ENVE 576
Indoor Air Pollution
Spring 2013

Lecture 6: February 19, 2013
Finishing gas-phase compounds: chemistry
Particulate matter: physics, size distributions, respiratory deposition

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HW updates

- HW 2 graded
  - A couple of you have not turned it in yet
  - I am also returning some back that missed a lot of points for not approaching problems correctly
    - If submitted by email, you've already gotten these back
    - If submitted by hand, I am returning now
  - You can fix the issues (which are partially my fault for not being clear)
    - And still get full credit
  - Helpful hints (doc cam)

- HW 3 was due today
  - Postponed until next week
  - Any questions?

Review from last time

- Last time we covered:
  - Adsorption/desorption of gas-phase compounds
  - Reactions of gas-phase compounds (finish today)
    - Heterogeneous (reactive deposition)
    - Homogeneous (gas-phase chemistry)

- Today we will begin ~3 weeks on particulate matter
  - Starting with:
    - Single particle physics
    - Particle size distributions
    - Respiratory deposition

- Start by discussing project expectations

Course project information

- Final project expectations document has been uploaded to BB

- Basic idea is to write a ‘conference paper’
  - Must combine literature review with modeling or measurement effort
  - Either is fine
  - A lot of freedom

Course project information

- 40% of your grade
- Report/paper due April 30, 2013
- Investigate a course topic in greater detail
  - Use what you've learned to critically analyze:
    - Contaminant(s)…
    - In particular environment(s), and…
    - Control strategies
  - Can move outside this boundary and focus on policy decisions
  - The point is for critical review + measurement/modeling effort
- Write a 'conference paper'
  - 8 pages single spaced
  - Fully referenced (although references don't count against word count)
- Present a 'conference presentation'
  - In class on April 30, 2013

Project topics

- 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

Potential project topics

- Energy impacts of gas or particle filtration
- Impact of LEED points on indoor air pollutants
- Exposures in indoor swimming pools
- Particle exposure during commuting or other activities
  - e.g. during cooking at home or in cafeteria
- Measurement of HVAC recirculation rates and estimates of particle filtration
- Infiltration and persistence of outdoor criteria pollutants
- Pollen exposures and control strategies for allergies
- Cookstove emissions in developing countries
- Indoor and outdoor traffic noise
- Particle exposure during religious ceremonies
- Impacts of mechanical ventilation on indoor air pollution
- Plants as air cleaners

Lab instrumentation: T/RH and power/energy

Temperature/RH

Data logging

Temperature

Heat flux

IR camera

Solar radiation

Electric power

Lab instrumentation: HVAC diagnostics

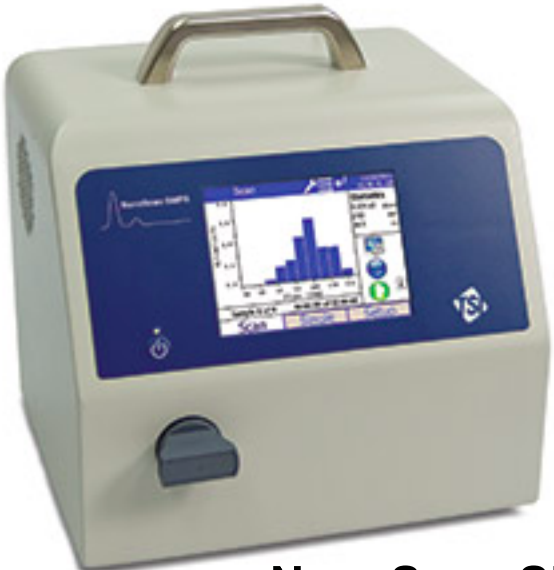
Blower door (envelope leakage)

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 µm

CO_2
(for AER)
CO

DustTrak
$PM_{2.5}/PM_{10}$

CPC
< 1 µm

CPC respirator fit tester
< 1 µm

Lab instrumentation: other

- Other items already in the lab:
  - Acoustics (microphones of all kinds, dB meters)
  - Lighting (lux/lumens)
  - Air speed

Topic justification (mid-March)

- 1/2 page
- 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 March 12**
- Criteria
  - Importance
  - Creativity
  - Justification
  - Reasonable scope

Tips on introduction and literature review

- 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 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

- 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

- Avoid passive voice, be active
- It is acceptable to use "I" or "we"
- Vary language:
  - Smith et al. (1972) measured …
  - Ezekoye and Shi (2003) 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

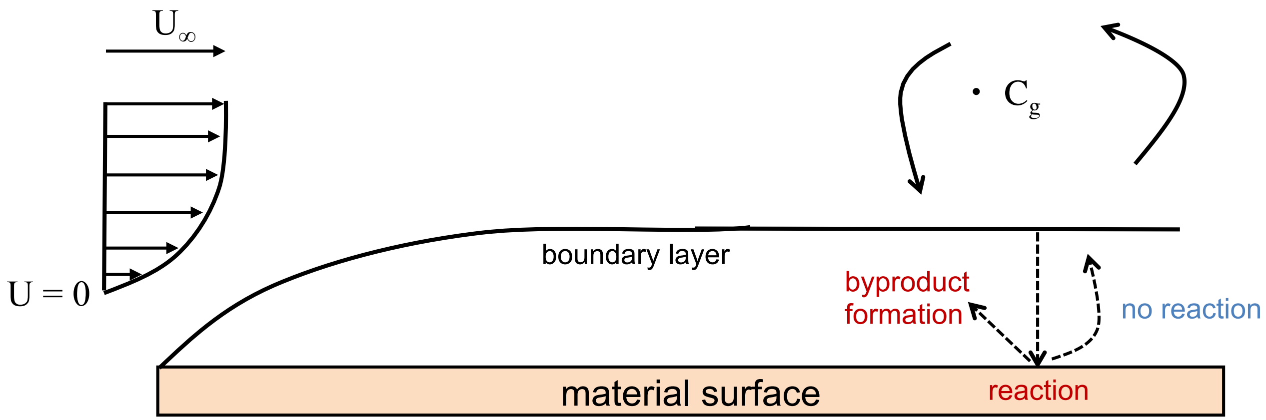
Rest of your paper

- 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 not required at all
  - No additional points for measurement vs. modeling study

REACTIVE DEPOSITION

Finishing up from last lecture

Reactive deposition: summary



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

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

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

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

v_s = surface-limited deposition velocity (m/hr)
v_t = transport-limited deposition velocity (m/hr)
γ = reaction probability (-)
$\langle v \rangle$ = Boltzmann velocity (m/hr)

Reactive deposition: byproduct formation

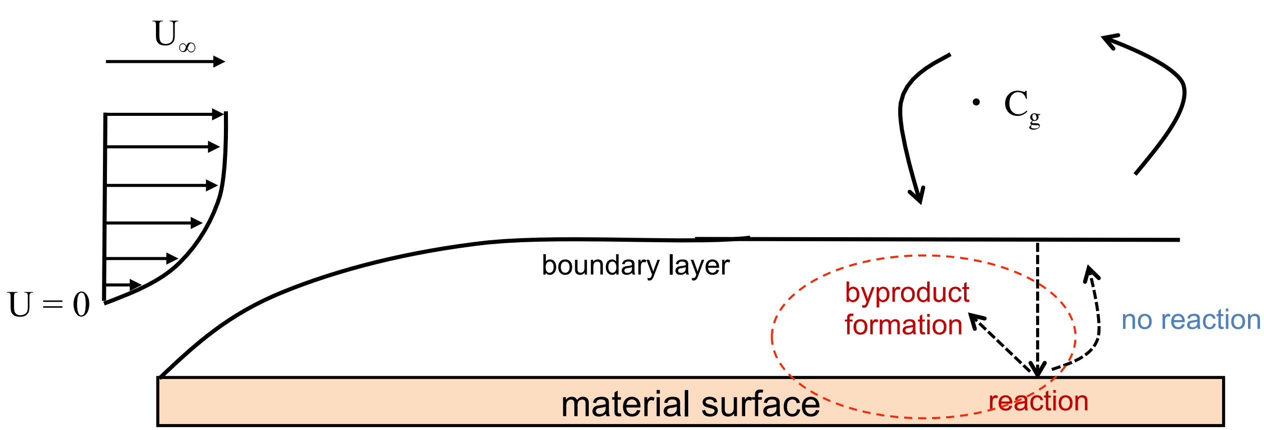
- Reactive deposition to surfaces removes indoor pollutants
  - Can also generate others in the form of reaction by-products

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

$R_{byproduct,i}$ = 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 $\frac{\mu g}{m^3}$ to $\frac{moles}{hour}$)



Byproduct formation: mass balance

- 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!

Example heterogeneous byproduct formation

- Ozone deposition velocity, yields, and secondary emission rates of aldehydes after ozone exposure in 4 homes

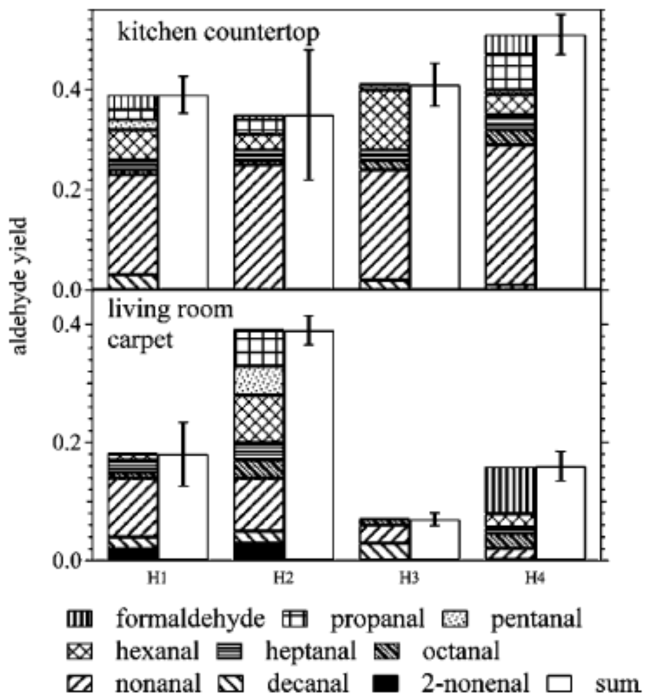
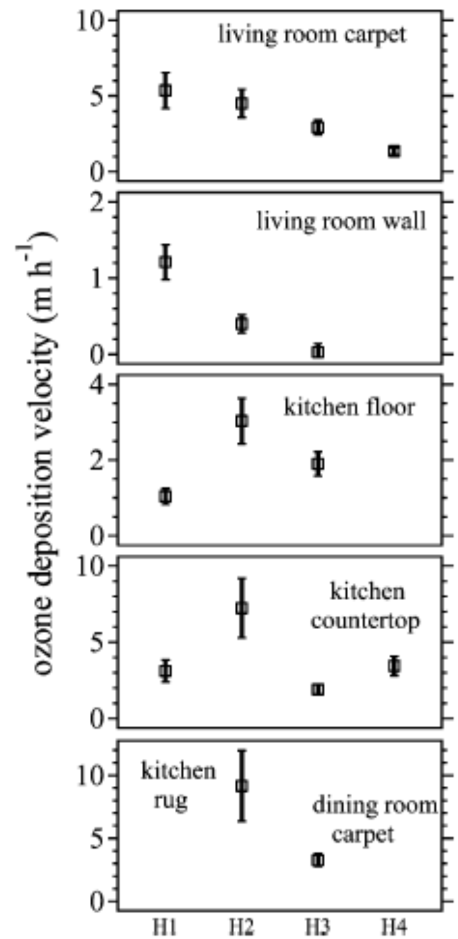
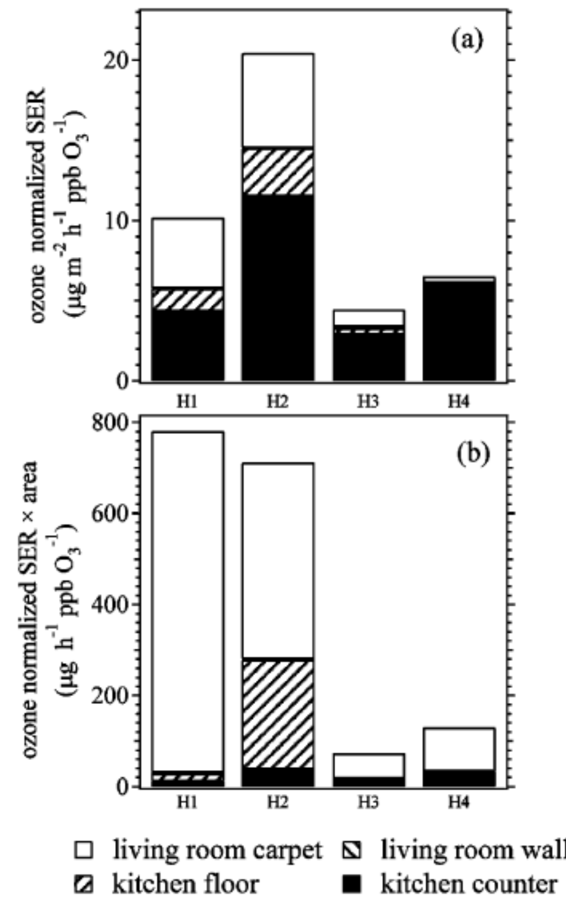


FIGURE 3. Ozone-induced aldehyde yields for kitchen countertop and living room carpet.



Ozone deposition velocity for each surface.

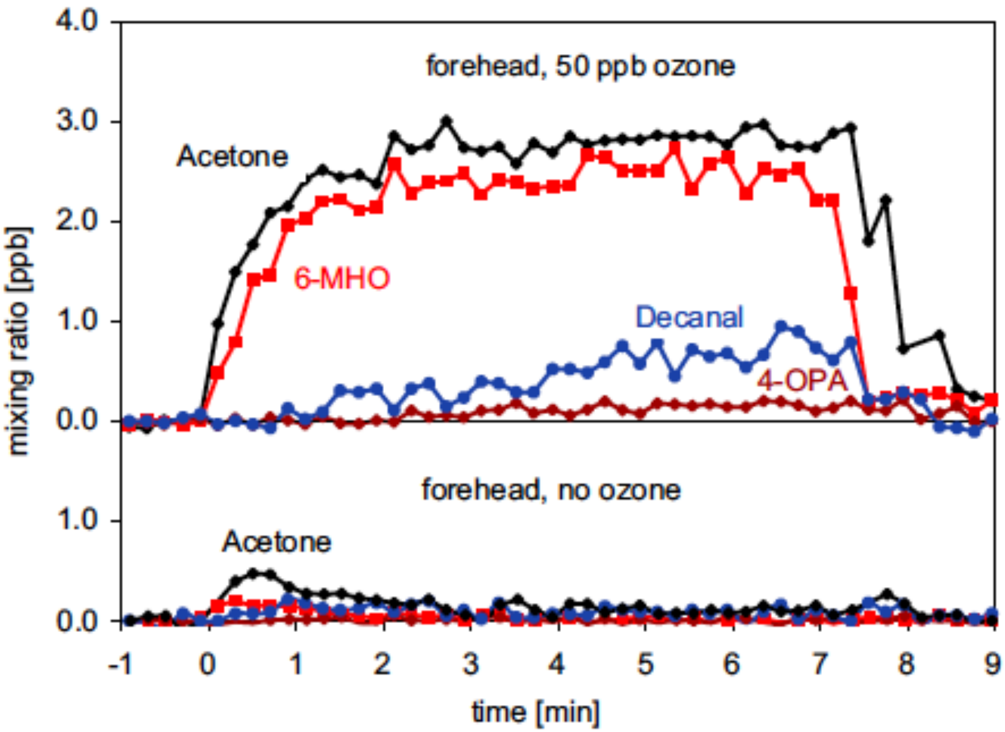


Normalized aldehyde emission rates for four homes.

Wang and Morrison, 2006 *Environ Sci Technol*

Example heterogeneous byproduct formation

- Skin oils have recently been identified as being potentially important for ozone chemistry



Acetone (C_3H_6O)
6-MHO (6-methyl-5-hepten-2-one)
Decanal ($C_{10}H_{20}O$)
4-OPA (4-oxo-pentanal)

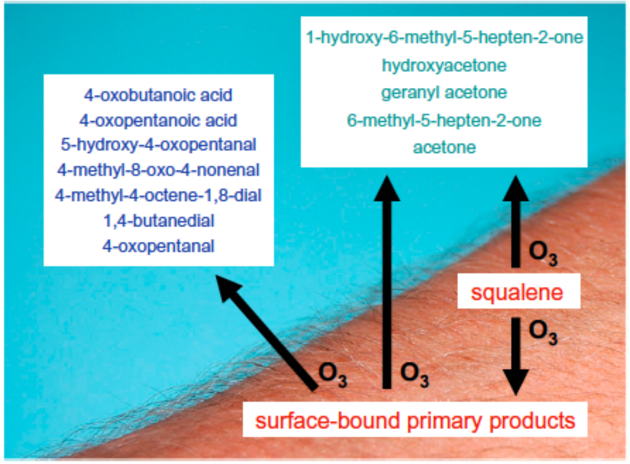


Fig. 4. Schematic of ozone reacting with squalene on exposed skin. The initial reaction produces both gas phase and surface-bound primary products. Ozone further reacts with surface bound primary products (see Table 3) to produce additional gas-phase products.

Wisthaler and Weschler, 2010 *Proc Nat'l Academy of Scienes*

HETEROGENEOUS CHEMISTRY

Quick overview

Homogeneous chemistry

- Homogeneous reactions also occur in indoor environments
  - Gas *i* + Gas *j* → Byproduct *k*

$$R_{\text{homogeneous}} = -k_{ij} C_i C_j V$$

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

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

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

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

Homogeneous chemistry

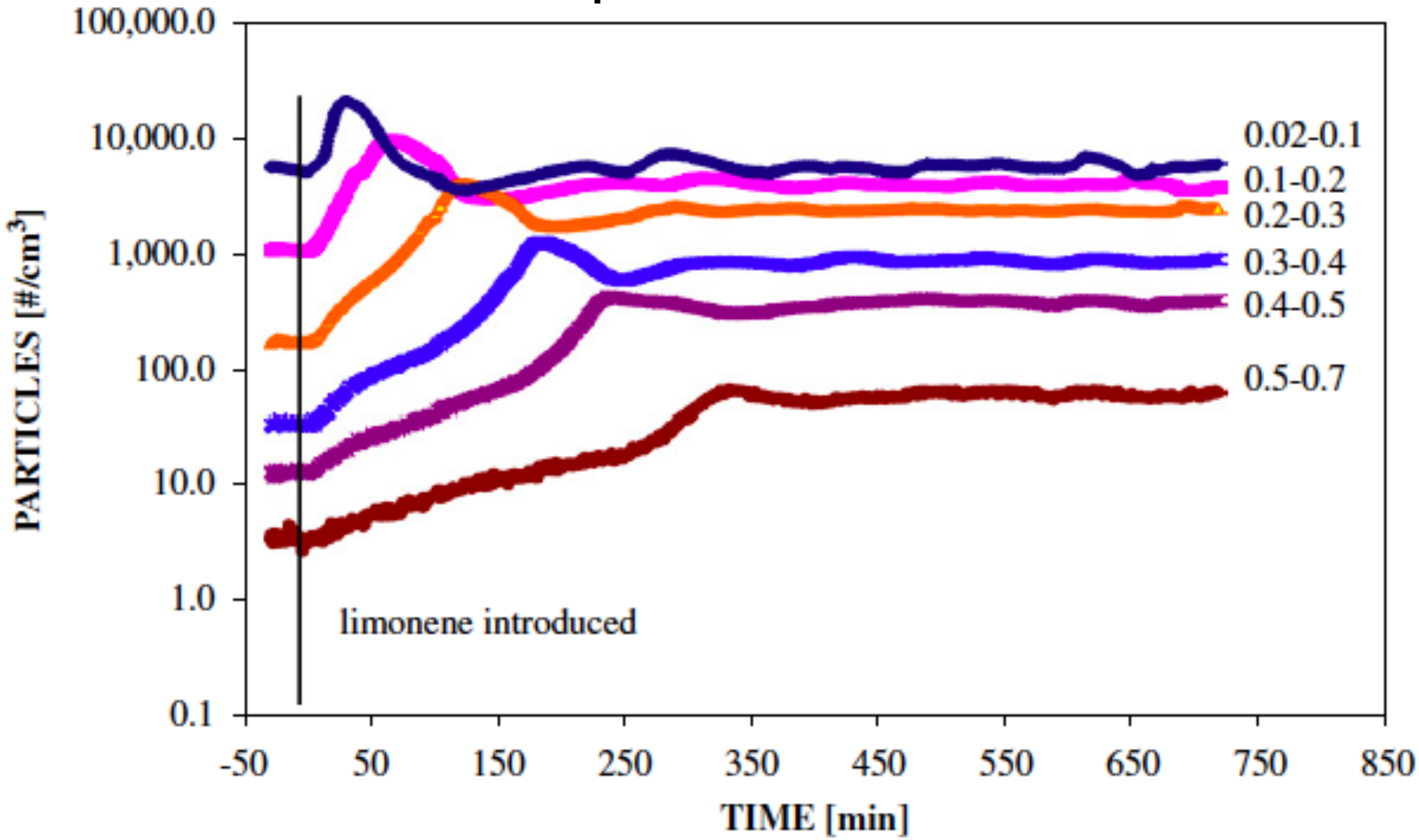
- Ozone: important driver of homogeneous chemistry indoors
  - Oxidation chemistry with unsaturated (C=C double bond) VOCs
  - Weschler (2000) *Indoor Air* provides great review of ozone chemistry
    - Including what reactants are important

  - Important reactants include:
    - Terpenes (limonene, pinene, and others)
      - Household cleaners, scented products
    - Fatty acids (oleic acid, linoleic acid)
    - Squalene

  - Important byproducts include:
    - Gas phase: aldehydes (including HCHO), carbonyls
    - Particle phase: secondary organic aerosols (low-vapor pressure species that self-nucleate to form small particles or condense on and increase the mass of existing particles)

SOA formation from homogeneous chemistry

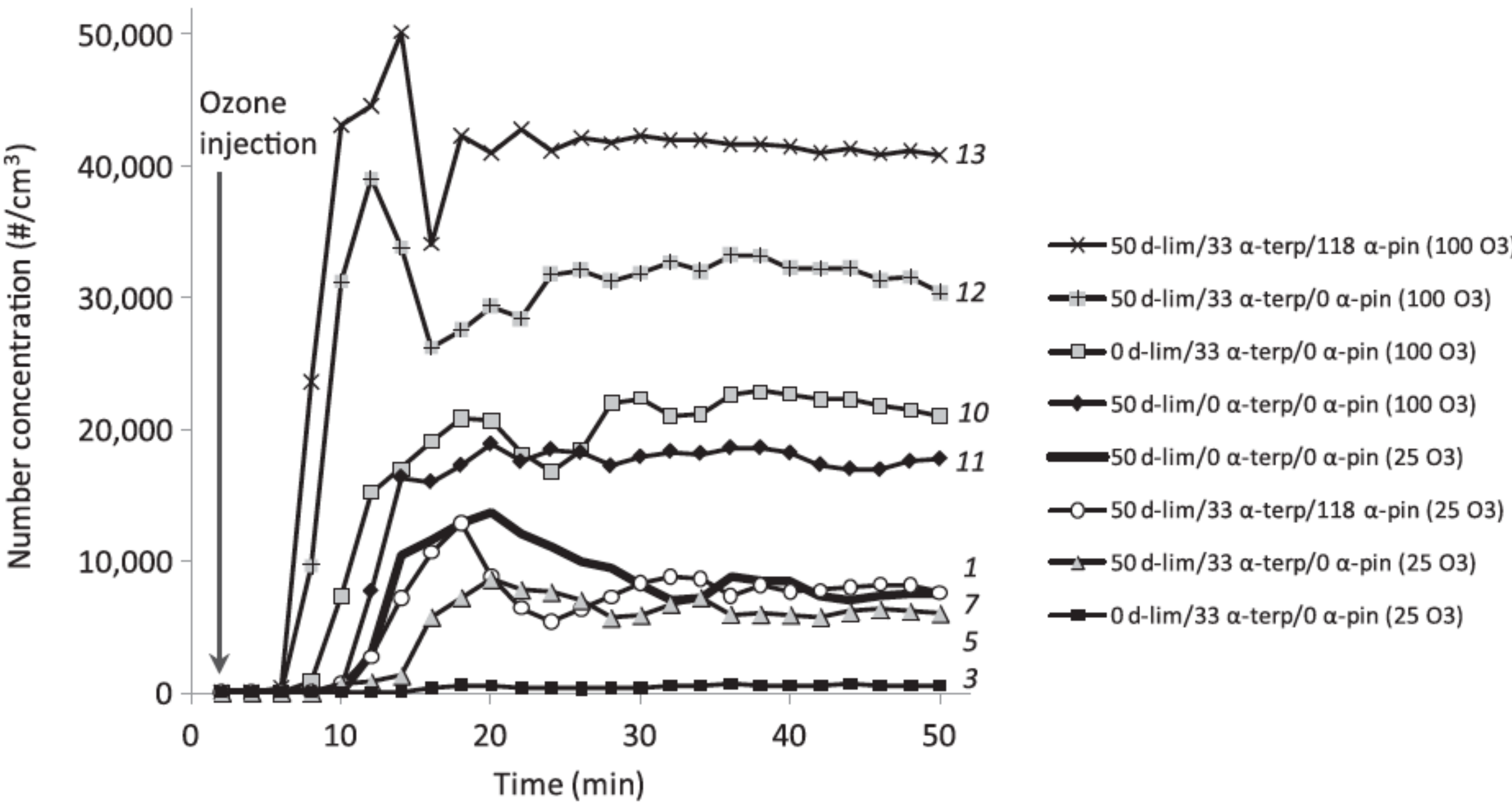
Limonene injection (air fresheners and perfumes) in the presence of ozone indoors



Sarwar et al., 2004 *Atmospheric Environment*

SOA formation from homogeneous chemistry

Chamber experiments with mixtures of terpenes and more realistic O_3
(10-500 nm particles)



Waring et al., 2011 *Atmospheric Environment*

Other homogeneous chemistry

- Hydroxyl radical ($\cdot OH$)
  - Formed during ozone-terpene chemistry
  - Strong oxidant and reacts with almost any hydrocarbon
  - Concentrations typically ppt
- Nitrate radical ($NO_3\cdot$)
  - Forms as product of reaction between O_3 and NO_2
  - Targets reactions with terpenes
  - Concentrations typically ppt
- Byproducts from indoor chemistry can be respiratory or skin irritants

Before moving on to particulate matter…

CONTROL OF GAS PHASE COMPOUNDS

Control of VOCs and inorganic gases

- There are a few important ways to control (i.e., remove) VOCs and inorganic gases:
  1. Source control
  2. Adsorption-based air-cleaning (e.g., activated carbon)
  3. Photocatalytic air-cleaning (e.g., UV/PCO)

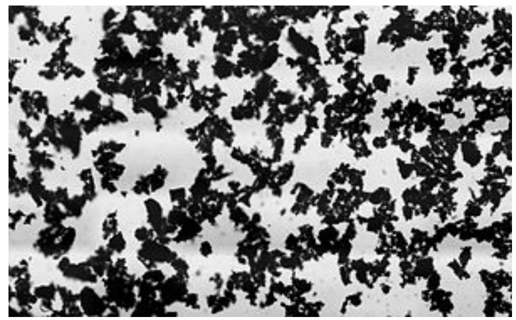
- We won't spend any time on these but we need to know they exist
  - You may incorporate into your final project too

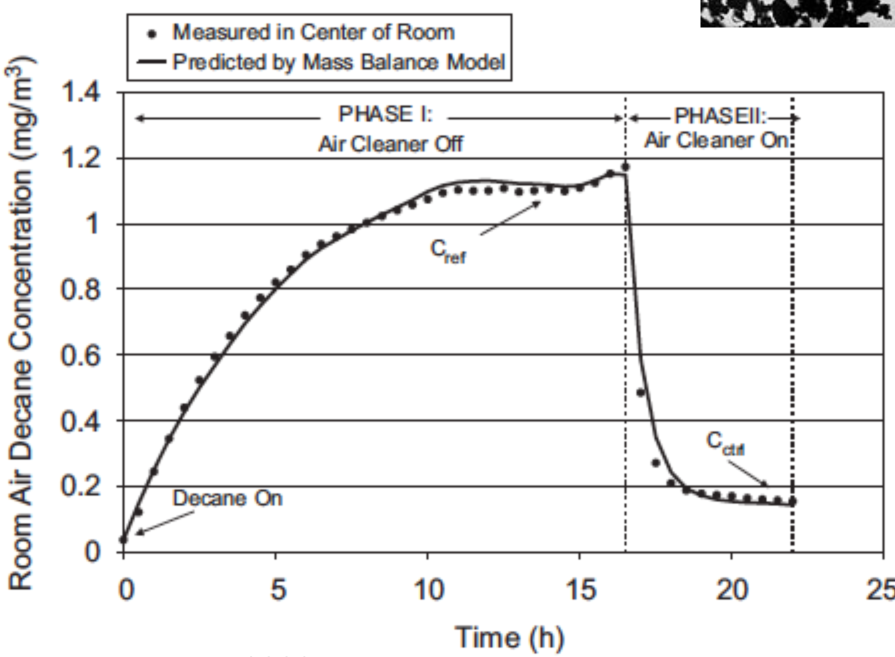
Source control/substitution

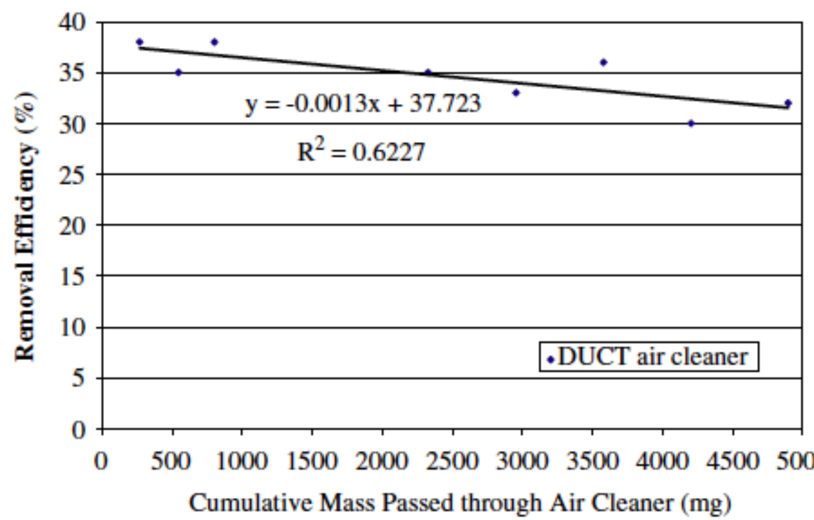
- Simple enough: this involves switching to low-emitting materials
  - We've discussed this already in some form

Adsorption: activated carbon

- Microporous activated carbon adsorbents
  - Very high surface areas
    - e.g., 800-2000 m^2/g



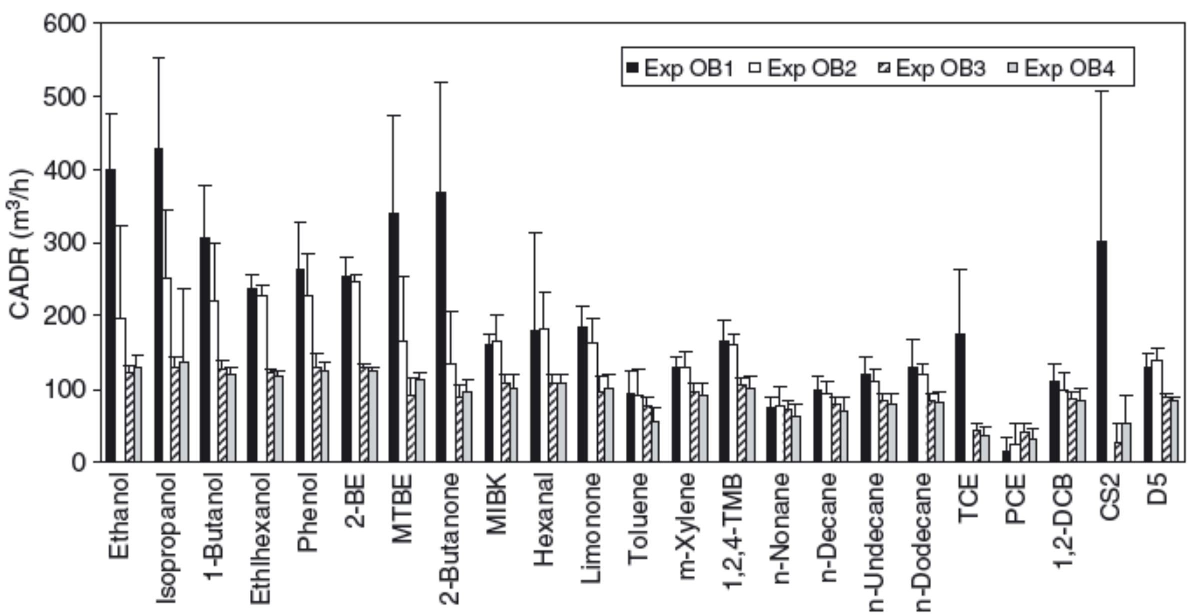


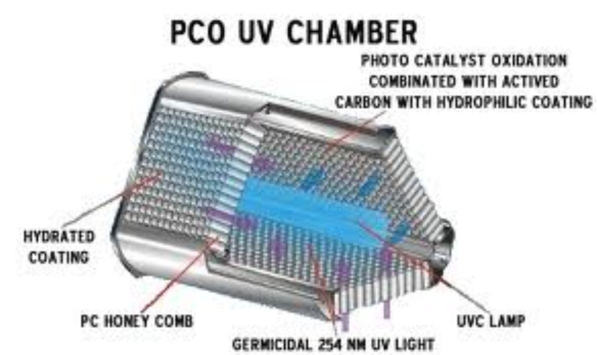


Howard-Reed et al., 2008 *Building and Environment*

UV+PCO

- Ultraviolet (UV) photocatalytic oxidation (PCO)
  - Honeycomb reactor coated with TiO_2
  - Structure is irradiated with UV light
  - VOCs adsorb reversibly on the catalyst
  - React to form CO_2 and water
    - TiO_2 semi-conductor sensitizes light-induced reactions





Hodgson et al., 2007 *Indoor Air*

PARTICULATE MATTER

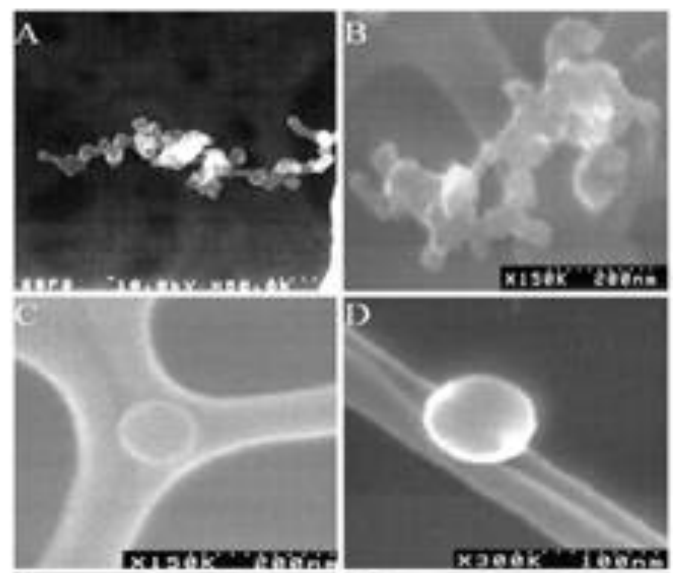
Overview, physics, size distributions, respiratory deposition

Particulate matter (PM)

- 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



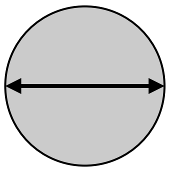
http://www.aerosols.wustl.edu/education/AerosolBasics/What%20is%20an%20aerosol.htm

Particle sizes

- Usually referring to a characteristic dimension
  - Diameter for sphere
  - Diameter for fibers (e.g. asbestos)
  - Equivalent diameter for non-spherical
- Micrometer (μm)
  - 1 μm = 10^{-6} m
- Nanometer (nm)
  - 1 nm = 10^{-9} m

- We usually treat particles as spherical:
  - Or 'equivalent' spheres

d_p



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

Particle sizes

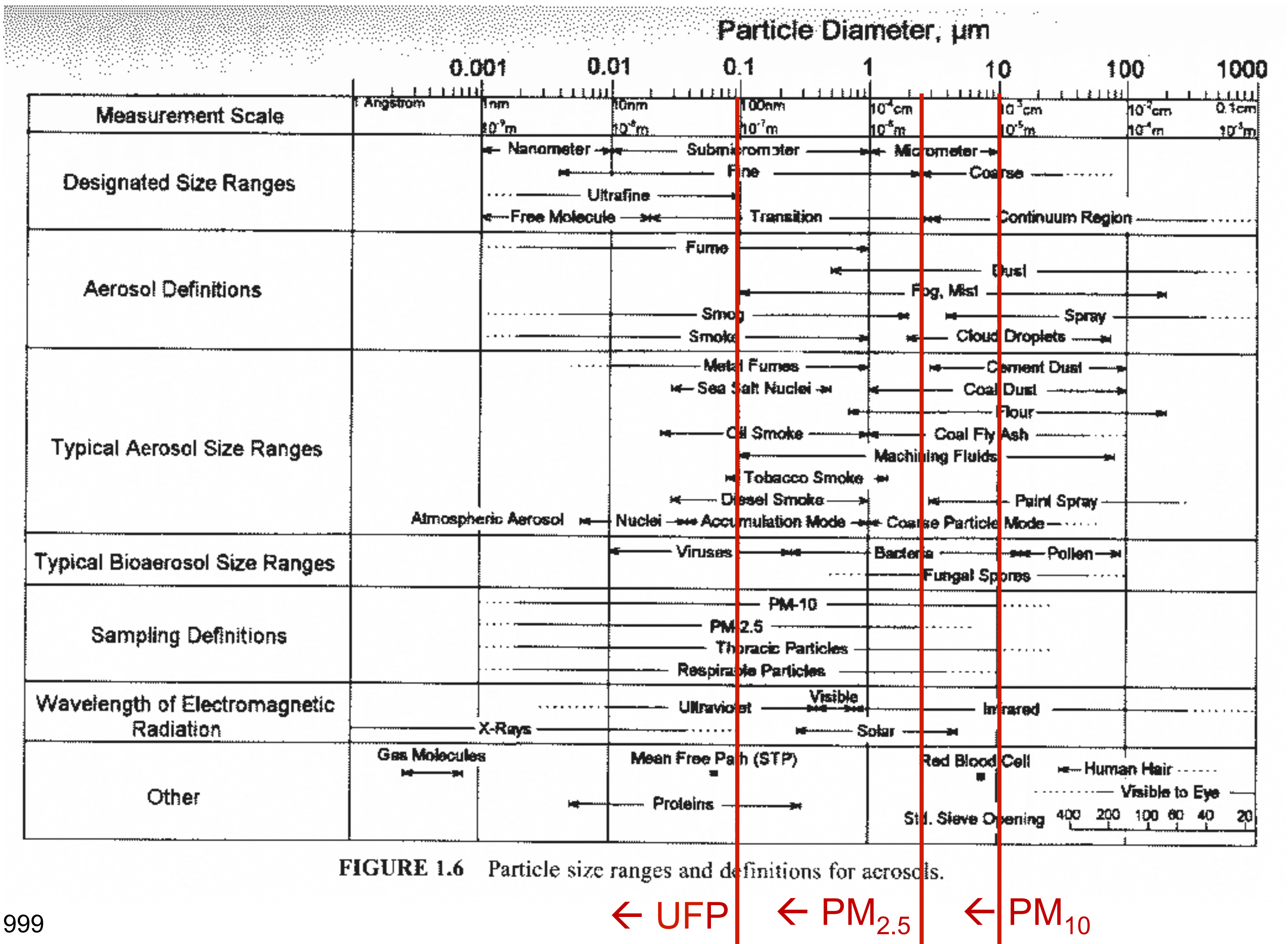
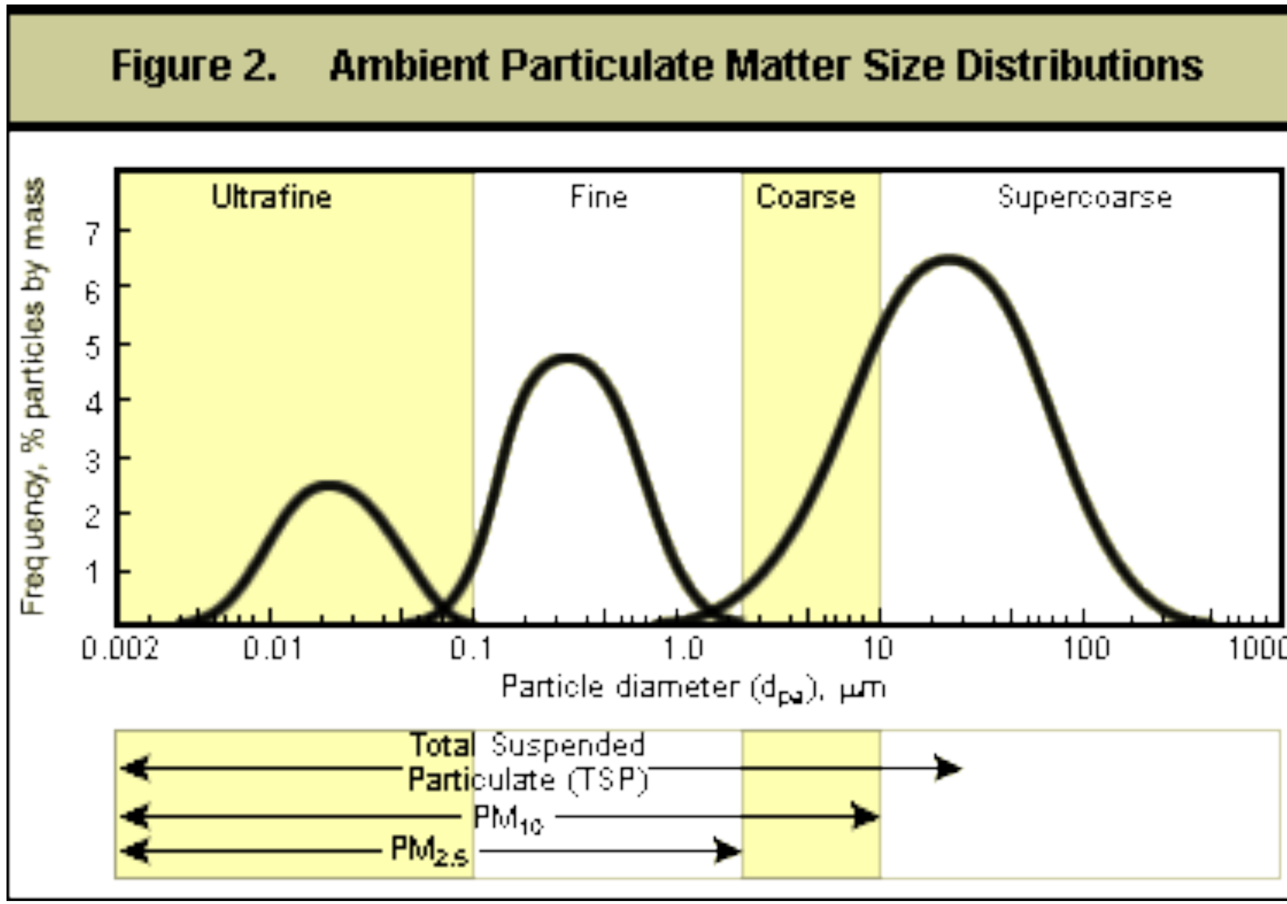


FIGURE 1.6 Particle size ranges and definitions for aerosols.

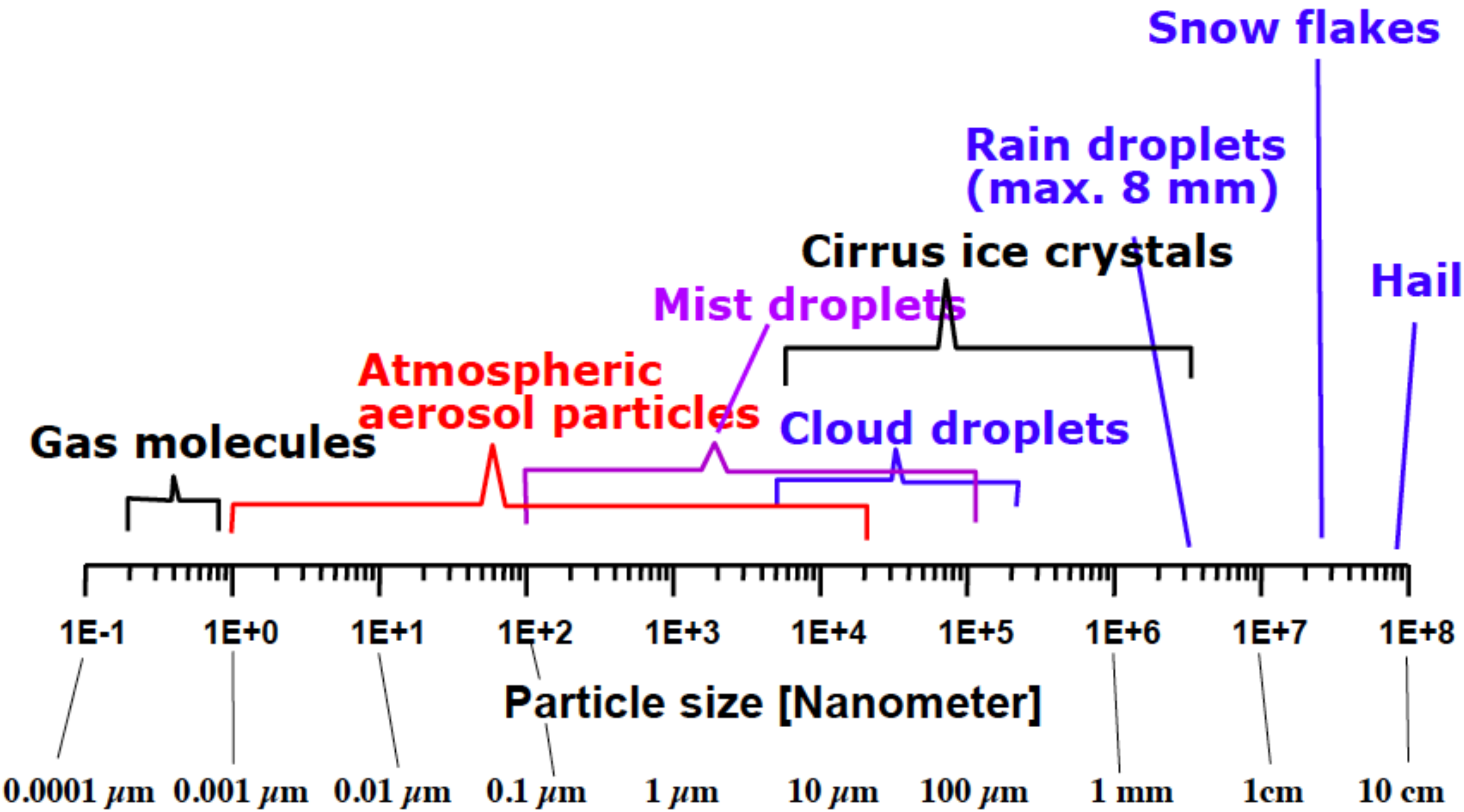
Hinds 1999

How are particle concentrations reported?

- Number
  - #/cm^3
  - UFP <100 nm
- Surface area
  - cm^2/cm^3
- Volume
  - m^3/m^3
- Mass
  - µg/m^3
  - $PM_{2.5}$
  - PM_{10}
  - $PM_{2.5\text{-}10}$
  - TSP
  - RSP

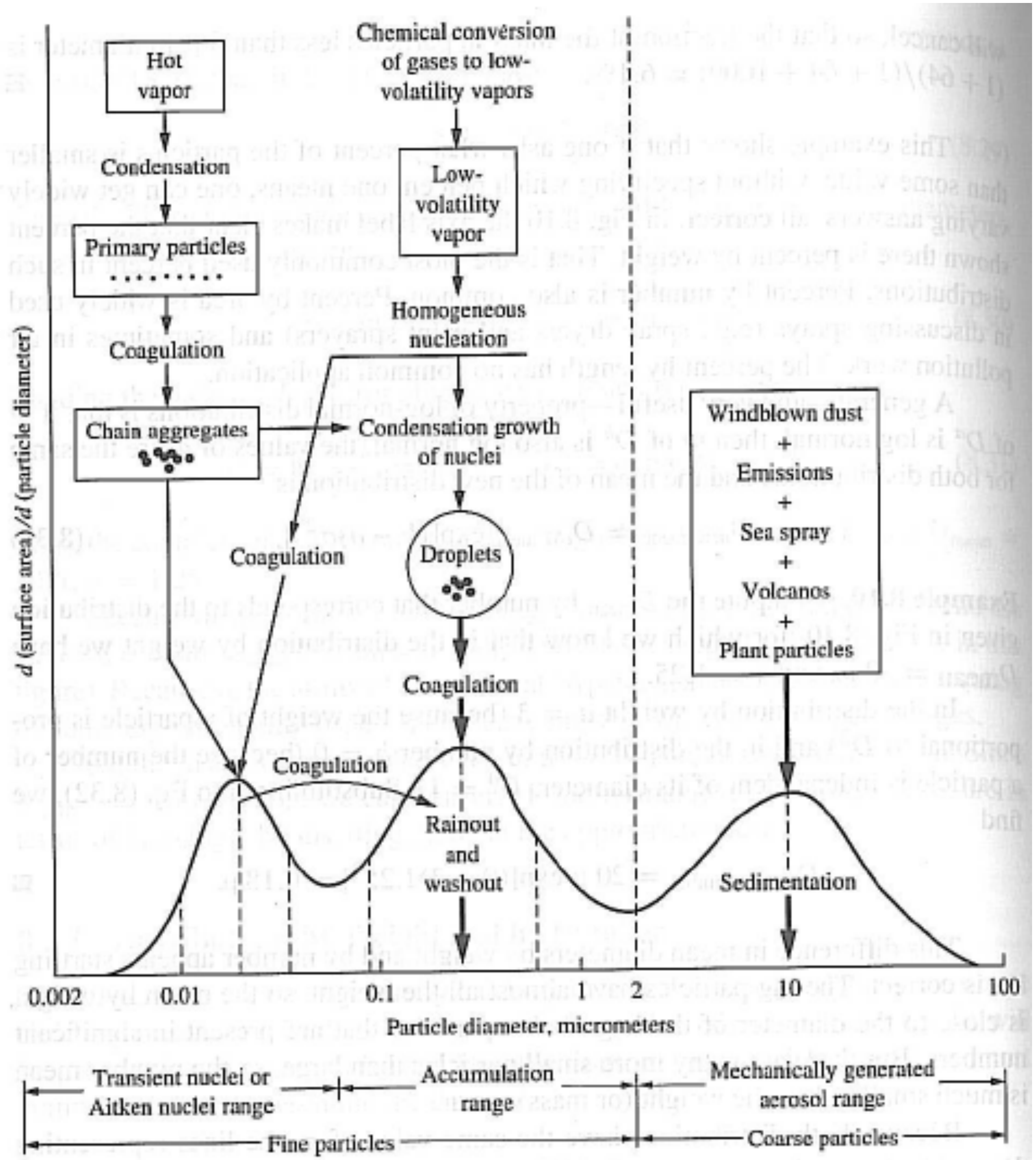


Particle sizes



Schneider, 2010

Particle formation mechanisms, surface area, and size



Seinfeld and Pandis, 2006

Particles: Typical concentrations

- How many 0.5 μm particles can fit into a cubic centimeter of air?
  - Ratio of 0.5 μm particle volume to cubic centimeter volume:

$$\frac{V_{air}}{V_{particle}} = \frac{1\ \mathrm{cm}^3}{\frac{\pi}{6} d_p^3} = \frac{10^{-6}\ \mathrm{m}^3}{\frac{\pi}{6}(0.5 \times 10^{-6}\,\mathrm{m})^3} \approx 10^{12}$$

~1 trillion 0.5 μm particles could exist within 1 m^3 of air (not counting void space)

- What do you think a typical concentration of 0.5 μm particles in indoor air is?
  - How about in this classroom right now?

PARTICLE MOTION

What affects the movement of particles?

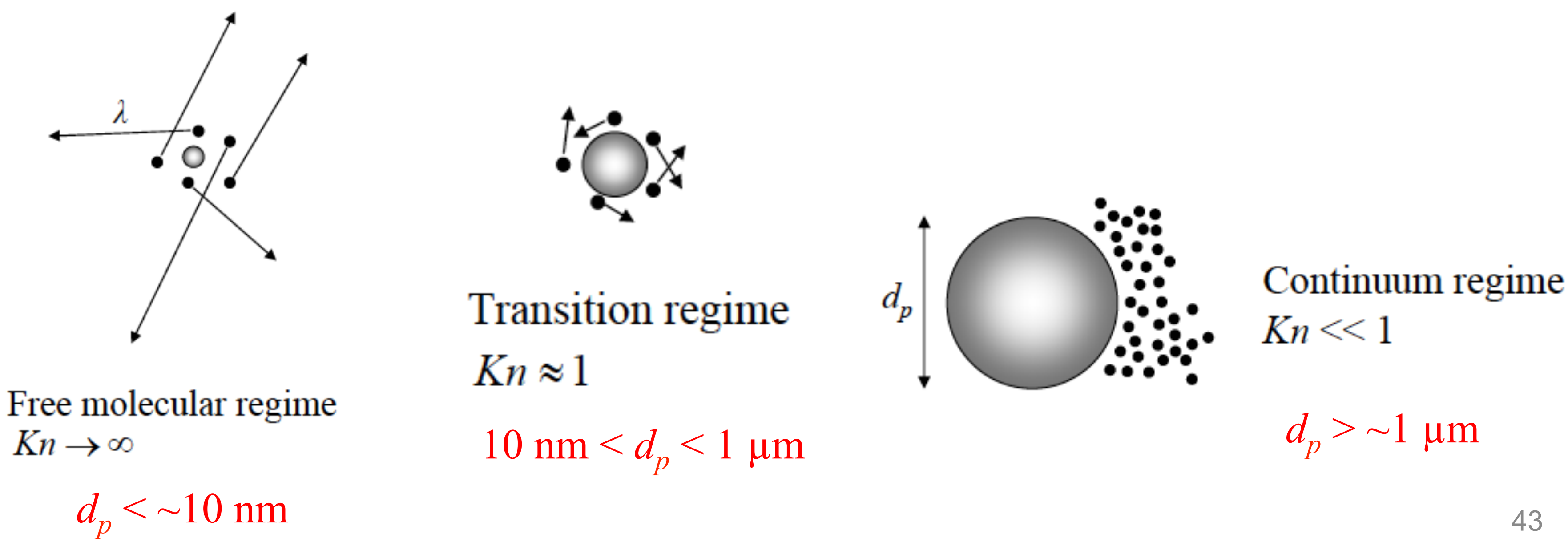
Particle motion in gases

- 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 (μm)

λ = mean free path of air (0.066 μm @ STP)



Seinfeld and Pandis, 2006; Schneider, 2010

Particle motion in gases

- 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:

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

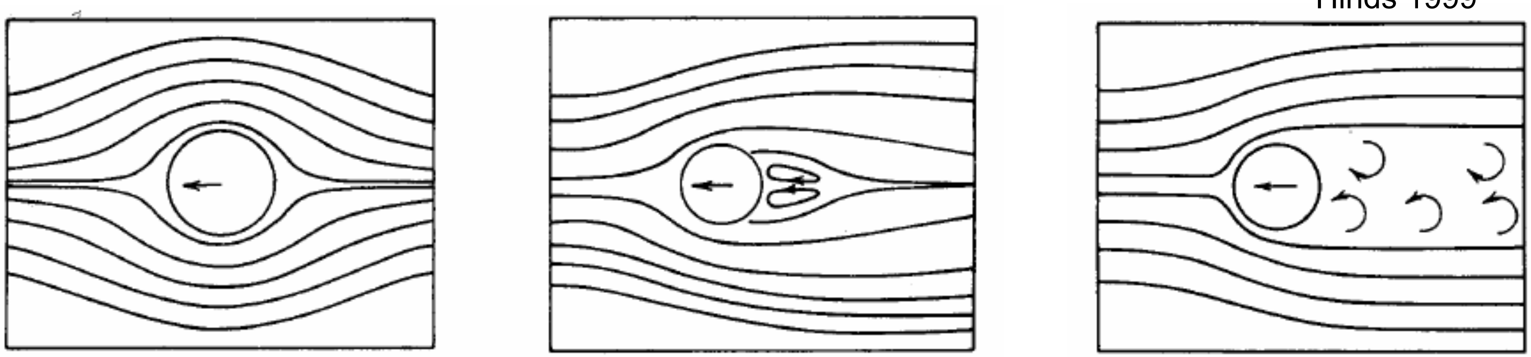
ρ_{air} = air density (kg/m^3)

V = relative velocity between particle and air (m/s)

μ = dynamic viscosity of air (1.8×10^{-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)

Hinds 1999



Re = 0.1 (a) Re = 2 (b) Re = 250 (c)

Particle motion in gases

- 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 = drag force (kg-m/s^2)
C_D = 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 **Stoke's Law**

Particle motion in gases

- Stoke's law states that:

$$F_D = 3\pi\mu V d_p$$

$$V = \text{particle velocity (m/s)}$$

  - Valid for laminar flow around a solid sphere
- Comparing Newton's and Stoke's laws:

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

$$C_D = \frac{24\mu}{\rho_{air} V d_p} = \frac{24}{\text{Re}}$$

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

Particle motion in gases

- Drag coefficient, C_D:

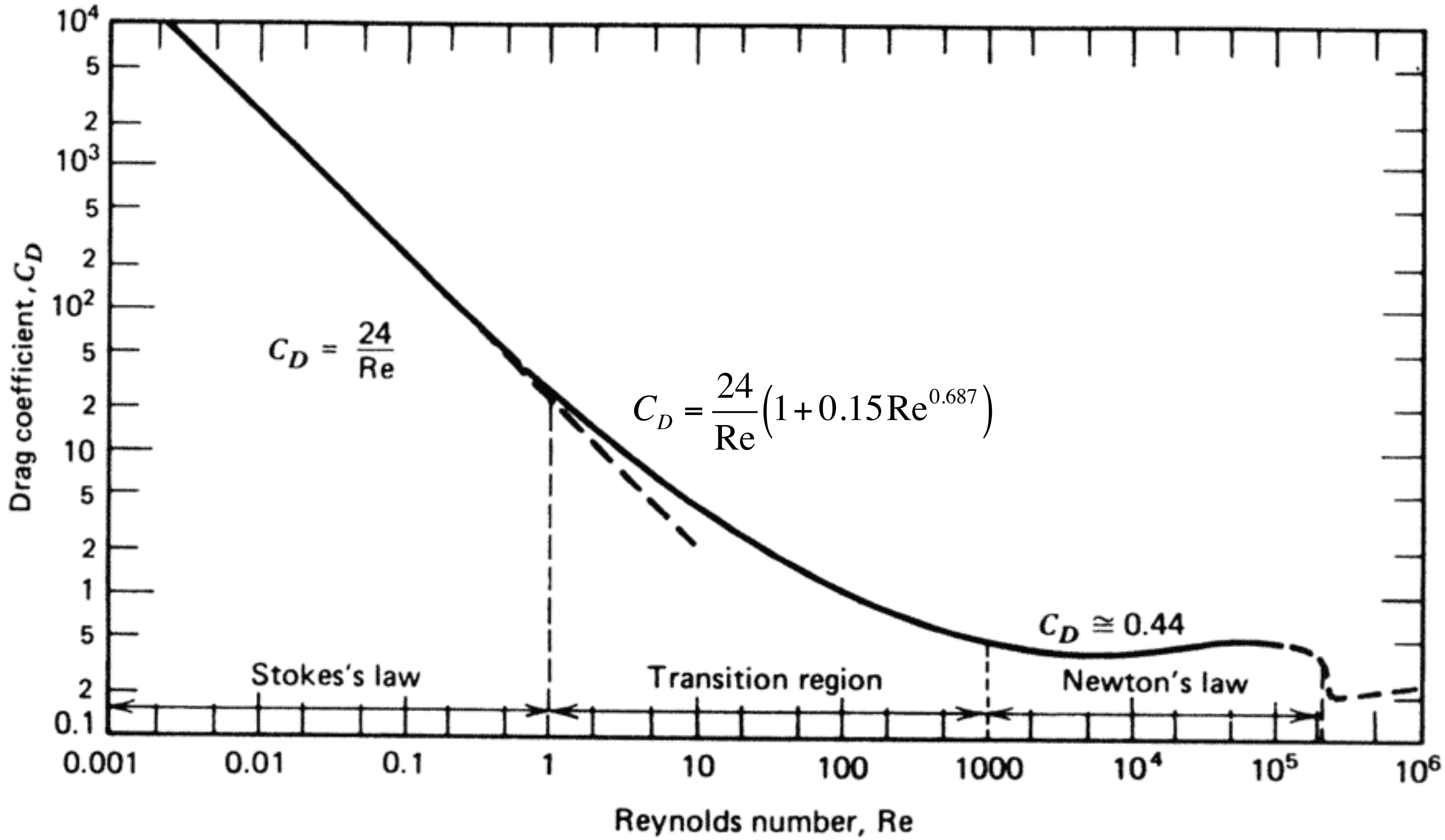


FIGURE 3.1 Drag coefficient versus Reynolds number for spheres.

Hinds 1999

Particle motion in gases

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

Diameter (μm)	*Re*
0.1	7×10^{-9}
1	2.8×10^{-6}
10	2.5×10^{-3}
20	0.02
60	0.4
100	2
300	20

  - Almost all atmospheric aerosols are in the Stoke's regime and Stoke's law can be applied (i.e., d_p < ~80 μm)

Hinds 1999

Particle motion in gases

- In the derivation of Stoke's 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 ≤ 1)
  - Particles less than about 1 μm
- Stoke's law has to be corrected for "slip" conditions:
  - Cunningham slip correction factor, C_C:

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

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

Based on Kn → lets you use Stoke's law for all regimes

Particle motion in gases

- Where are we going with this?

- Settling velocity
  - When a particle is released into the air, it quickly reaches its "terminal settling velocity"
    - 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

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

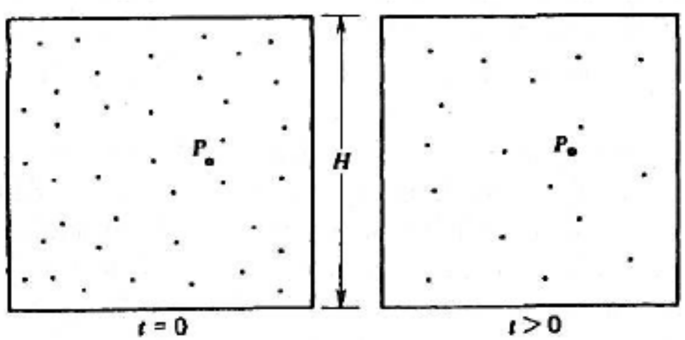
$$\frac{\pi}{6}\rho_p d_p^3 g = \frac{3\pi\mu V d_p}{C_C}$$

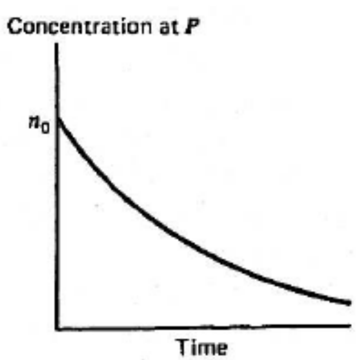
$$\boxed{V_{TS} = \frac{\rho_p d_p^2 g C_C}{18\mu}}$$

Particle motion in gases

- Terminal settling velocity for particles at STP

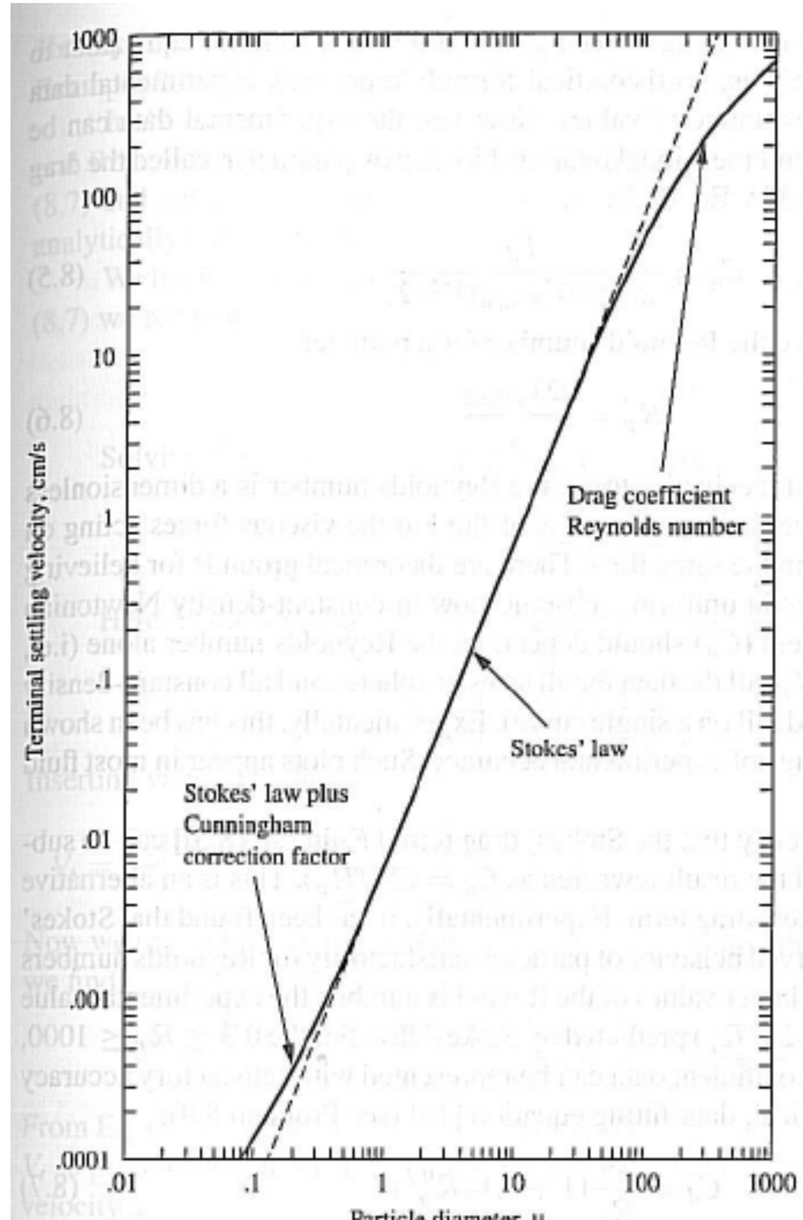
- What can we use V_{TS} for?
- Imagine "stirred settling"





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

Larger particles settle out of the air faster!



Particle motion in gases

- Other forces governing particle motion
  - Gravity (already covered)
  - Inertial impaction
  - Brownian diffusion
  - Electrophoretic
  - Thermophoretic

- A couple of other important particle properties also exist
  - Let's define these first:
    - 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, χ:

Shape	Dynamic Shape Factor,[a] χ	Axial Ratio 2	5	10
Geometric Shapes				
Sphere	1.00			
Cube[b]	1.08			
Cylinder[b]				
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[c]		1.10	1.35	1.68
Compact cluster				
Three spheres	1.15			
Four spheres	1.17			
Dusts				
Bituminous coal[d]	1.05–1.11			
Quartz[d]	1.36			
Sand[d]	1.57			
Talc[e]	1.88			

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

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

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

χ = 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

- Two other equivalent diameters are commonly used
- The aerodynamic diameter (d_a) is the diameter of a spherical particles having the density of water (1 g/cm^3) 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

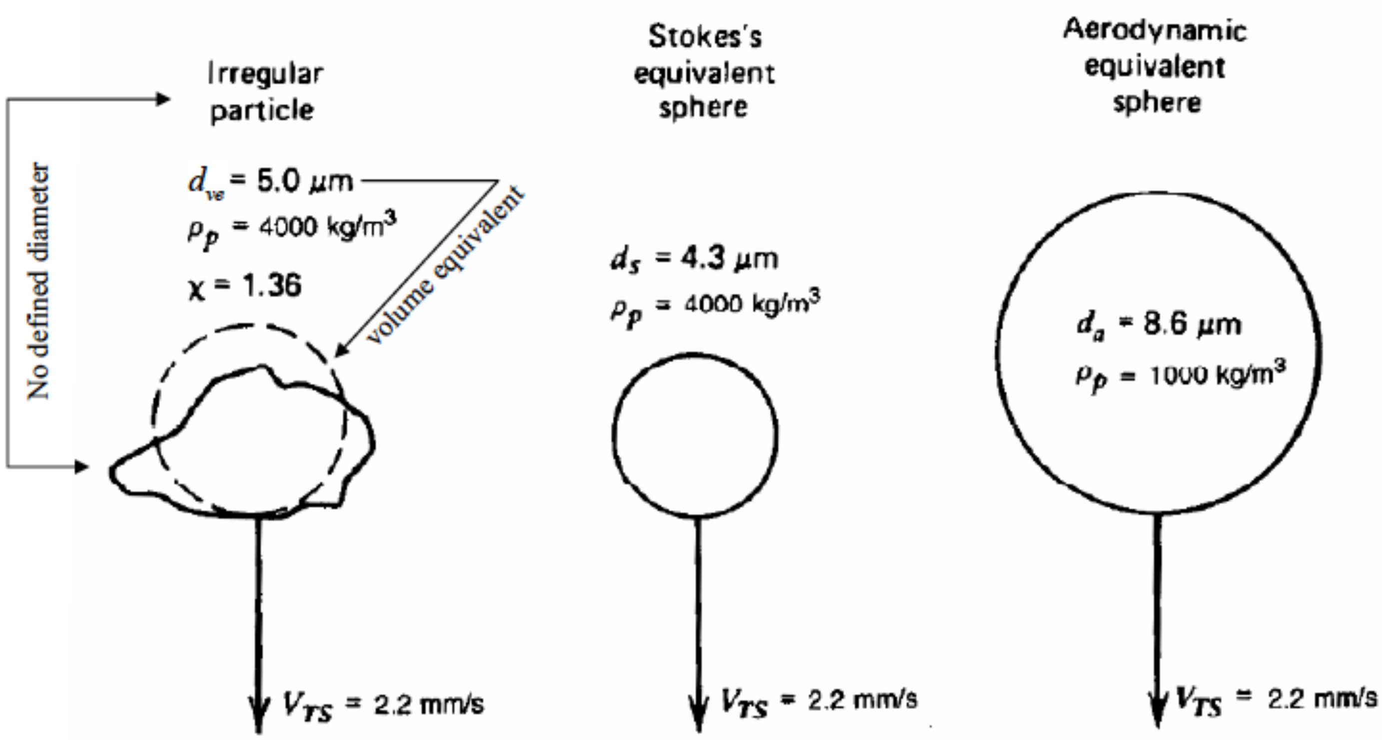
$$V_{TS} = \frac{\rho_p g C_C(d_e) d_e^2}{18\mu\chi} = \frac{\rho_0 g C_C(d_a) d_a^2}{18\mu} = \frac{\rho_p g C_C(d_s) d_s^2}{18\mu}$$

  – Note that C_C has to be calculated as functions of the diameter you're using

Aerodynamic and Stokes diameters

- For particles with $d_p > 1$ µm 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

- We don’t have time to cover these in full detail
  - Inertial impaction
  - Brownian diffusion
  - Electrophoretic/electrostatic forces
  - Thermophoretic
- But I will provide basic concepts and equations so we can understand what removes 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
  - Particle deposition rate onto surfaces (1/hr): $k_{dep} = \frac{v_d A}{V}$

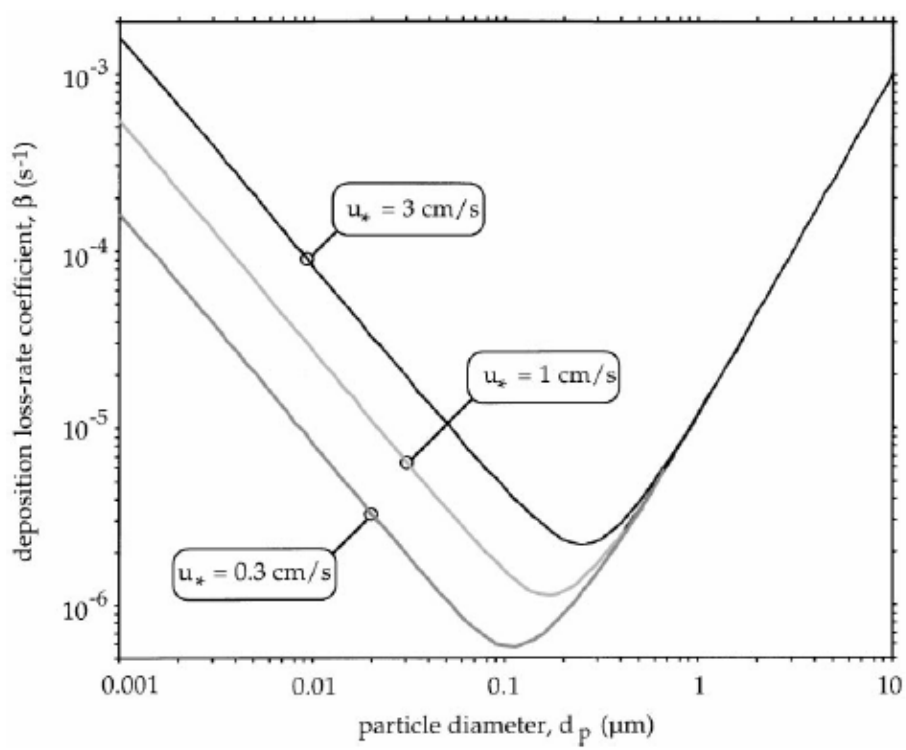


Fig. 5. Particle deposition loss-rate coefficient, β, for typical room dimensions (3 m high × 4 m × 5 m) according to the current model. Friction velocities of 0.3–3 cm s^{-1} approximately span the range expected for mechanically ventilated indoor spaces. Predictions assume air pressure is 1 atm, temperature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

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

Lai and Nazaroff 2000 *J Aerosol Sci*

PARTICLE SIZE DISTRIBUTIONS

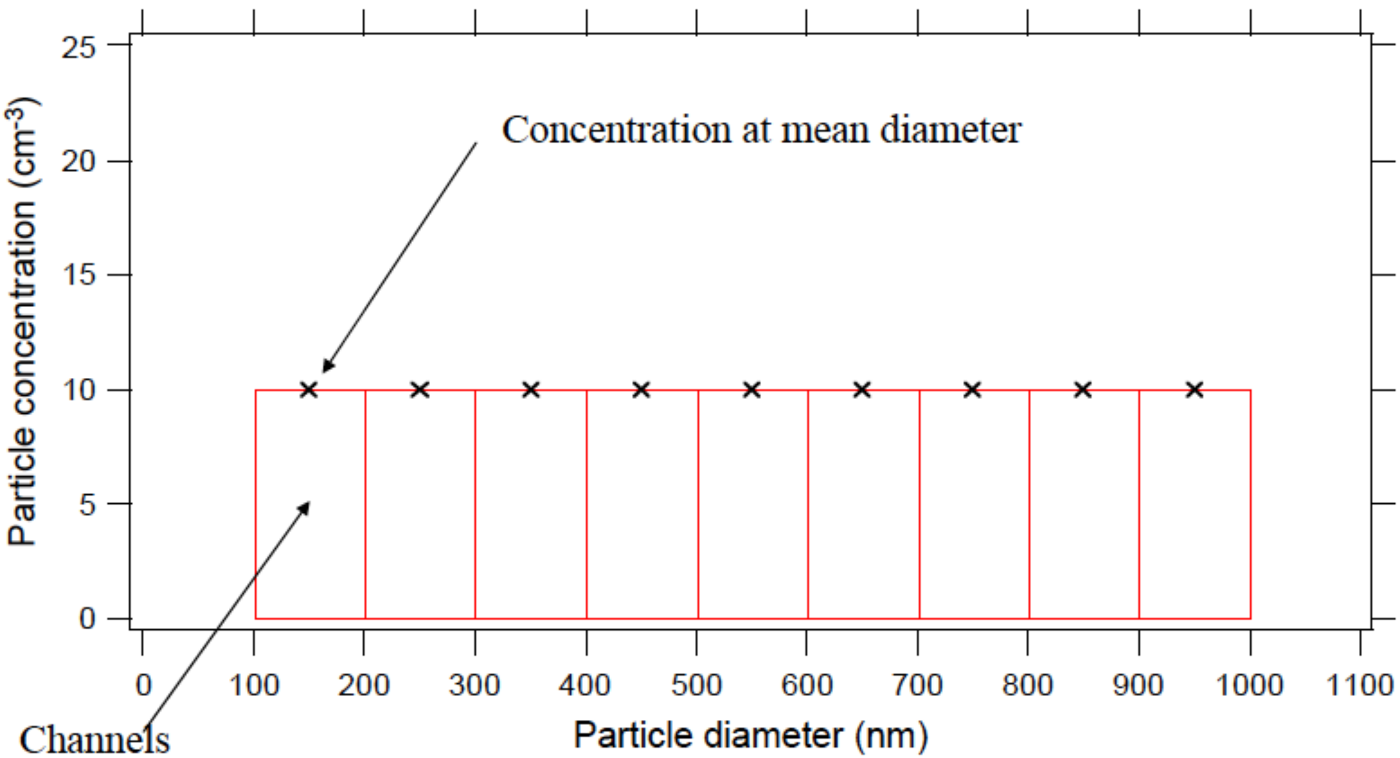
Size distributions

- 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 size distribution, 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 Δd_p or dd_p
    - Number of particles with diameters between d_{p2} and d_{p1}

Size distributions

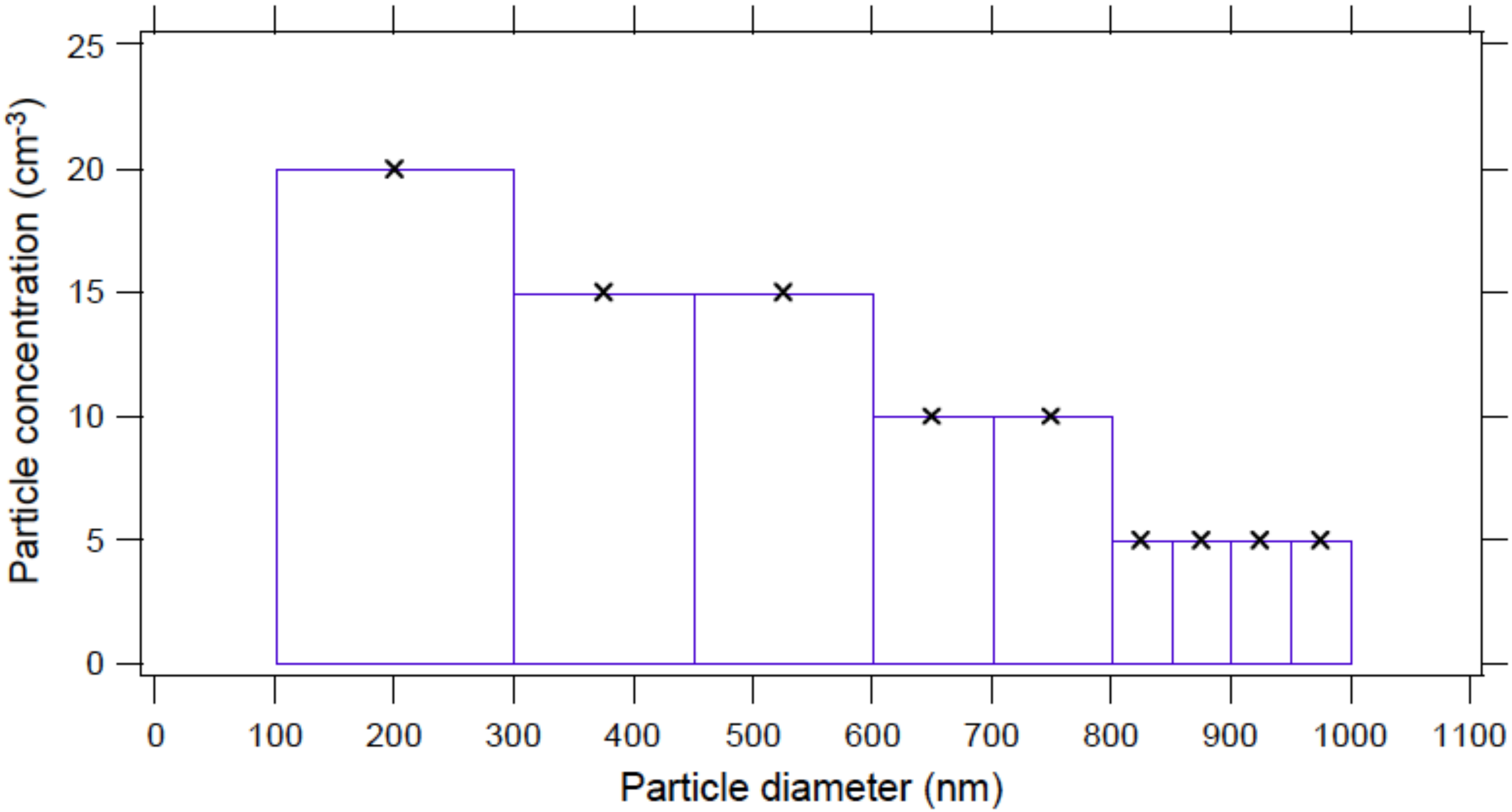
- 9 size channels, width of 100 nm each, each with 10 particles per cm^3
- We consider the measured concentration as dN in each channel



Schneider, 2010

Size distributions

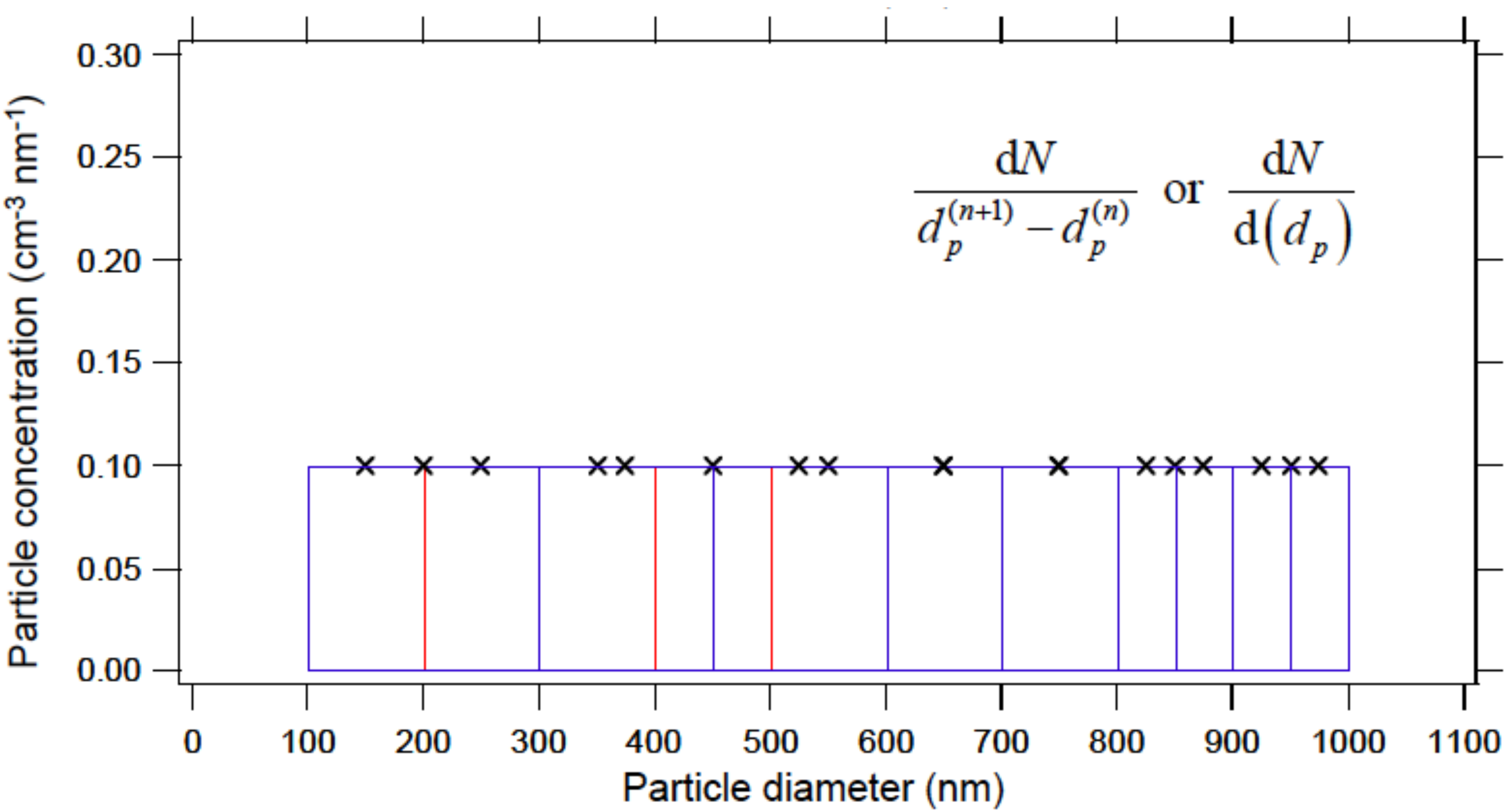
- If we use a different instrument with different channel widths, the shape of the distribution changes:



Schneider, 2010

Size distributions

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



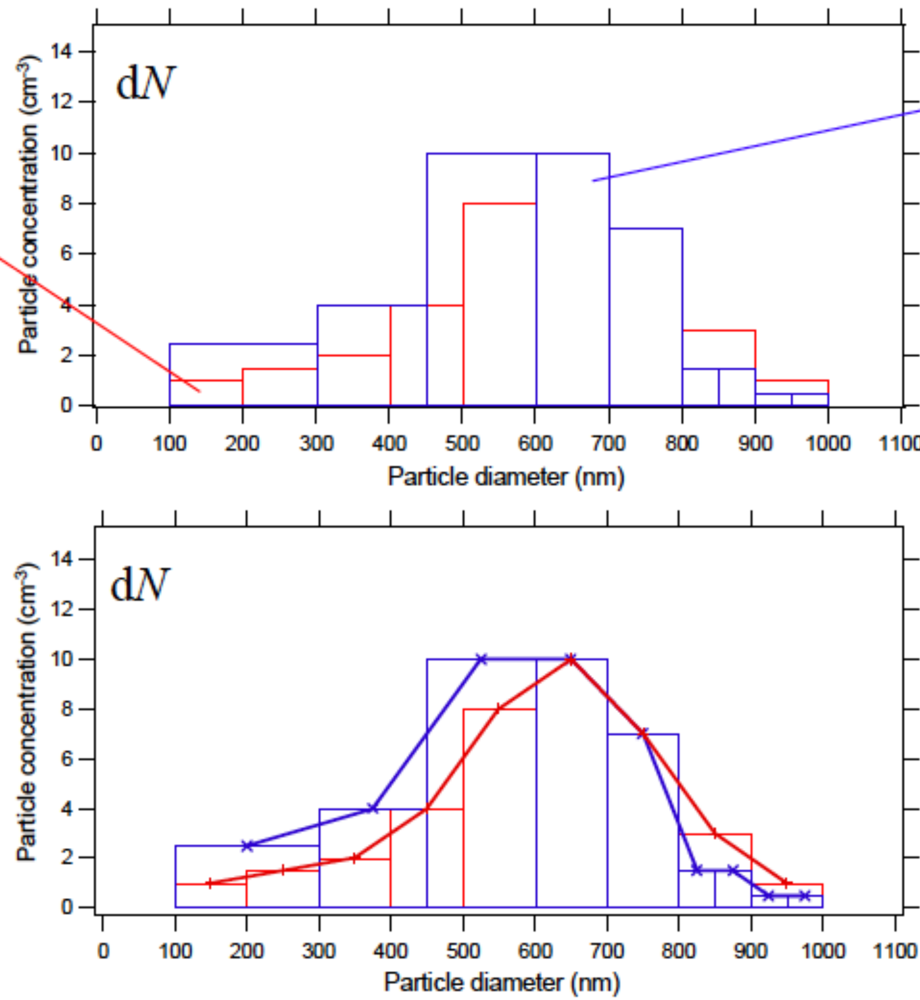
Schneider, 2010

Size distributions

- Similar example but for a more realistic size distribution

"Instrument 1"

Channel	N (cm^{-3})
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



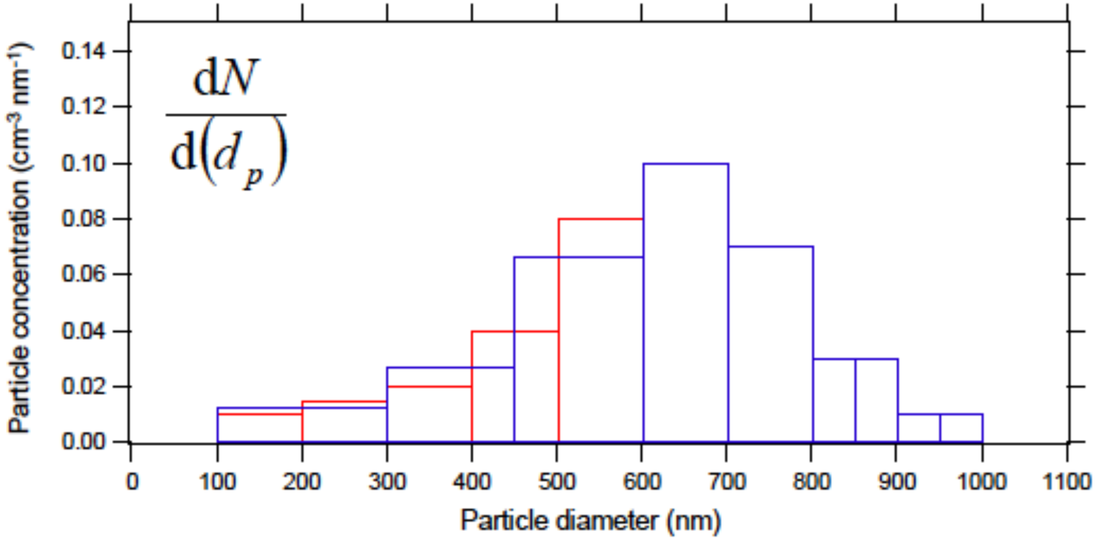
"Instrument 2"

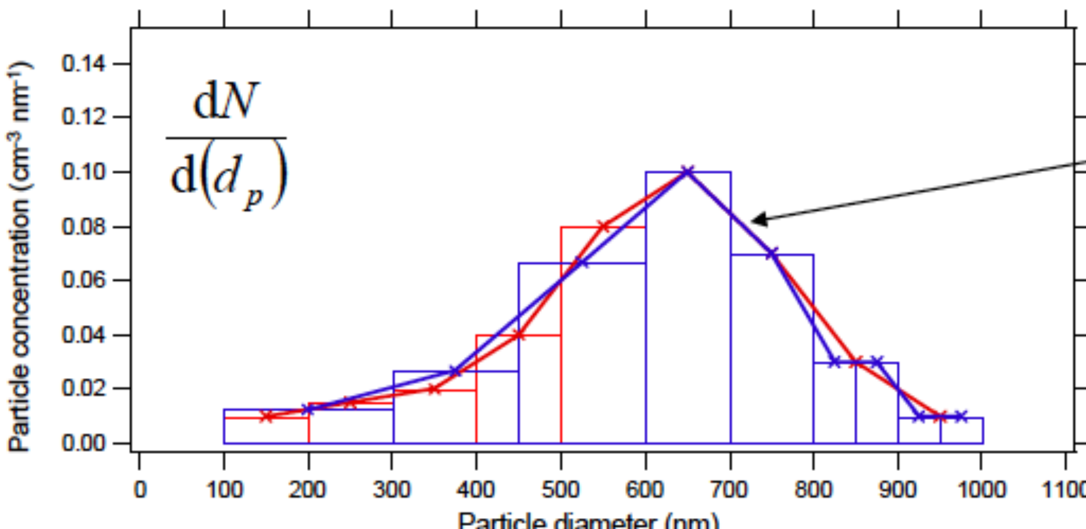
Channel	N (cm^{-3})
100-300	2.5
300-450	4
450-600	10
600-700	10
700-800	7
800-850	1.5
850-900	1.5
900-950	0.5
950-1000	0.5

Schneider, 2010

Size distributions

- Divide by the channel widths





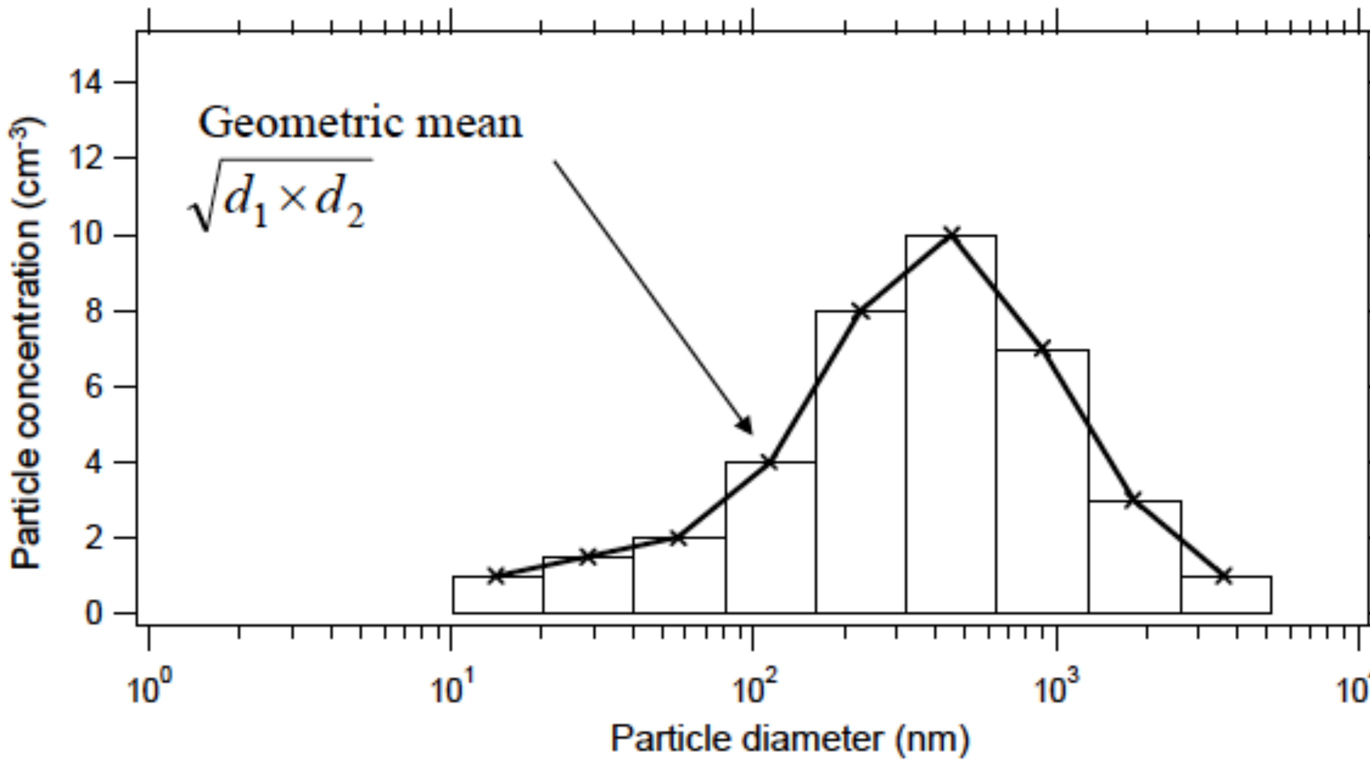
Almost the same distribution despite different measurement channels for the two instruments

Schneider, 2010

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)

Channel	N (cm^{-3})
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



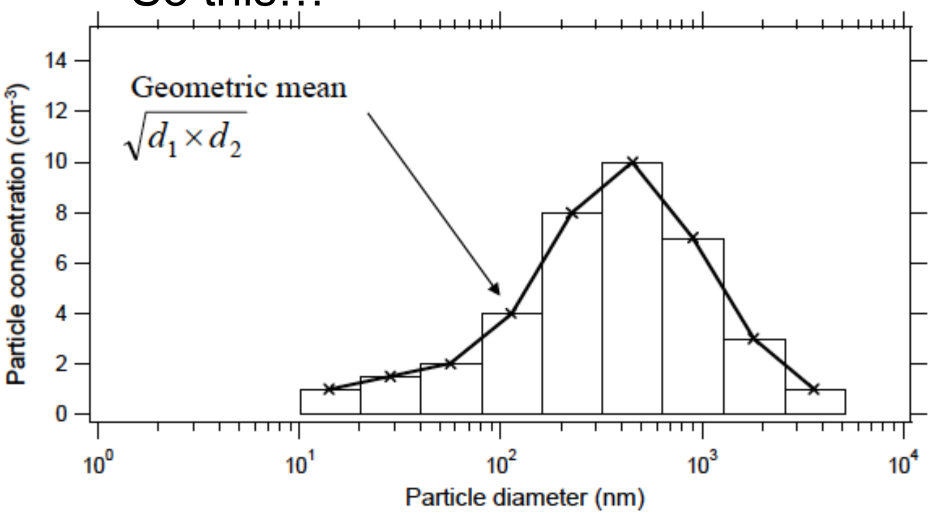
Schneider, 2010

Size distributions

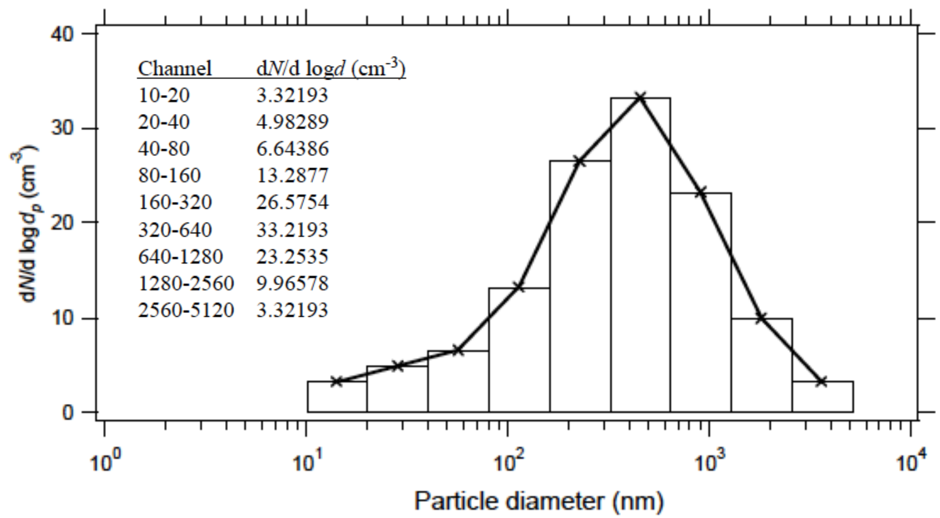
- For log scales we need to account for the channel width differently:

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

So this…



Becomes this…

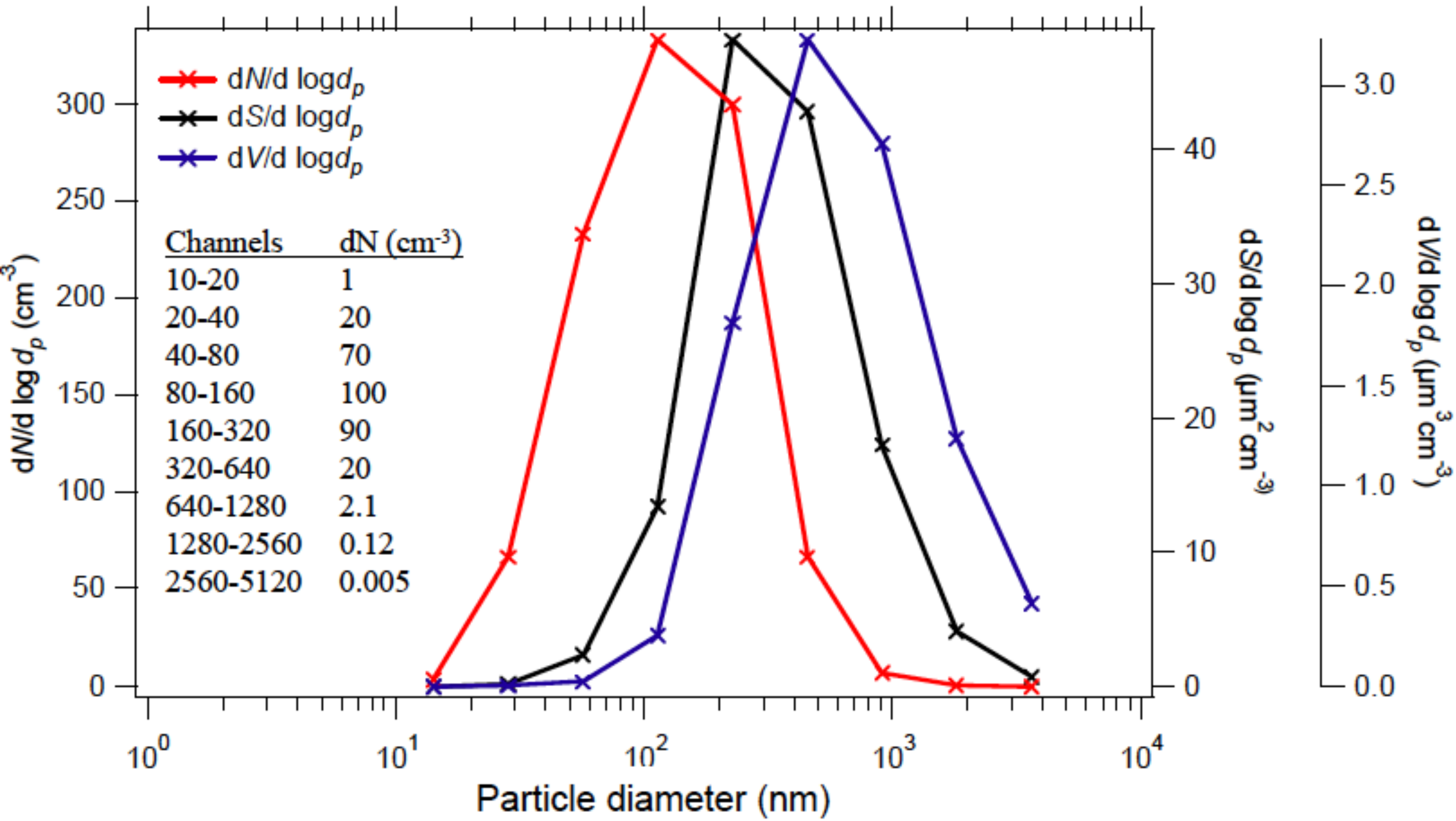


Schneider, 2010

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 (µm2 per cm^3): $dS = \pi d_p^2 dN$
- Volume (µm^3 per cm^3): $dV = \frac{\pi}{6} d_p^3 dN$
- If we know particle density
  - We can estimate the mass distribution (µg per cm^3): $dM = \rho_p \frac{\pi}{6} d_p^3 dN$

Number, surface area, volume, and mass distributions



Schneider, 2010

Describing distributions

- Arithmetic mean particle diameter = 'count mean diameter'

$$CMD = d_{mean} = \bar{d}_p = \frac{1}{N_{tot}} \sum_{k=1}^{n} d_{p,k} N_k$$

n: number of size channels $d_{p,k}$: mean channel diameters,
N_k: number concentrations, N_{tot} : integrated number concentration.

- For continuous distribution $N(d_p)$:

$$\bar{d}_p = \frac{1}{N_{tot}} \int_0^{\infty} d_p N\left(d_p\right) \mathrm{d}d_p$$

- Geometric mean particle diameter (d_g)

$$\log d_g = \frac{1}{N_{tot}} \sum_{k=1}^{n} \log d_{p,k} N_k$$

Schneider, 2010

Describing distributions

- Atmospheric aerosols are often described by a lognormal distribution
  - Allows for characterization of an aerosol with only 3 parameters
- Normal distribution: $$n(x) = \frac{N}{\sqrt{2\pi\sigma}} e^{\left(-\frac{(x-\bar{x})^2}{2\sigma^2}\right)}$$
- Lognormal distribution: $$\frac{\mathrm{d}N}{\mathrm{d}\log d_p} = \frac{N}{\sqrt{2\pi}\log\sigma_g} e^{\left(-\frac{\left(\log d_p - \log\bar{d}_g\right)^2}{2\left(\log\sigma_g\right)^2}\right)}$$
  - Where:

N: Total particle number concentration

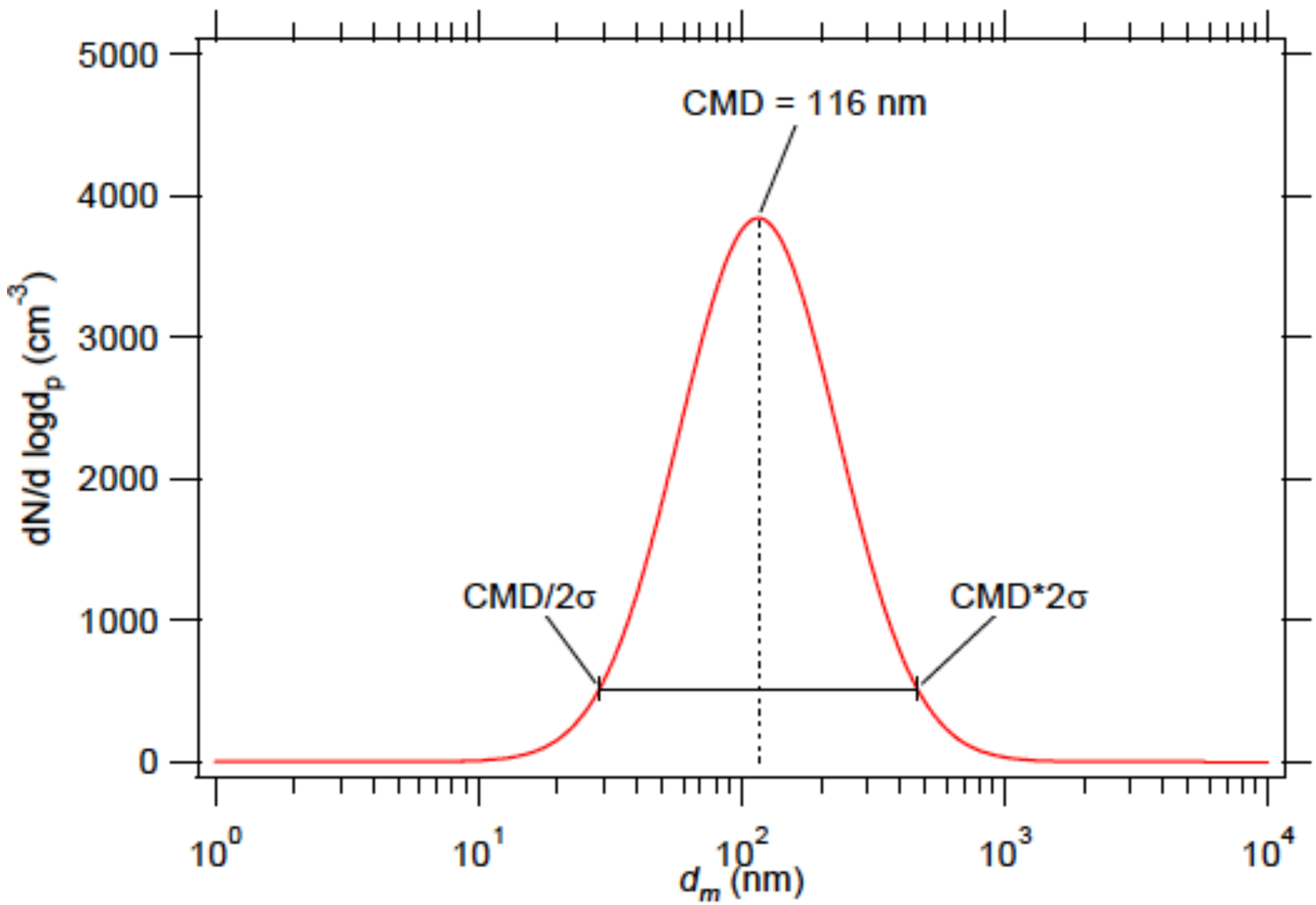
σ_g: Geometric standard deviation

$\bar{d}_g$: Geometric mean diameter: $\log\bar{d}_g = \frac{\sum n_i \log d_i}{N}$

Schneider, 2010

Lognormal distribution

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



Schneider, 2010

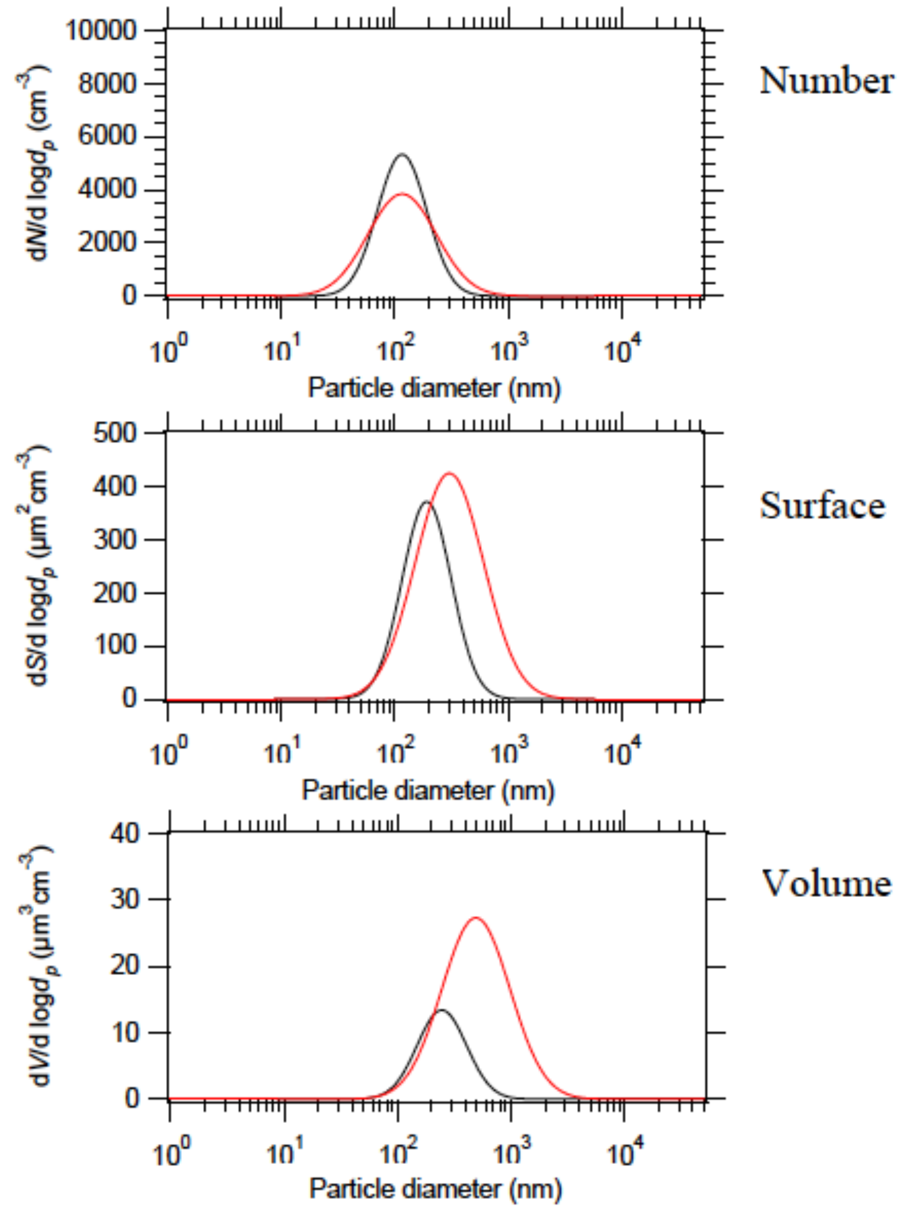
Lognormal distribution

- Example distribution for one ‘mode’:

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

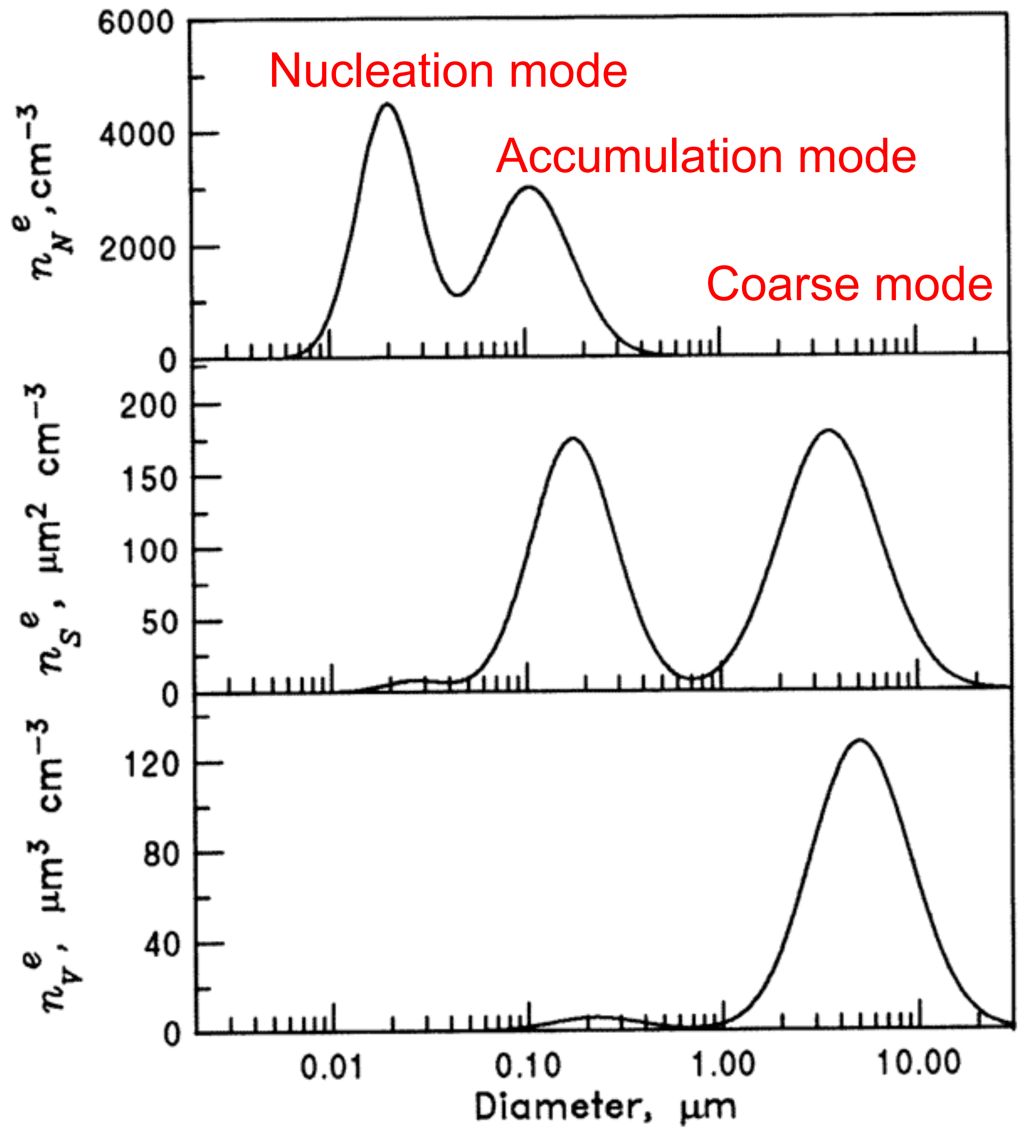
$$\cancel{\sigma_g = 1.65}\quad \sigma_g = 2.0$$

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



Schneider, 2010

Typical aerosol distributions



Lognormal distributions: summing across modes

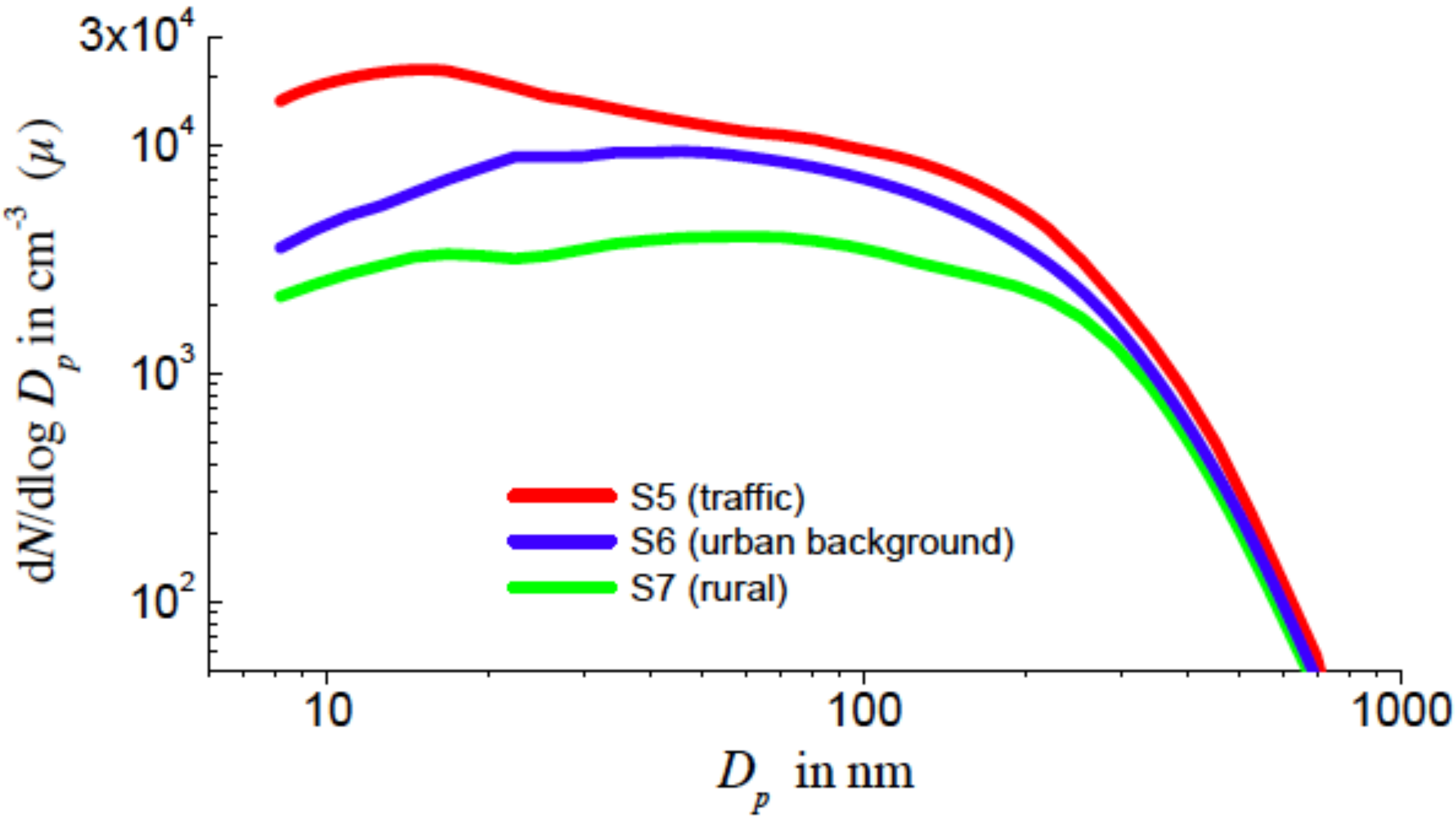
$$\frac{dN}{d\log d_p} = \sum_{i=1}^{n} \frac{N_i}{\sqrt{2\pi}\log\sigma_i} e^{\left(-\frac{\left(\log d_p - \log \bar{d}_{g,i}\right)^2}{2(\log\sigma_i)^2}\right)}$$

	Mode I			Mode II			Mode III		
Type	N (cm^{-3})	D_p (μm)	$\log\sigma$	N (cm^{-3})	D_p (μm)	$\log\sigma$	N (cm^{-3})	D_p (μm)	$\log\sigma$
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).

Typical aerosol distributions

- Submicron particles in Germany



Costabile et al. 2009 *Atmos Chem Phys*

RESPIRATORY DEPOSITION

Why are we so concerned about particle size?

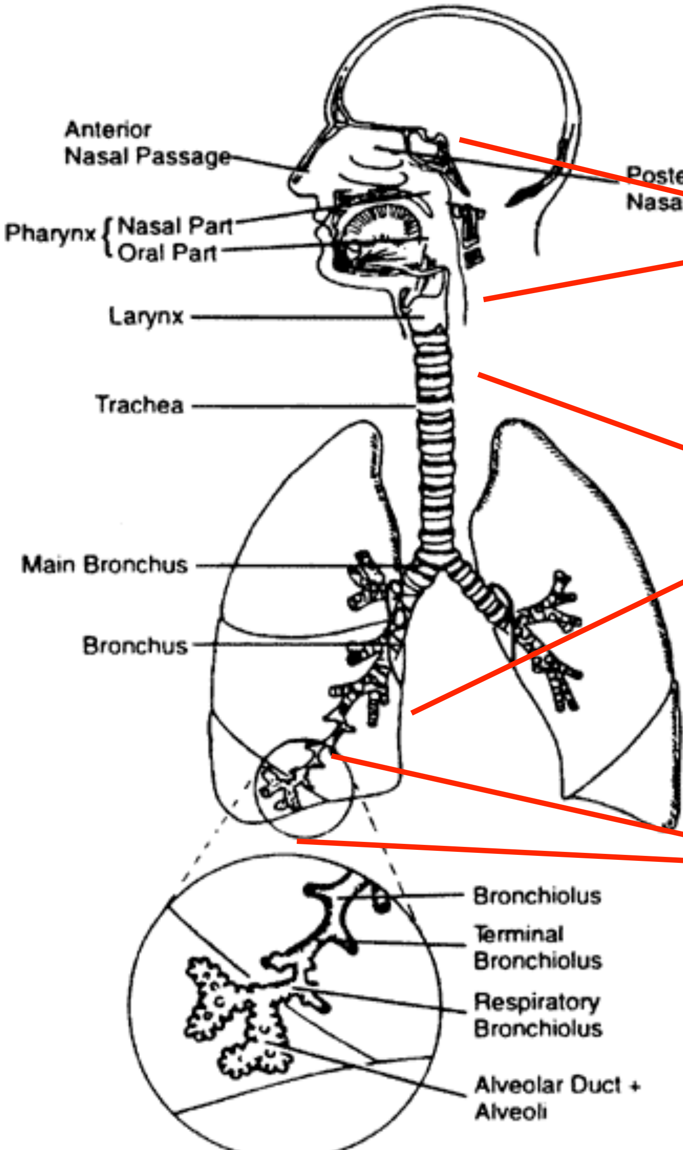
- One reason is because particles of different sizes deposit in different areas of our respiratory system with different efficiencies

- Humans breathe 10-25 m^3/day
  ~0.5 L/breath at rest
  ~12 breaths/minute at rest

- Surface area of lung devoted to gas exchange is ~75 m^2
  – ½ area of singles tennis court in alveolar region

- Velocities range from cm/s to mm/s

Human respiratory system



Nasopharyngeal

Tracheobronchial

(N&T regions "cleaned" by mucus)

Alveolar

Hinds, 1999 Ch. 11

Lung parameters

TABLE 11.1 Characteristics of Selected Regions of the Lung[a]

Airway	Generation	Number per Generation	Diameter (mm)	Length (mm)	Total Cross Section (cm^2)	Velocity[a] (mm/s)	Residence Time[b] (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	0.26×10^6	0.50	1.2	530	19	60
Alveolar duct	21	2×10^6	0.43	0.7	3200	3.2	210
Alveolar sac	23	8×10^6	0.41	0.5	72,000	0.9	550
Alveoli		300×10^6	0.28	0.2			

[a]Based on Weibel's model A; regular dichotomy average adult lung with volume. 0.0048 m^3 [4800 cm^3] at about three-fourths maximal inflation. Table adapted from Lippmann (1995).
[b]At a flow rate of 3.6 m^3/hr [1.0 L/s].

Note: based on steady flow

Hinds, 1999 Ch. 11

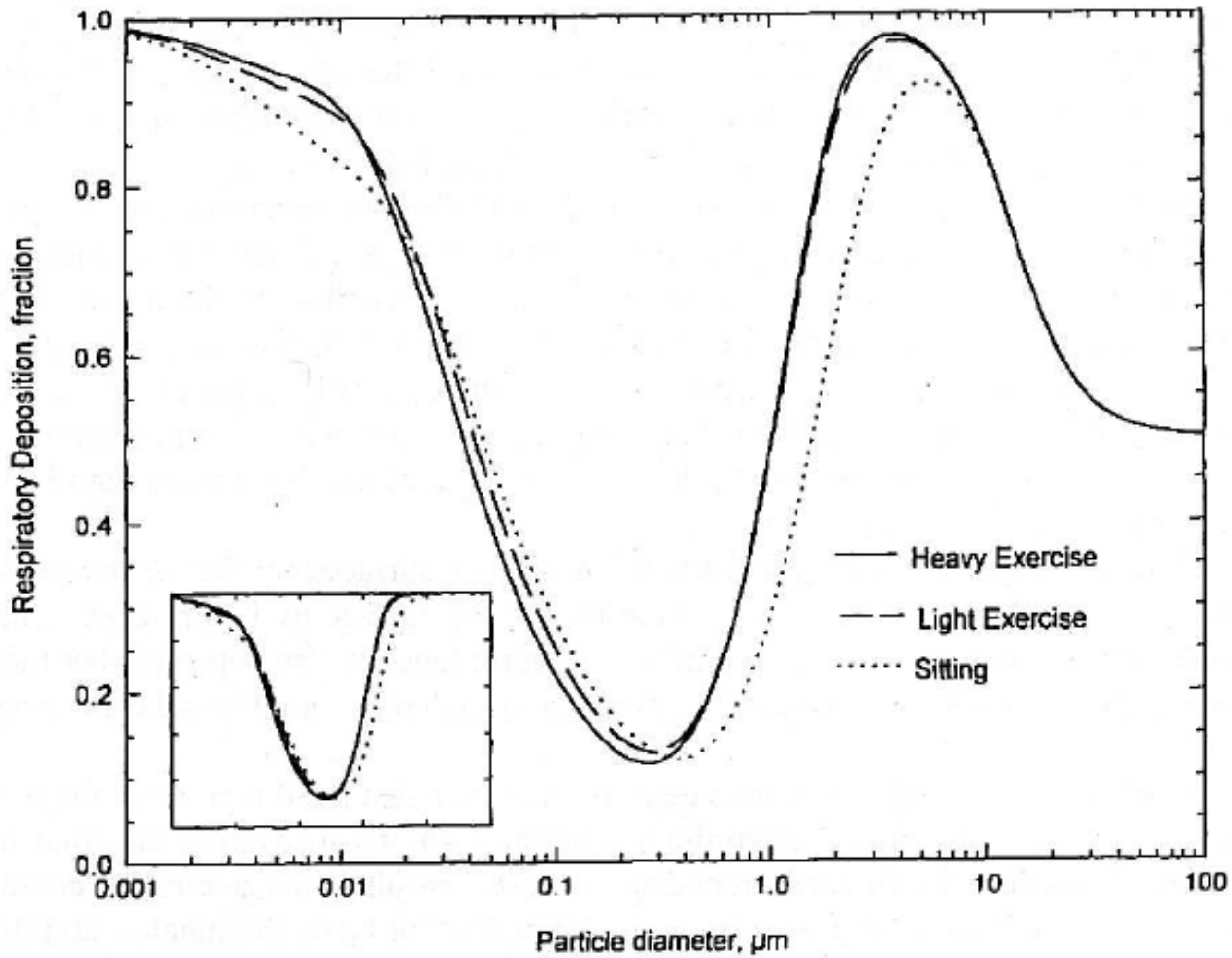
Particle deposition in lungs

- 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



Hinds, 1999 Ch. 11

Respiratory deposition by region

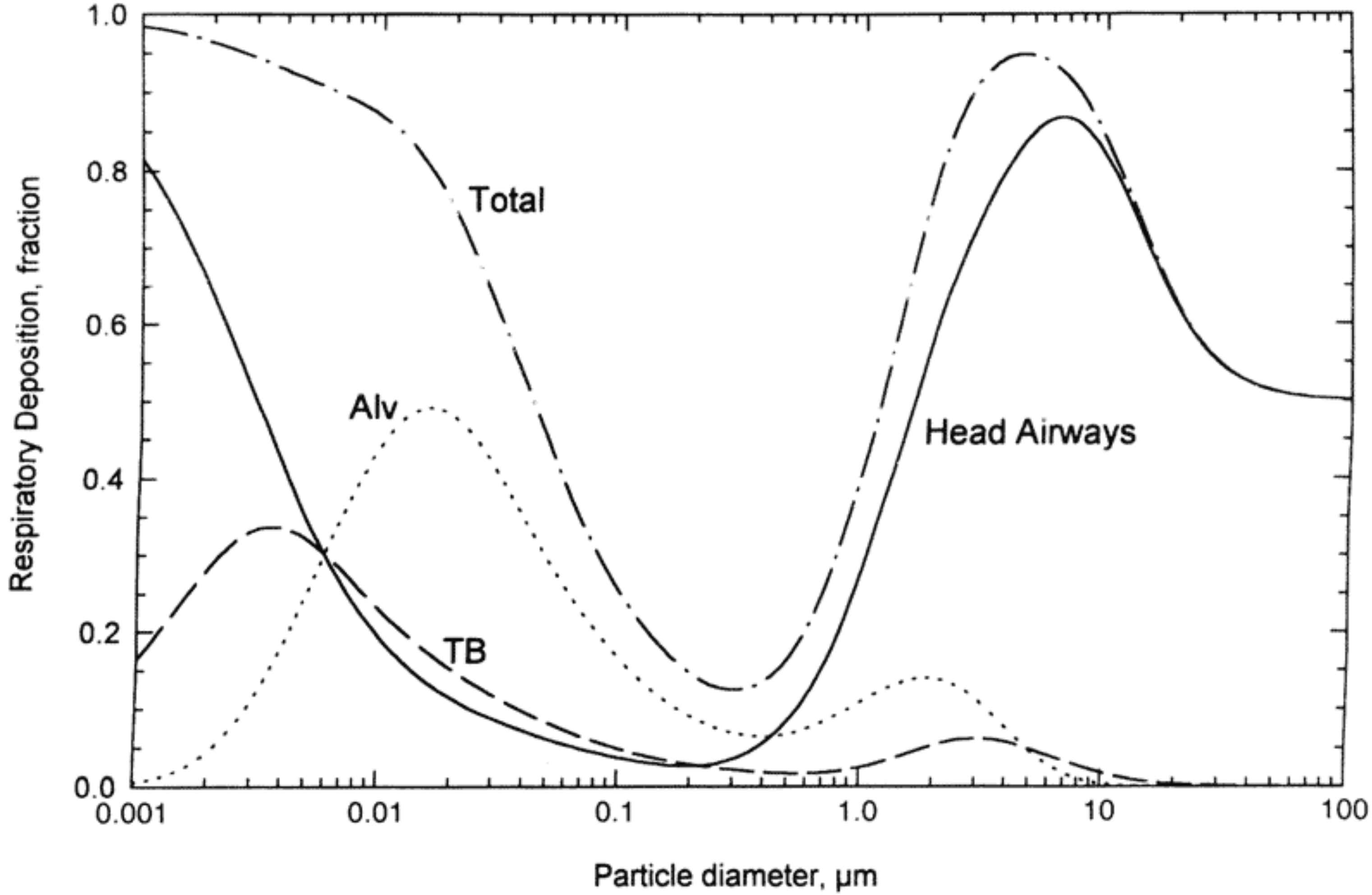


FIGURE 11.3 Predicted total and regional deposition for light exercise (nose breathing) based on ICRP deposition model. Average data for males and females.

Hinds, 1999 Ch. 11

Alveolar deposition

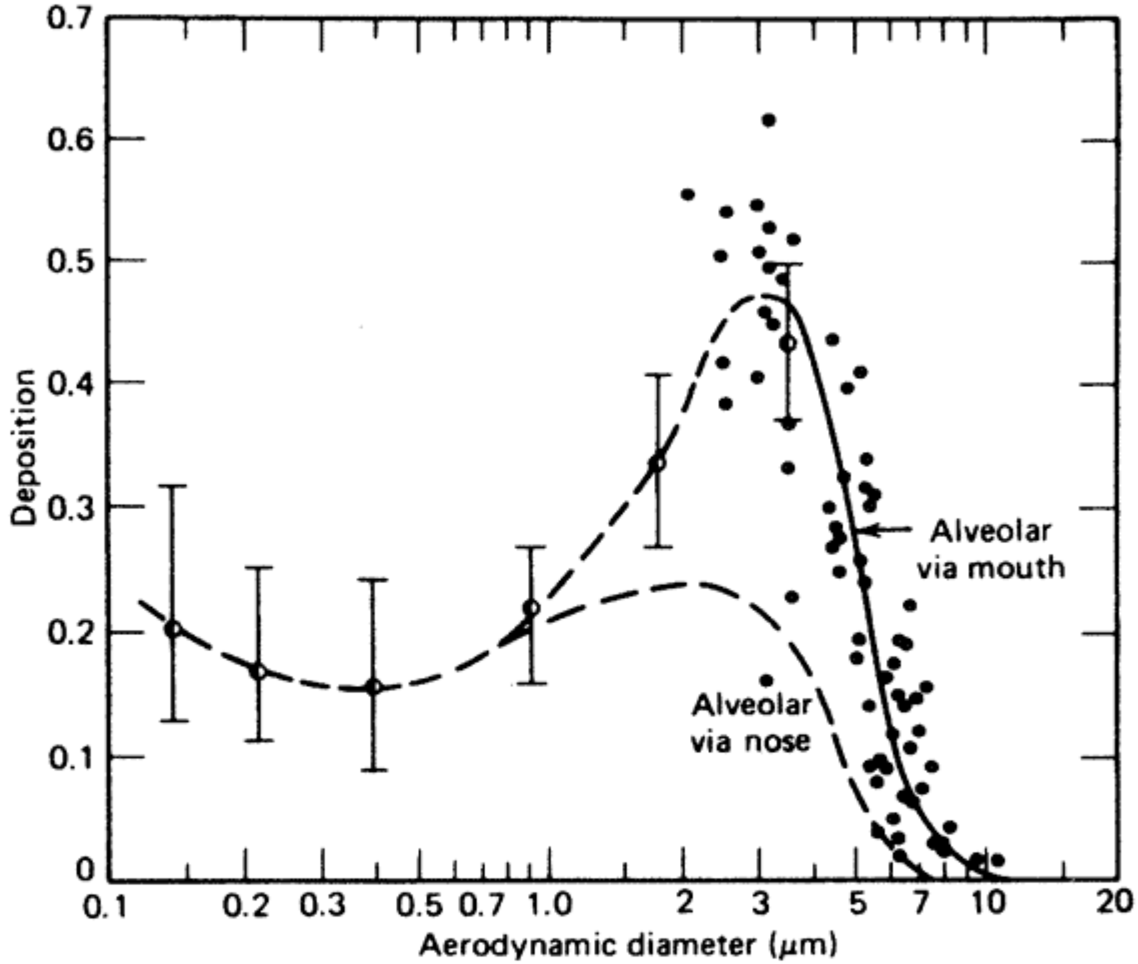


FIGURE 11.4 Experimental data for deposition in the alveolar region. Deposition is expressed as a fraction of mouthpiece inhalation versus aerodynamic diameter (geometric diameter used below 0.5 μm). Reprinted with permission from Lippmann (1977).

Hinds, 1999 Ch. 11

So what?

- We can examine different sources
  - e.g., ETS or cooking particles
- What particles will deposit in lungs?
  - In which region?

ETS lung penetration

- 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
  - Use lung deposition model to examine where ETS particles end up

Emissions from ETS

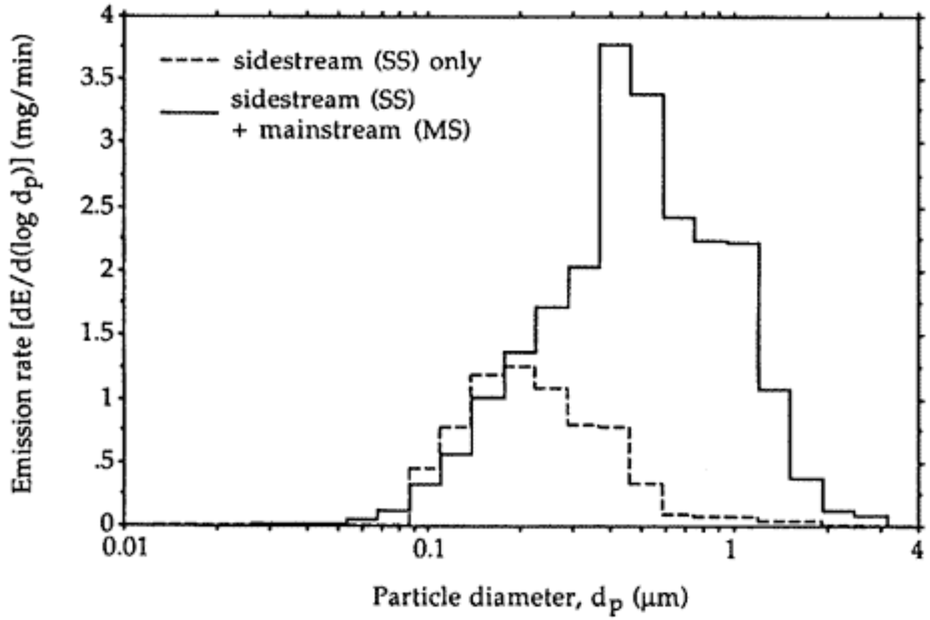


FIGURE 1. Effective particle emission rate from a burning cigarette as a function of particle diameter. The form of the figure is such that the area under a curve between two particle sizes is proportional to the mass emission rate of all particles within those size limits. These experiments were reported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

Nazaroff et al., 1993 *AS&T*

Modeled indoor concentrations from ETS

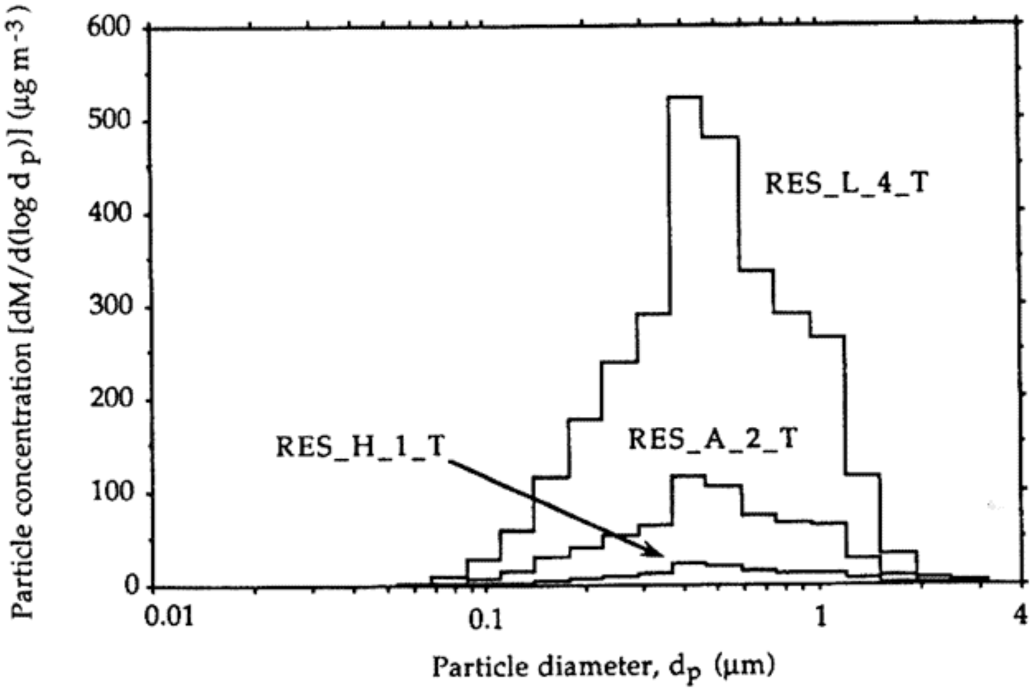


FIGURE 4. Average environmental tobacco smoke particle size distribution over 24-h period for three residential simulations corresponding

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^{-1}; **A** = 0.68 h^{-1}; **L** = 0.28 h^{-1}
cigarette smoking frequency: **1**, **2**, or **4** per hour

Nazaroff et al., 1993 *AS&T*

ETS lung deposition

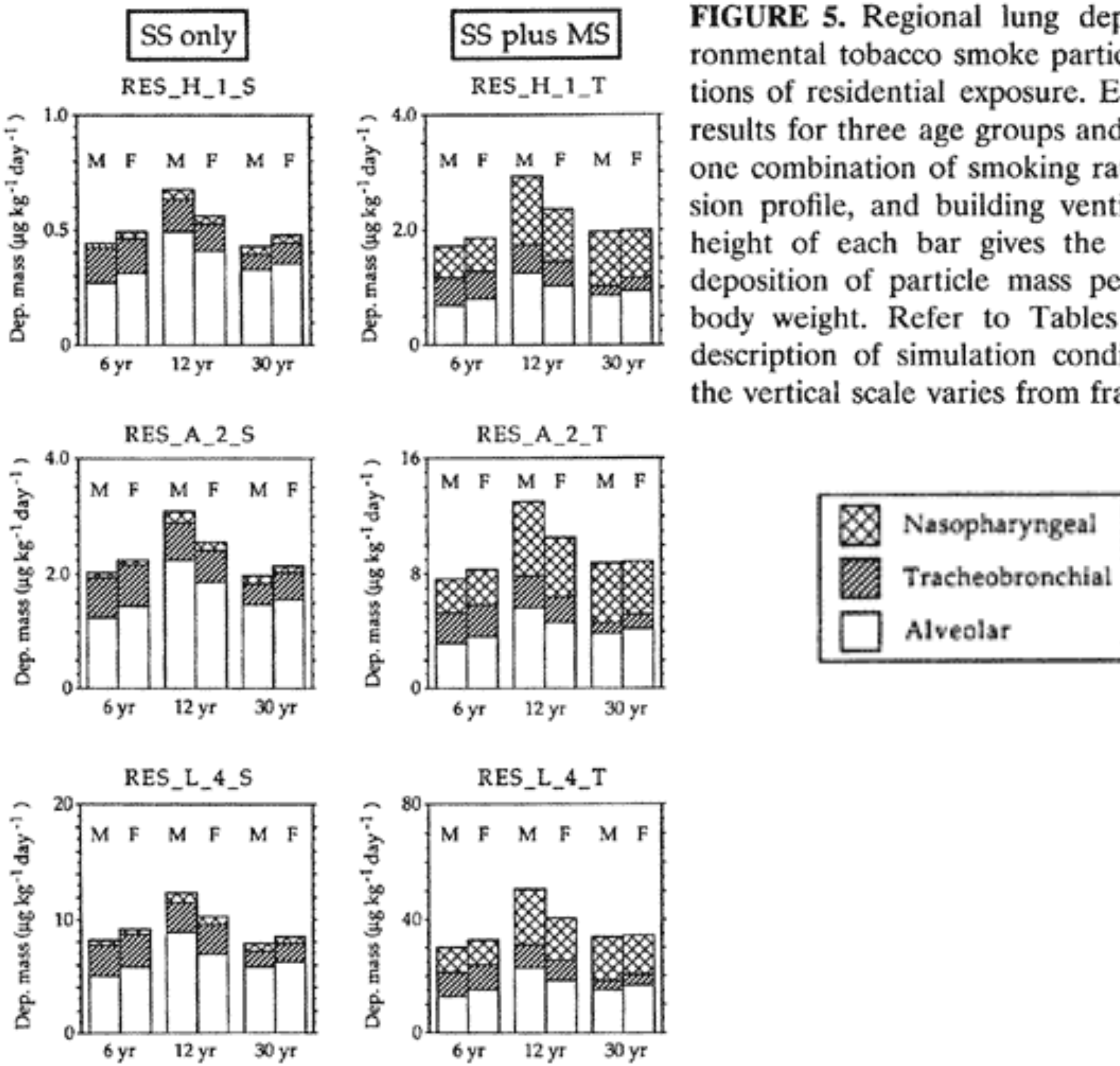


FIGURE 5. Regional lung deposition of environmental tobacco smoke particles from simulations of residential exposure. Each frame shows results for three age groups and each gender for one combination of smoking rate, particle emission profile, and building ventilation rate. The height of each bar gives 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.

Nazaroff et al., 1993 *AS&T*

ETS lung deposition

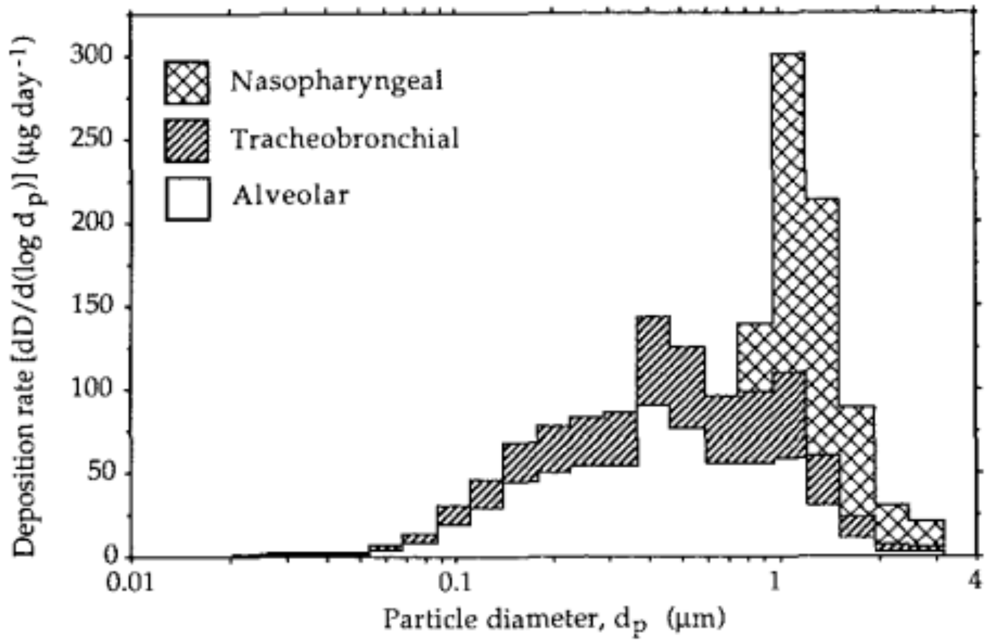


FIGURE 6. Size distribution of deposited mass of environmental tobacco smoke particles in 6-year-old boy for simulation RES_A_2_T. The form of the figure is such that the shaded area between two particle sizes is proportional to the average 24-h mass deposition rate of particles within those size limits. See Tables 1 and 2 for a description of simulation conditions.

Nazaroff et al., 1993 *AS&T*

Next time

- No HW assigned today

- Next time: particle sources, deposition, and resuspension