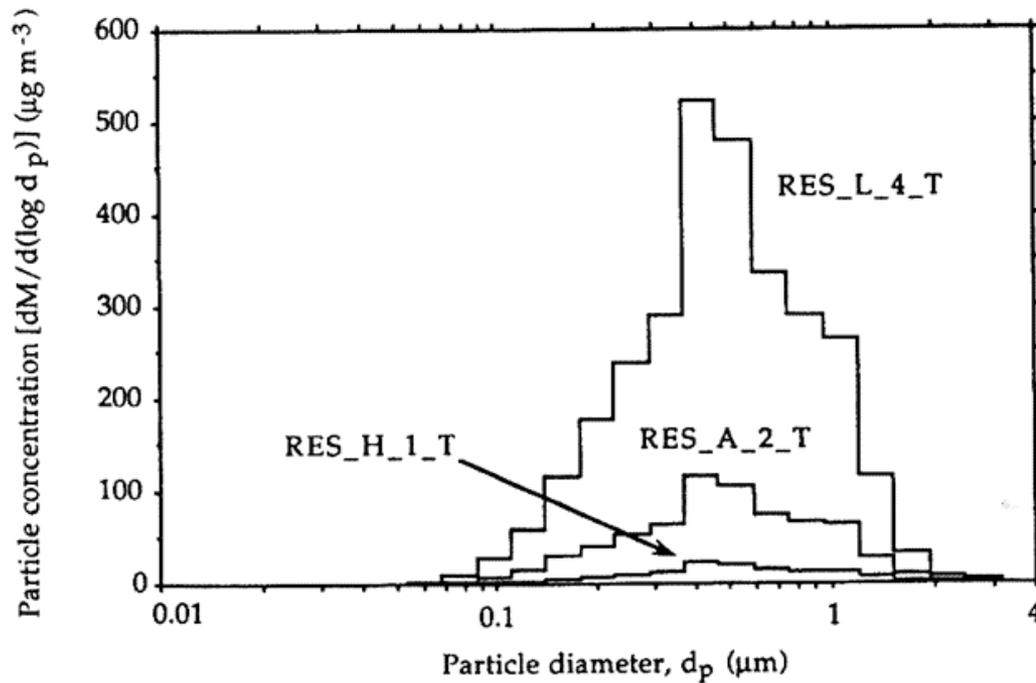
RES\_A\_2\_T

RES\_L\_4\_T

air-exchange rate:  $H = 1.7 \text{ h}^{-1}$ ;  $A = 0.68 \text{ h}^{-1}$ ;  $L = 0.28 \text{ h}^{-1}$

cigarette smoking frequency: 1, 2, or 4 per hour

# Mean indoor concentrations from ETS



**FIGURE 4.** Average environmental tobacco smoke particle size distribution over 24-h period for three residential simulations corresponding

*Simulation designations*

**RES\_H\_1\_S**

**RES\_A\_2\_S**

**RES\_L\_4\_S**

**RES\_H\_1\_T**

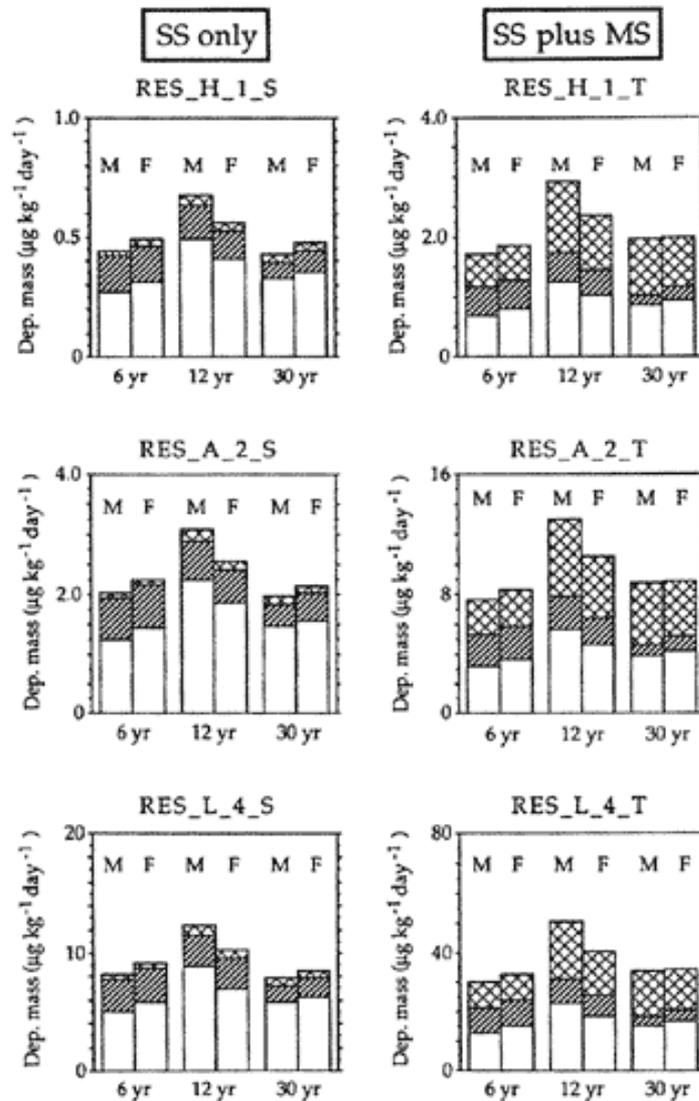
**RES\_A\_2\_T**

**RES\_L\_4\_T**

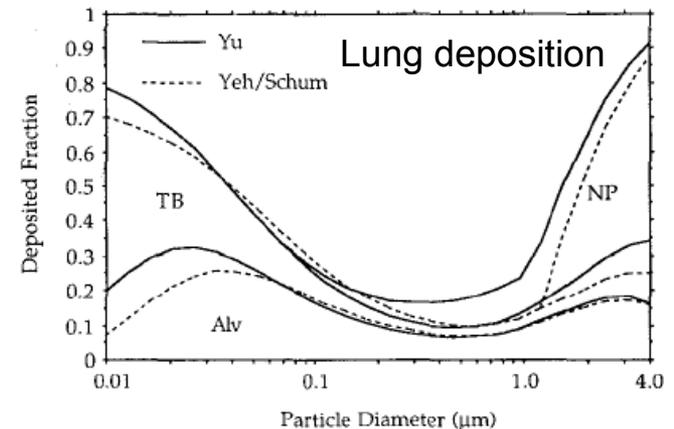
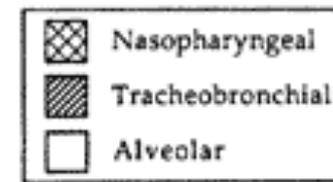
air-exchange rate: **H** = 1.7 h<sup>-1</sup>; **A** = 0.68 h<sup>-1</sup>; **L** = 0.28 h<sup>-1</sup>

cigarette smoking frequency: **1**, **2**, or **4** per hour

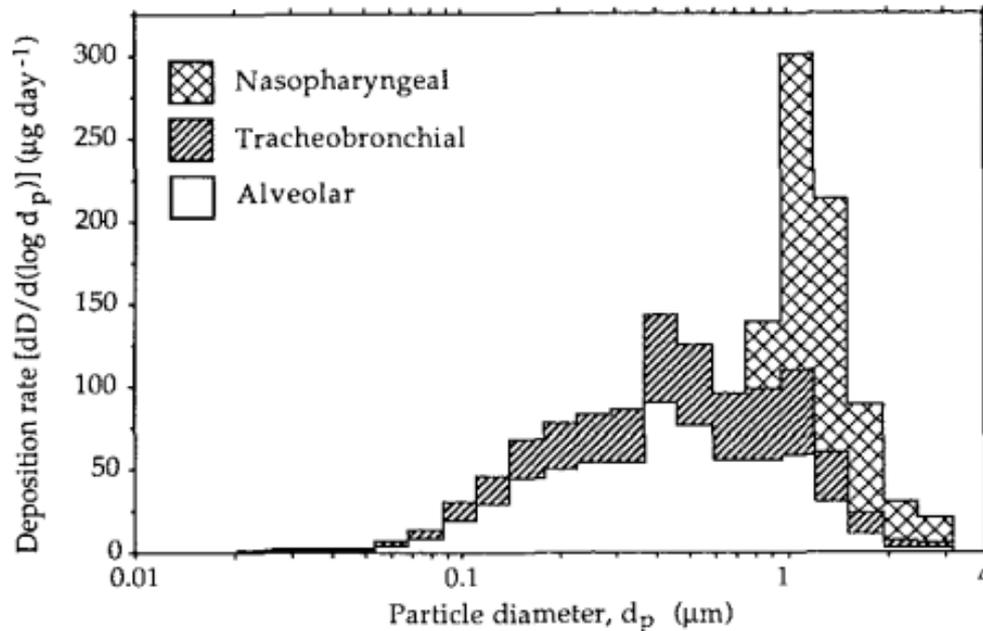
# ETS lung deposition



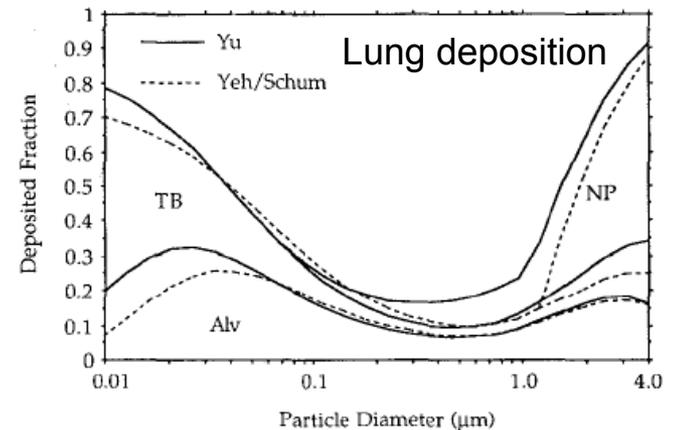
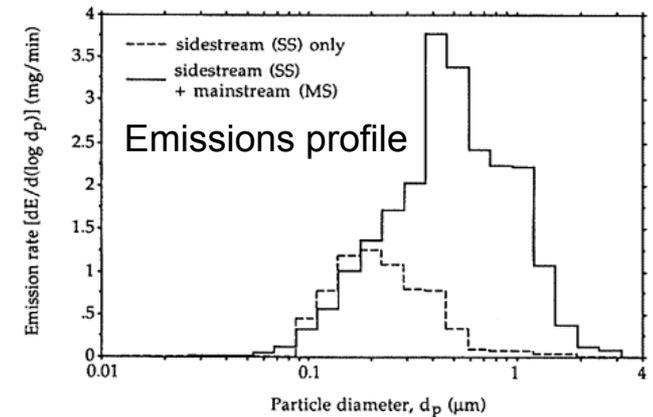
**FIGURE 5.** Regional lung deposition of environmental tobacco smoke particles from simulations of residential exposure. Each frame shows results for three age groups and each gender for one combination of smoking rate, particle emission profile, and building ventilation rate. The height of each bar gives the total respiratory deposition of particle mass per day per kg of body weight. Refer to Tables 1 and 2 for a description of simulation conditions. Note that the vertical scale varies from frame to frame.



# ETS lung deposition



**FIGURE 6.** Size distribution of deposited mass of environmental tobacco smoke particles in 6-year-old boy for simulation RES\_A\_2\_T. The form of the figure is such that the shaded area between two particle sizes is proportional to the average 24-h mass deposition rate of particles within those size limits. See Tables 1 and 2 for a description of simulation conditions.



# Next time

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- Particle emission source characteristics, deposition, resuspension, and penetration through cracks
- HW #3 is assigned, due next class period