Introduction to aerosol modelling with UKCA

Dan Grosvenor
Met Office, CEMAC at U. Leeds

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Based (with thanks!) on slides from **Cat Scott**, **Kirsty Pringle** and **Graham Mann,** Institute for Climate and Atmospheric Science, University of Leeds

With contributions from: Ken Carslaw, Carly Reddington, Sandip Dhomse, Steven Turnock, Dominick Spracklen, Anja Schmidt, Colin Johnson, Mohit Dalvi, Jane Mulcahy Philip Stier, Rosalind West, Zak Kipling, Nicolas Bellouin, Luke Abraham, Paul Telford, Peter Braesicke, Alex Archibald, John Pyle

What is an aerosol particle

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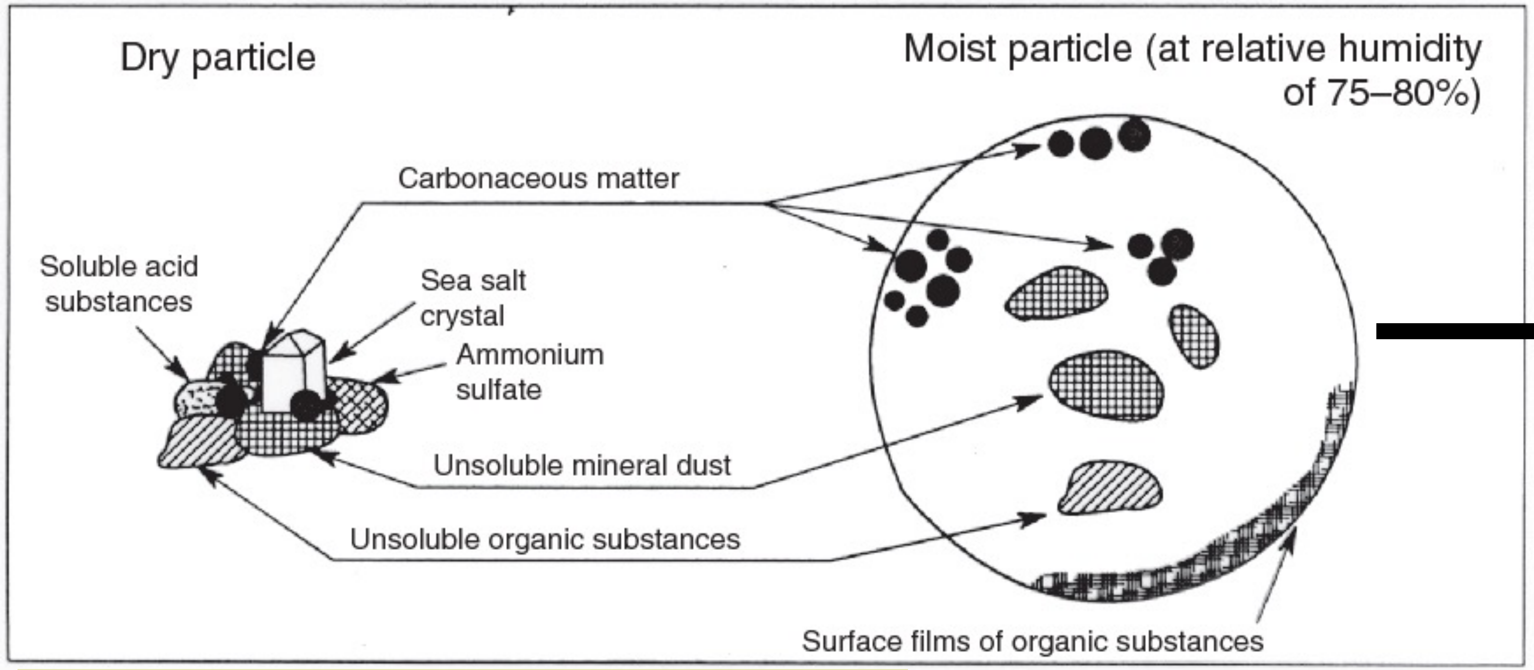
- Wikipedia: "An aerosol is a suspension of fine **solid particles** or **liquid droplets** in air or another gas."

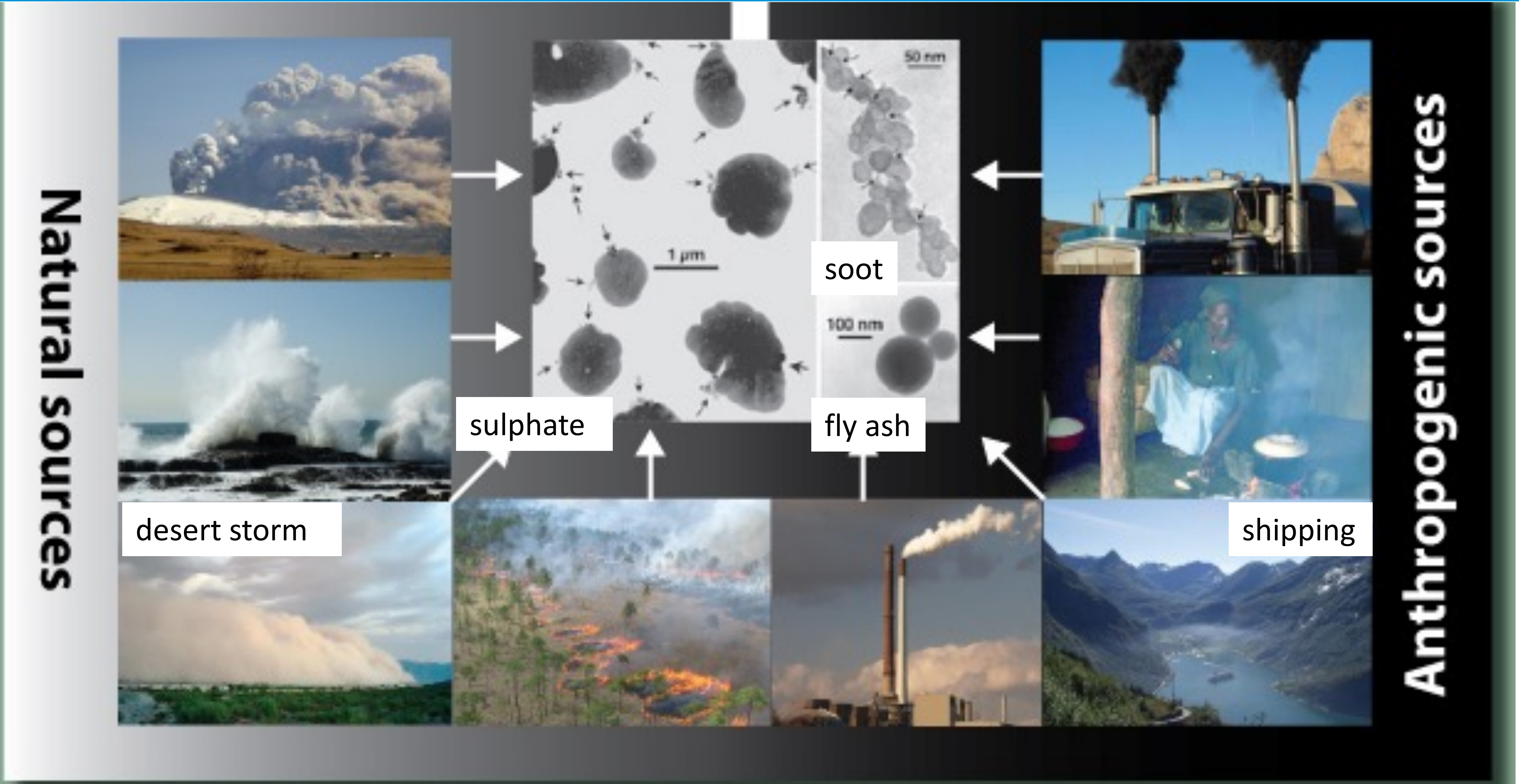


Claudio Tomasi, Sandro Fuzzi, Alexander Kokhanovsky (2016) Primary and Secondary Sources of Atmospheric Aerosol; (Book) https://doi.org/10.1002/9783527336449.

"Activation" into cloud droplets

Aerosol swelling

Aerosol sources



Myhre, G., Myhre, C. E.L., Samset, B. H. & Storelvmo, T. (2013) Aerosols and their Relation to Global Climate and Climate Sensitivity. Nature Education Knowledge 4(5):7

The Global Aerosol Distribution

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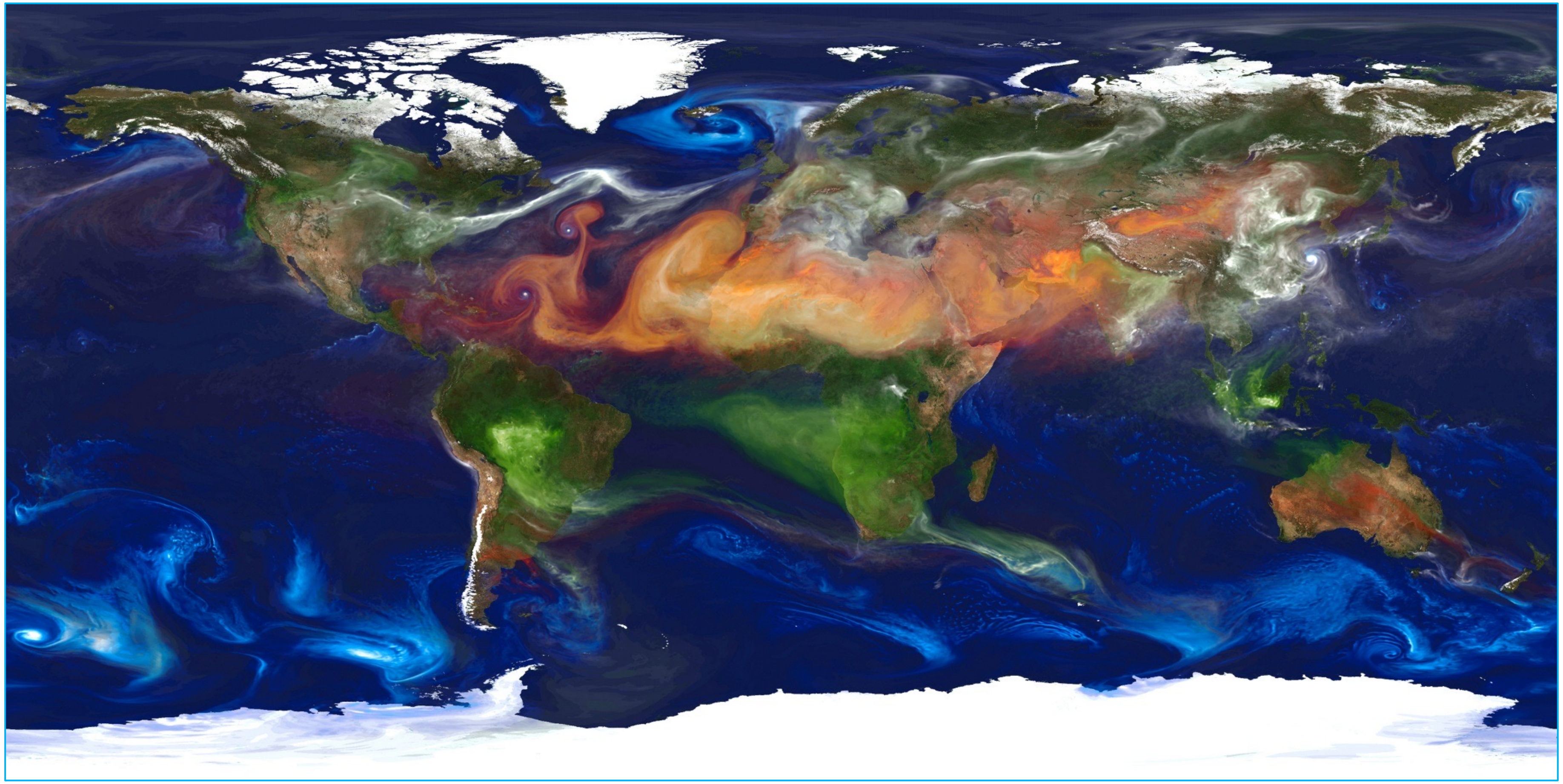

https://www.youtube.com/watch?v=oRsY_UviBPE

NASA: A portrait of global aerosol.
Composite of satellite and model data.

Green: Smoke, Orange: Dust
Blue: Sea spray, White: Sulfates

Why model aerosol?

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- **Aerosol-radiation interactions (direct forcing)**
- Aerosol can absorb and scatter solar radiation.

- **Aerosol-cloud interactions (indirect forcing)**
- Aerosol can act as cloud condensation nuclei and change cloud brightness and lifetime.

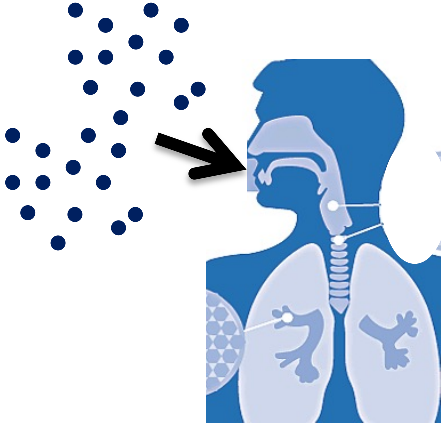
- **Atmospheric chemistry**
- Aerosol provide a surface area for chemical reactions.

Biogeochemical cycles

- Aerosols interact with living species in many ways, e.g. some aerosol provide nutrients to nutrient poor regions.

Health Effects

- Increases in aerosol concentration linked to increased likelihood of ca and heart disease.



How do aerosols affect climate?

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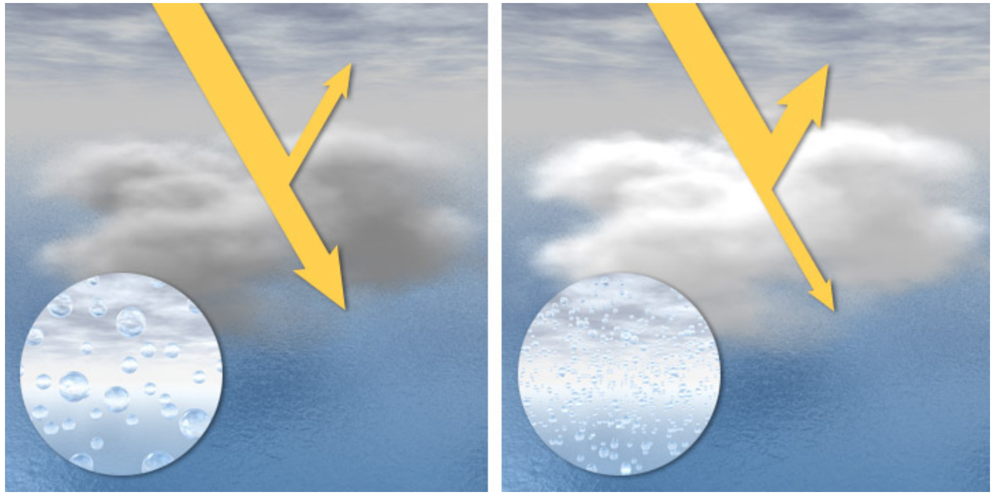
Aerosol direct radiative effects

Aerosols scatter and absorb radiation

Aerosol cloud brightening effect

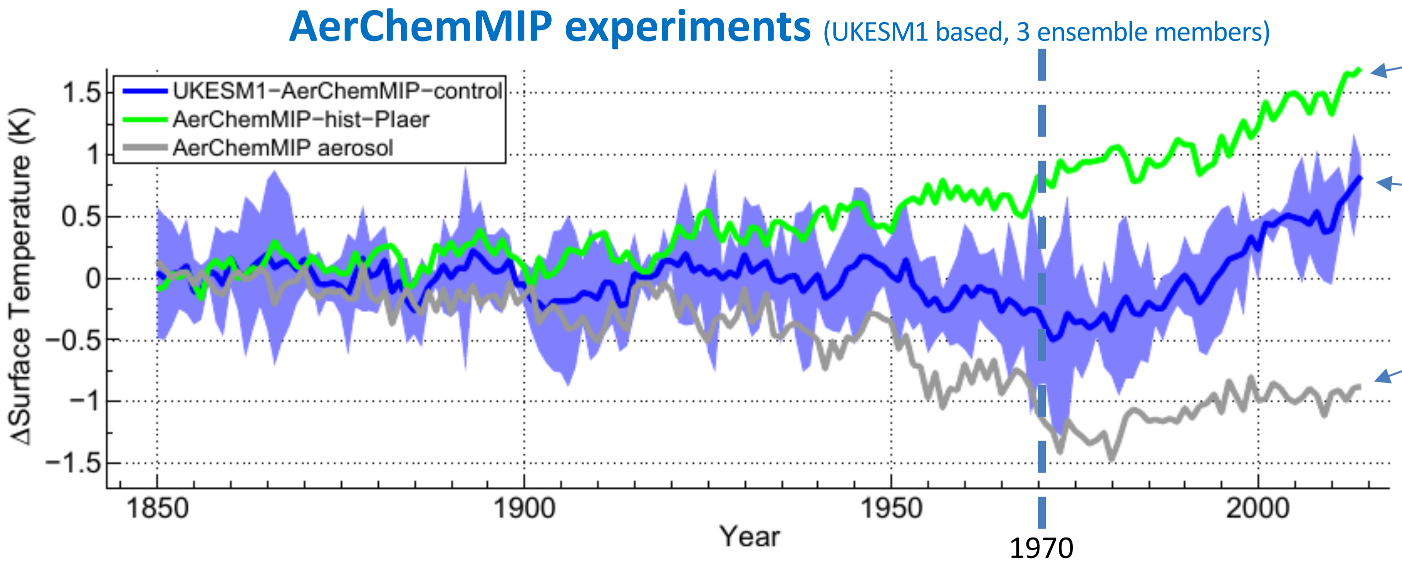
a.k.a. Twomey effect, 1st indirect effect (Constant cloud liquid water content).



Plus can aerosols can change cloud coverage and thickness

Cloud-aerosol "adjustment" effects

Aerosols vs Greenhouse gases in the UKESM1 climate model.



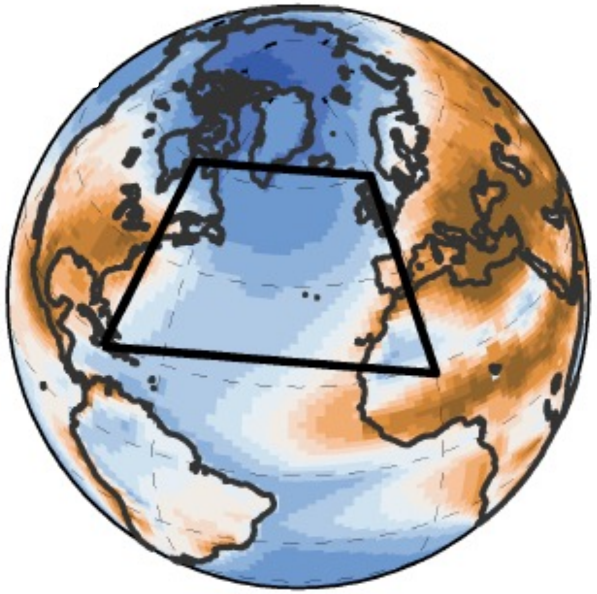
Greenhouse Gas-only proxy (AerChemMIP-piAer; all emissions except aerosols)

UKESM1 (aerosols+greenhouse), same 3 ensemble members as for AerChemMIP

Aerosol-only proxy (**UKESM1** minus **AerChemMIP-piAer**)

1850-1970: Aerosol cooling and greenhouse warming roughly cancel out.

1970-2013: Aerosol emissions have decreased to give a small warming.
Rapid greenhouse warming.



Grosvenor and Carslaw (ACP, 2023) Change from aerosol-driven to cloud-feedback-driven trend in short-wave radiative flux over the North Atlantic.

Big uncertainty in climate impact

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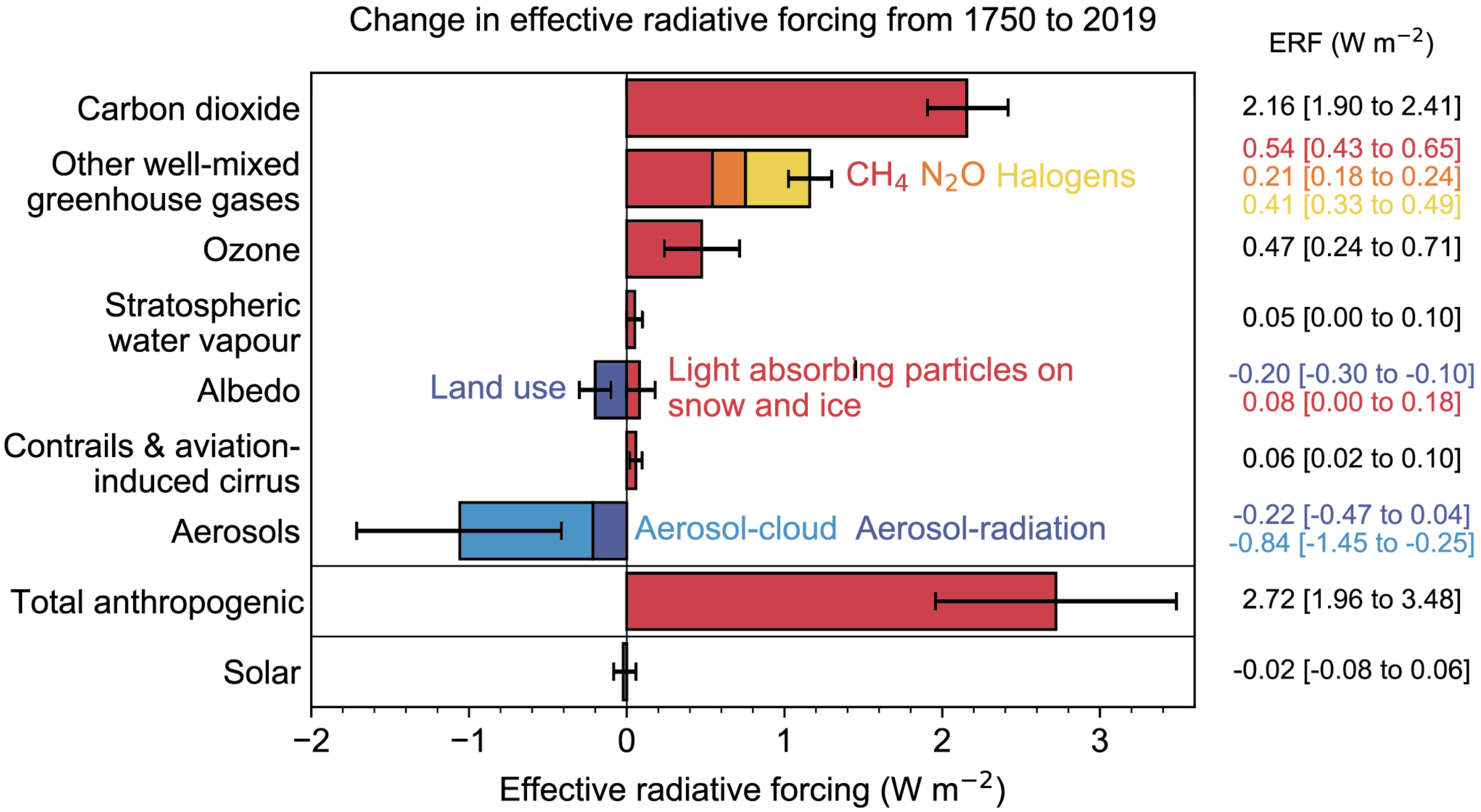

- Figure 7.6, WGI, AR6, IPCC (2021)

Why model aerosol?

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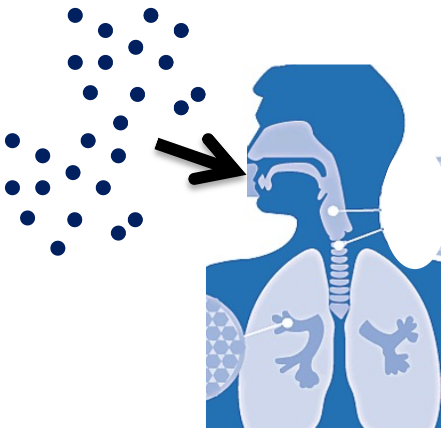

Building a Global Aerosol Model

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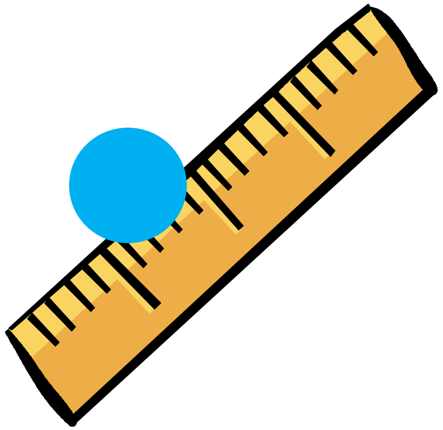
Model design needs to consider the degree of representation necessary to represent this complexity with **sufficient** accuracy.

Challenge 1: Large range in aerosol sizes, particles range from a few nanometres (10^{-9} m) to tens of micrometres (1 μm is 10^{-6} m).



Aerosol size

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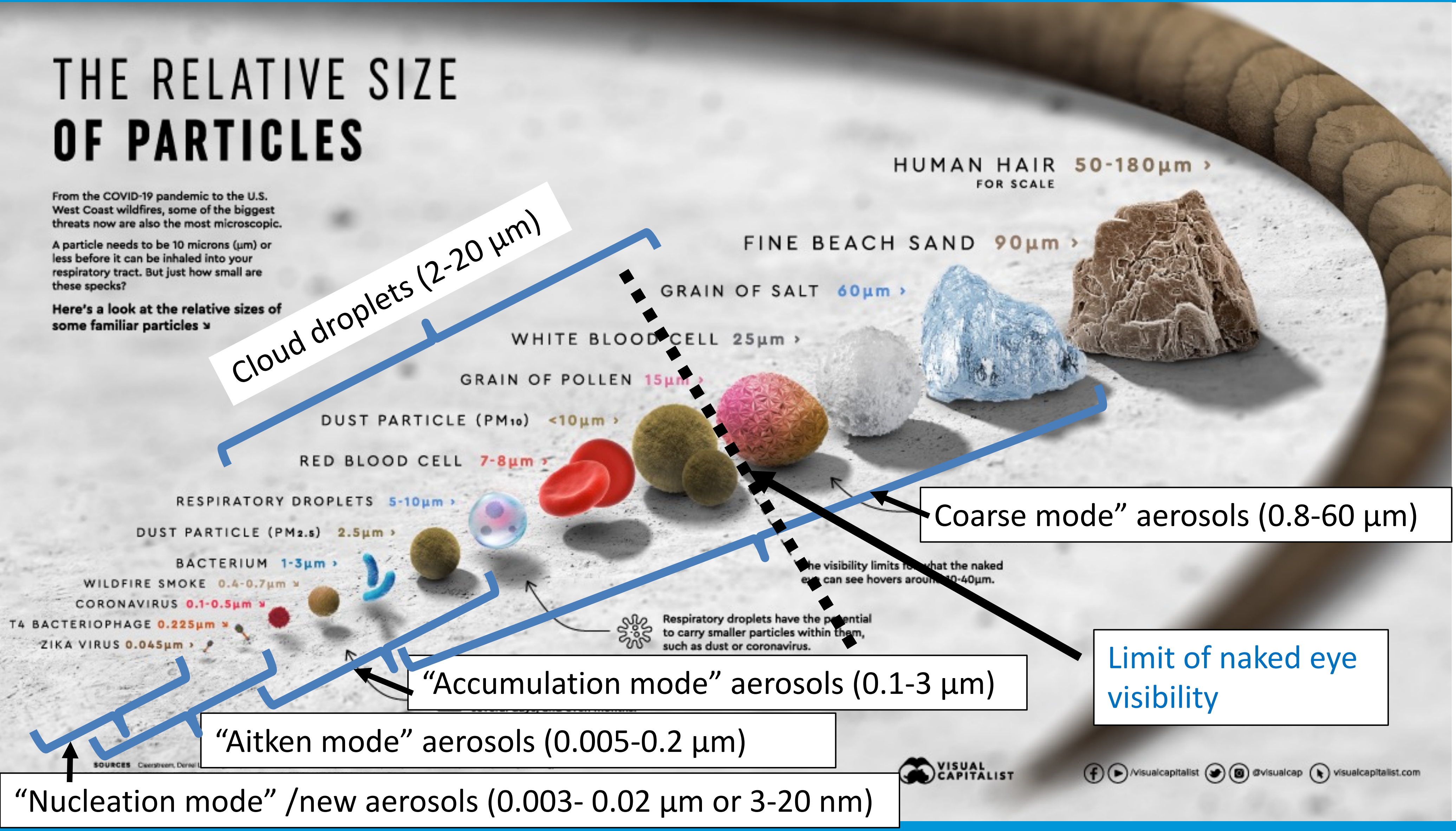

Visual Capitalist
https://www.visualcapitalist.com/visualizing-relative-size-of-particles/

Typical size distributions can vary regionally

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Measured size distributions at locations around the world:

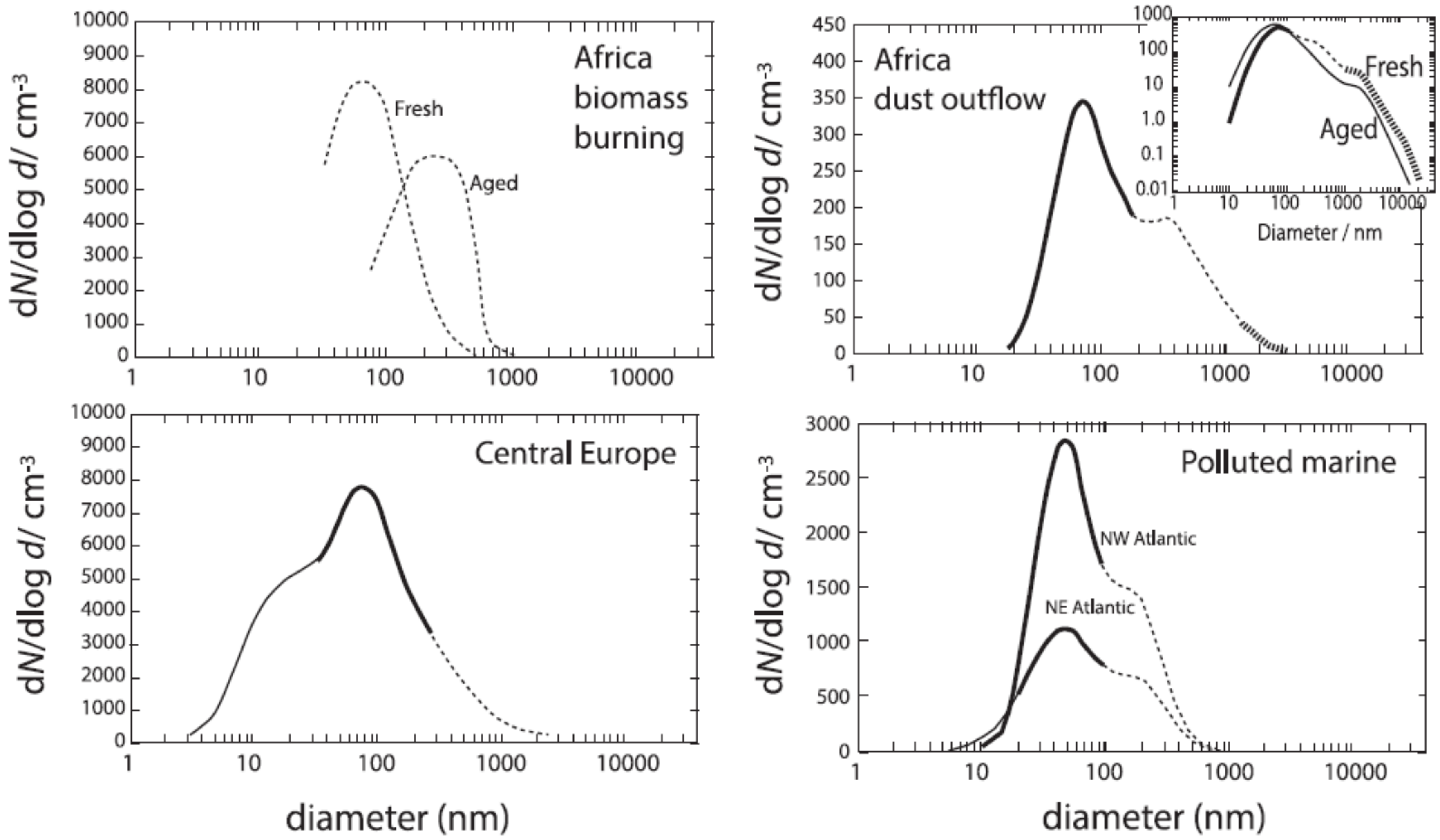
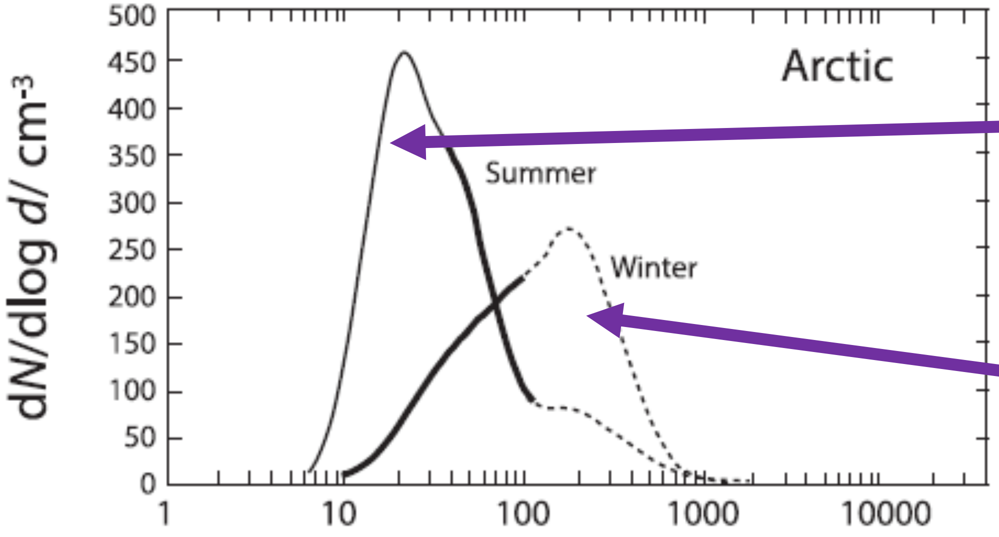


Fig 4.9 from Chapter 4 by Carslaw & Pringle, in "Aerosols and Climate", 2022, Elsevier

Area under the curves gives total number of particles.

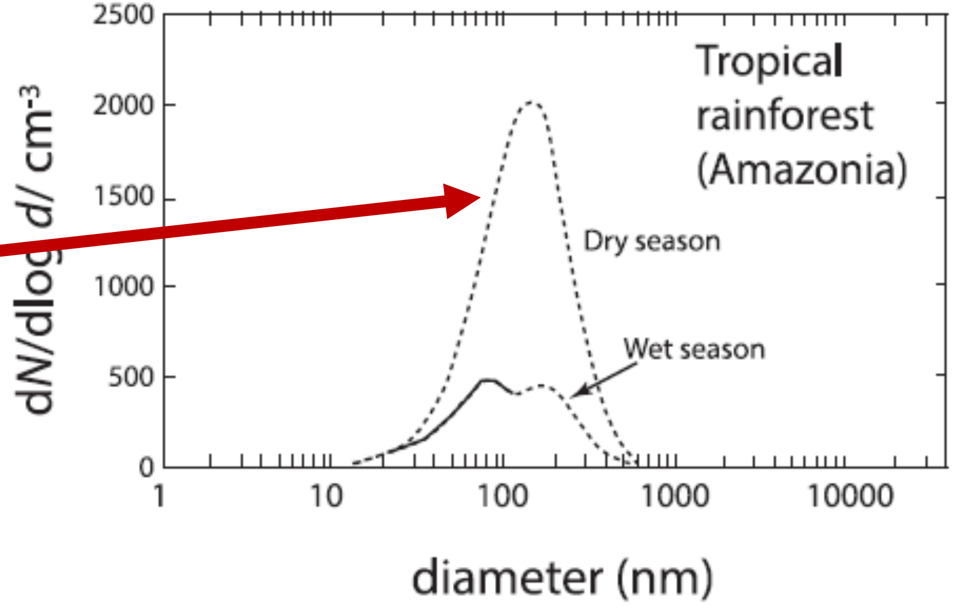
….but also seasonally in the same location



Local formation of new particles during summer

Winter / spring see effective transport from mid-latitudes

Dry season dominated by biomass burning emission (of black carbon and organic matter) into accumulation mode



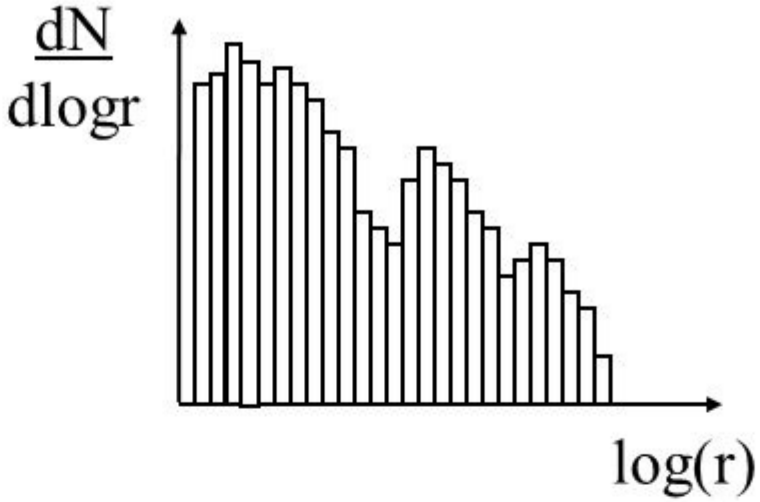
Area under the curves gives total number of particles.

Fig 4.9 from Chapter 4 by Carslaw & Pringle, in "Aerosols and Climate", 2022, Elsevier

Representing the aerosol size distribution in models

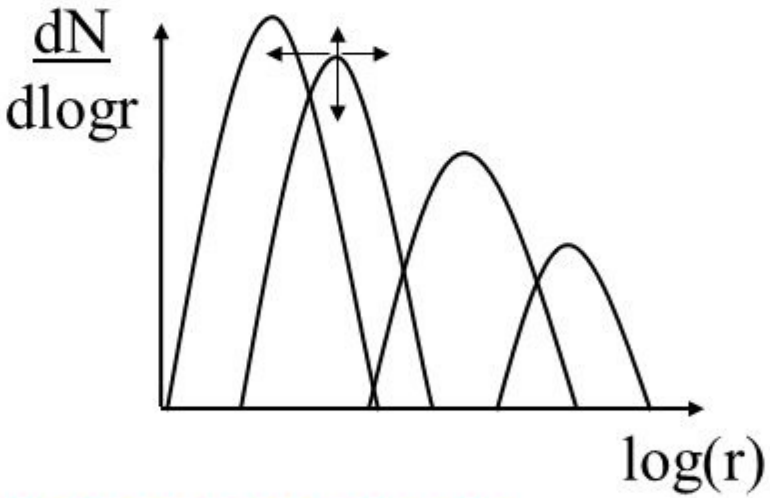
Sectional or Bin Schemes

- Divide the range of aerosol sizes into a number of **interacting** sections (or bins)
- Bins can have one or two prognostic variables (mass and number)
- No assumptions are made about the shape of the distribution
- Too computationally expensive for ESMs



Modal Schemes

- Represent the size distribution using a number of **interacting** log normal distributions.
- Each mode have two prognostic variables (mass and number)
- Cannot capture some potential detail in the distribution.
- Computationally cheaper
- Used in the UKCA (GLOMAP).



Schematic GLOMAP-Mode size distribution

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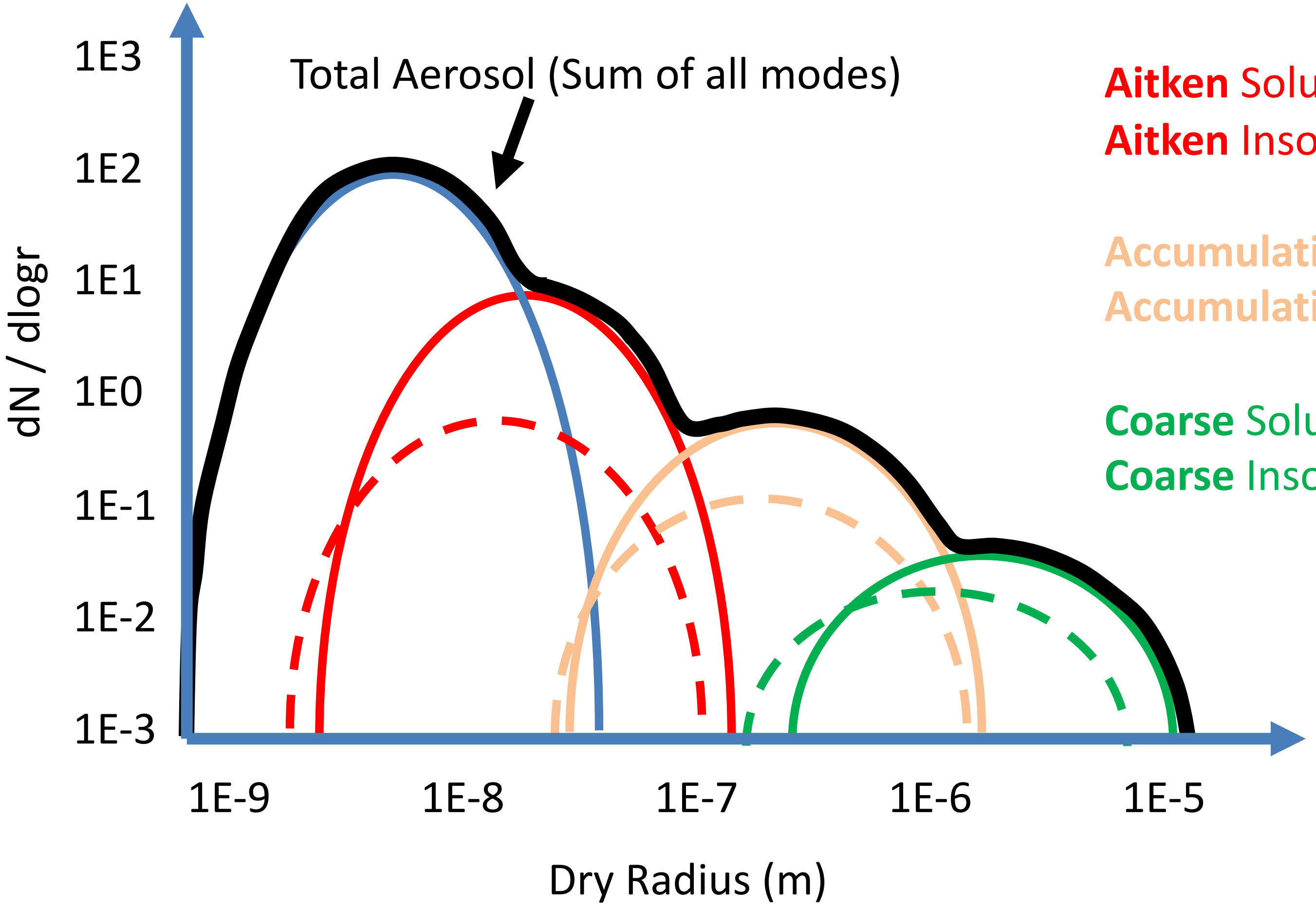
UKCA uses GLOMAP-Mode aerosol scheme.



Nucleation Soluble (solid line)

Aitken Soluble (solid line)
Aitken Insoluble (dashed line)

Accumulation Soluble (solid line)
Accumulation Insoluble (dashed line)

Coarse Soluble (solid line)
Coarse Insoluble (dashed line)

Each gridbox contains information on the mass, radius and composition of each of the (up to) 7 modes; can use this to calculate the simulated aerosol size distribution.

Building a Global Aerosol Model

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Model design needs to consider the degree of representation necessary to represent this complexity with **sufficient** accuracy.

Challenge 1: Large range in aerosol sizes, particles range from a few nanometres (10^{-9} m) to tens of micrometres (1 µm is 10^{-6} m).

Challenge 2: Particles vary in composition – different species mix together.

Particle composition varies regionally

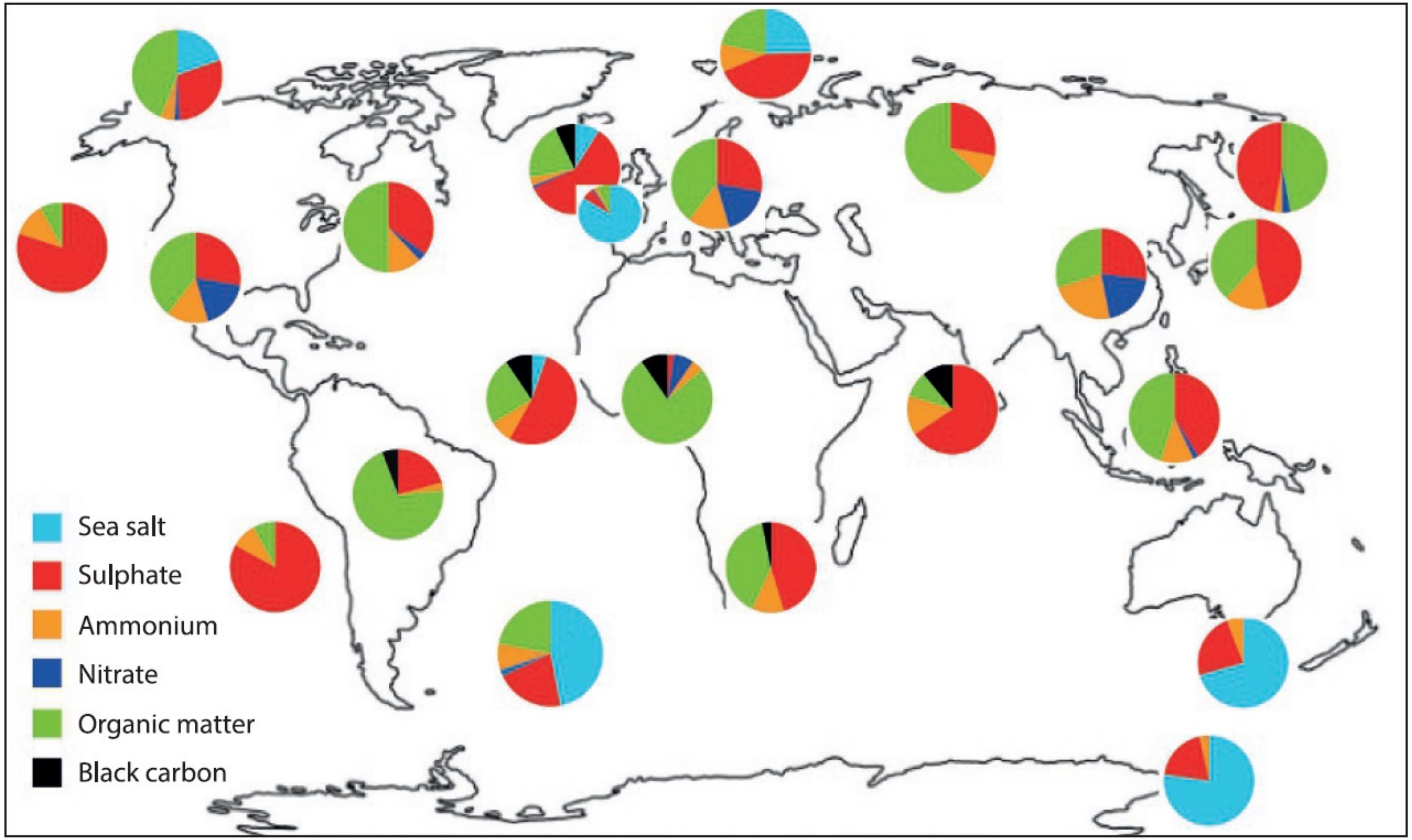
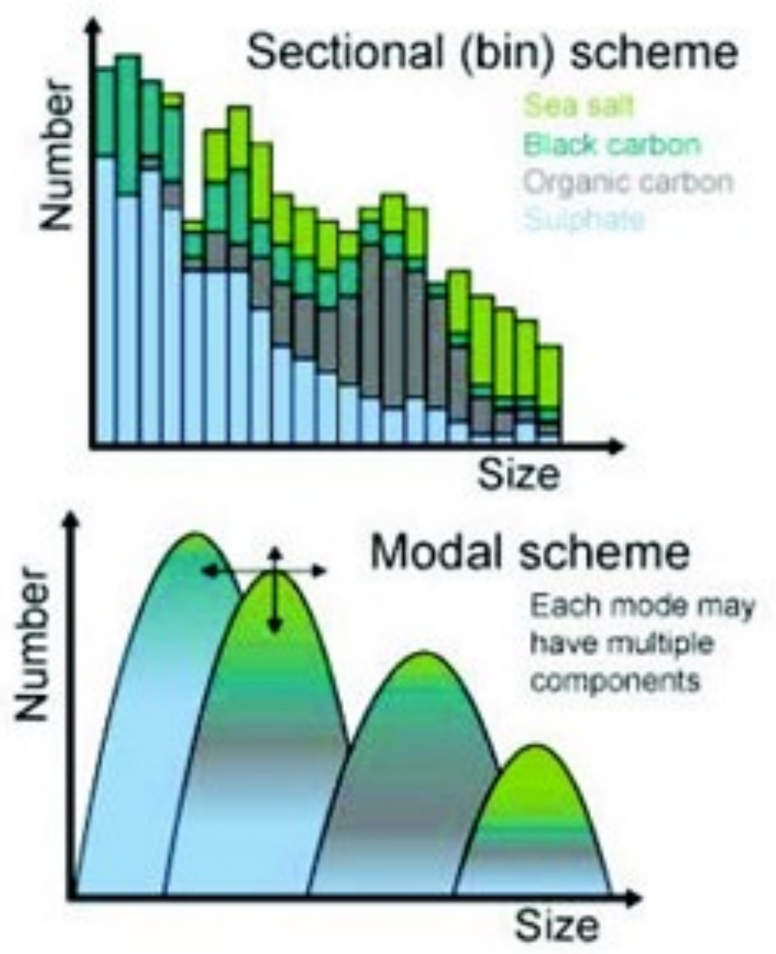


Fig 4.8 from Chapter 4 by Carslaw & Pringle, in "Aerosols and Climate", 2022, Elsevier

Modelling the aerosol size distribution



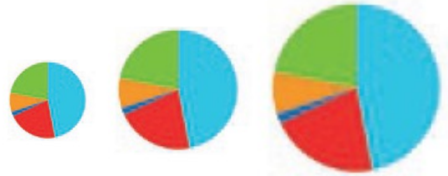
UKCA: Uses GLOMAP-Mode aerosol.

- Composition can vary between modes.
- All aerosol sizes within a mode are assumed to have the same composition (internally mixed)
- Each mode has only one number concentration, but different mass values for each species.
- The number fraction of each species within a mode is assumed to be proportional to the mass fraction.

Limitations:

- Assumes a degree of instantaneous mixing.
- Cannot account for varying composition with size within a mode.
- Mode width is fixed.

Within one mode:



Increasing size, but same composition

“Standard” 5-mode UKCA/UKESM Aerosol Scheme

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Mode name	Mean radius range nm	Species Permitted in Mode
Nucleation Soluble	< 5	SO_4, OM
Aitken Soluble	5 -50	SO_4, BC, OM, NH_4, NO_3
Accumulation Soluble	50 – 250	SO_4, BC, OM, SS, DU, NH_4, NO_3, NN
Coarse Soluble	> 250	SO_4, BC, OM, SS, DU, NH_4, NO_3, NN
Aitken Insoluble	5 – 50	BC, OM
Accumulation Insoluble	50 – 500	DU
Coarse Insoluble	> 500	DU

Standard setup of UKCA uses 5 modes and treats 4 chemical species:

1. Sulphate aerosol (SO_4 or SU)
2. Organic matter (OM)
3. Black carbon (BC)
4. Sea salt (SS)
5. Dust (DU; treated separately in UKESM, although the next version may use UKCA/GLOMAP modal dust)

6. Ammonium (NH4)
7. Nitrate (NO3)
8. Sodium nitrate (NN)

} Nitrate scheme should be used in the next UKESM climate model

Model design needs to consider the degree of representation necessary to represent this complexity with **sufficient** accuracy.

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Challenge 2: Particles vary in composition – different species mix together.

Challenge 3: Microphysical processes change the aerosol size distribution.

Processes controlling and shaping the size distribution

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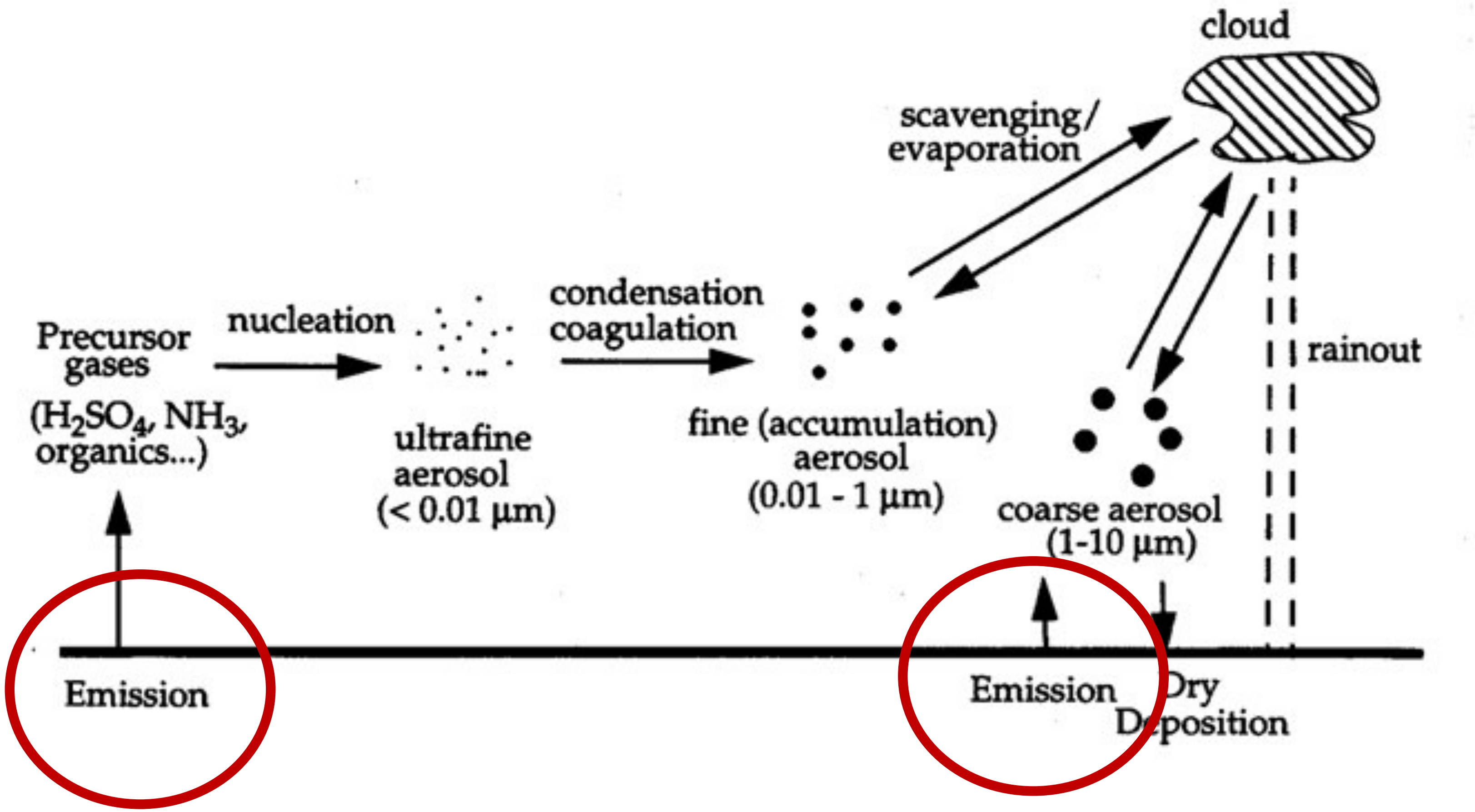

Jacob, Introduction to Atmospheric Chemistry, 2000.

- e.g., black carbon aerosols from wildfires
- organic carbon or sea-salt from sea-spray
- dust from deserts

Primary Emission

Off-line emissions may be read in from ancillary files, e.g.:

- Gas phase sulphur species: DMS, SO_2 (natural and anthropogenic; some natural are interactive in UKESM).
- A fraction of the SO_2 is assumed to be particulate when emitted (Aitken / accumulation size).
- Gas phase biogenic volatile organic compounds (BVOCs; interactive in UKESM).
- Black and Organic Carbon: biofuel, fossil fuel and biomass burning into Aitken mode.
    - Sensitivity of results to assumed size.
- How offline emissions inventories are developed:

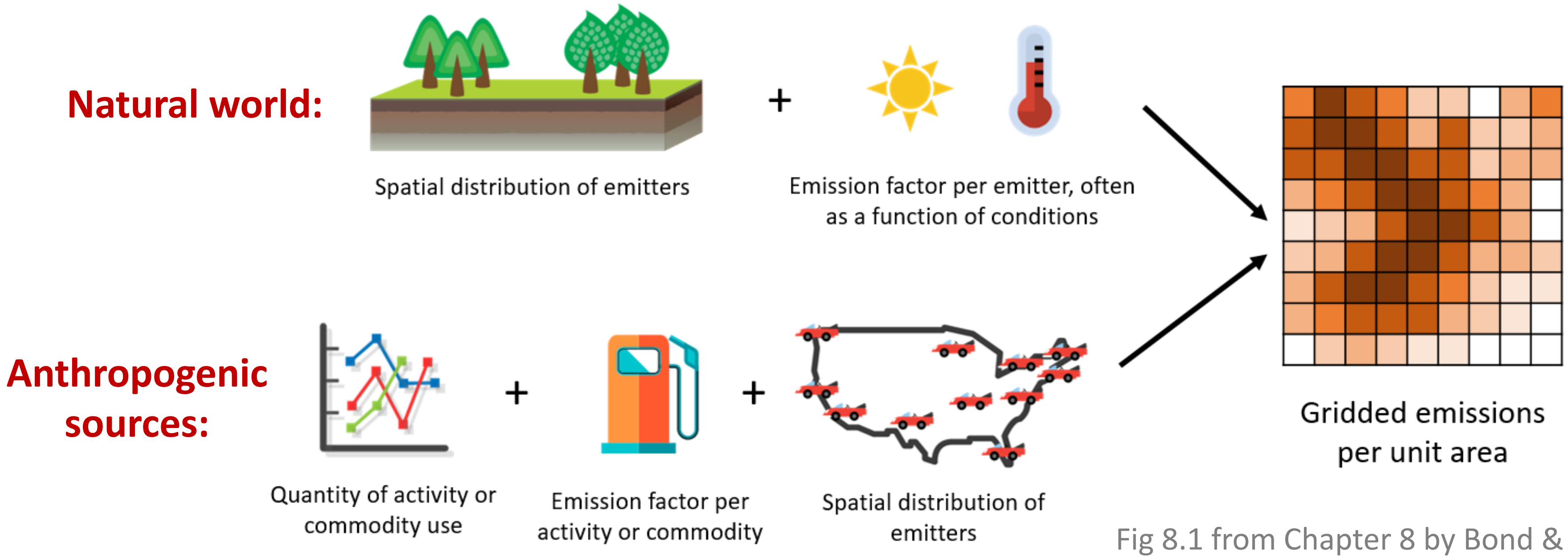

Fig 8.1 from Chapter 8 by Bond & Scott, in “Aerosols and Climate”, 2022, Elsevier

Primary Emission

Online/interactive emissions, calculated in the model, e.g.:

Sea spray:

- Calculated as a function of wind speed.
- Emitted into the accumulation and coarse soluble modes

Mineral Dust:

- Calculated depending on wind speed and soil moisture, land type (Woodward).
- Often dust is carried in 6 bins, that do not interact with the other species. Can also be treated in UKCA-Mode.

BVOCs:

- Is an option to calculation emissions based on temperature, etc.

Processes controlling and shaping the size distribution

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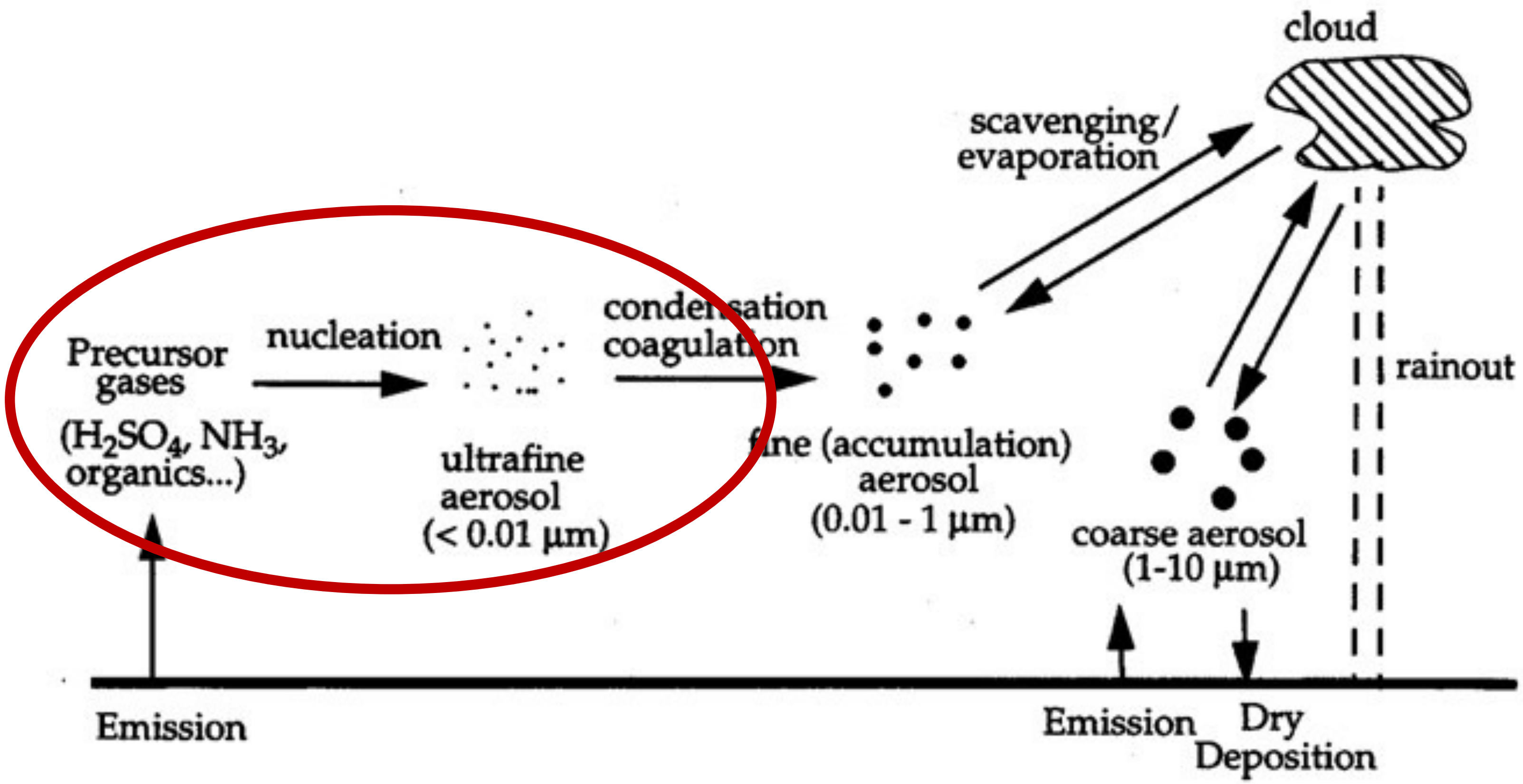
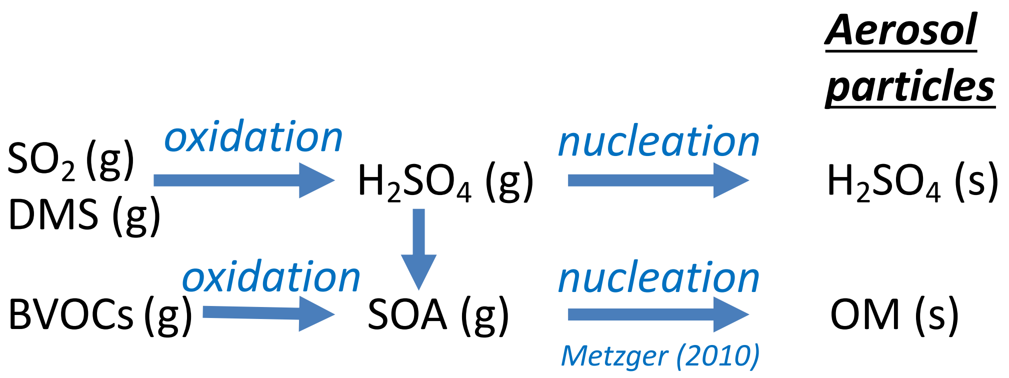


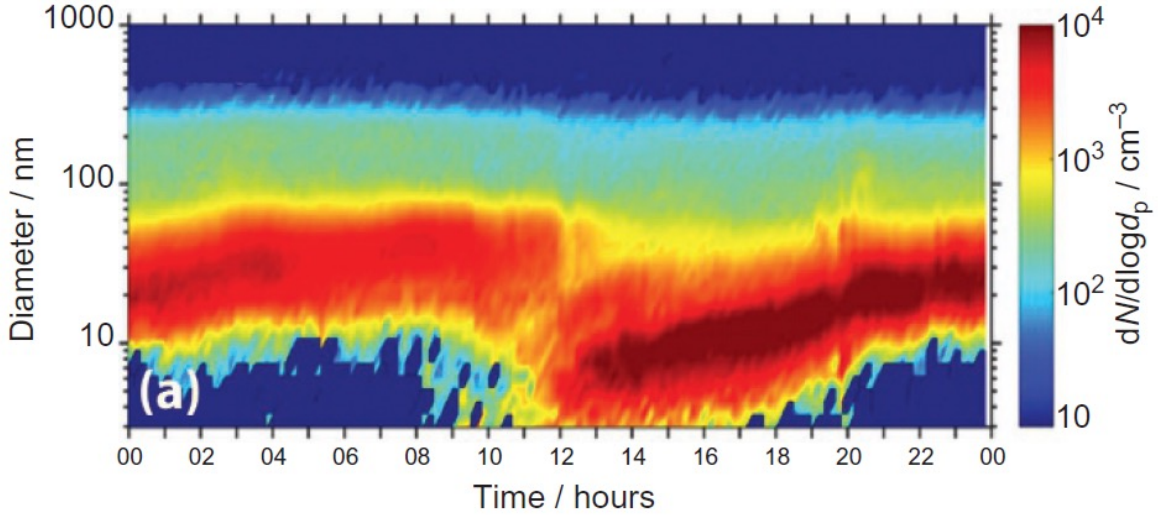
Jacob, Introduction to Atmospheric Chemistry, 2000.

Nucleation (new particle formation)

- **Upper Tropospheric Nucleation**
- In the cold, clean, air of the upper troposphere semi-volatile gases can nucleate new aerosol particulates.
- Vehkamaki et al (2002), Kulmala et al (1998)

- **Boundary Layer Nucleation**
- Thought to involve additional vapours, e.g. organics (from BVOC oxidation) and/or ammonia.
- Metzger (2010), Riccobono (2014), Kirkby (2016)

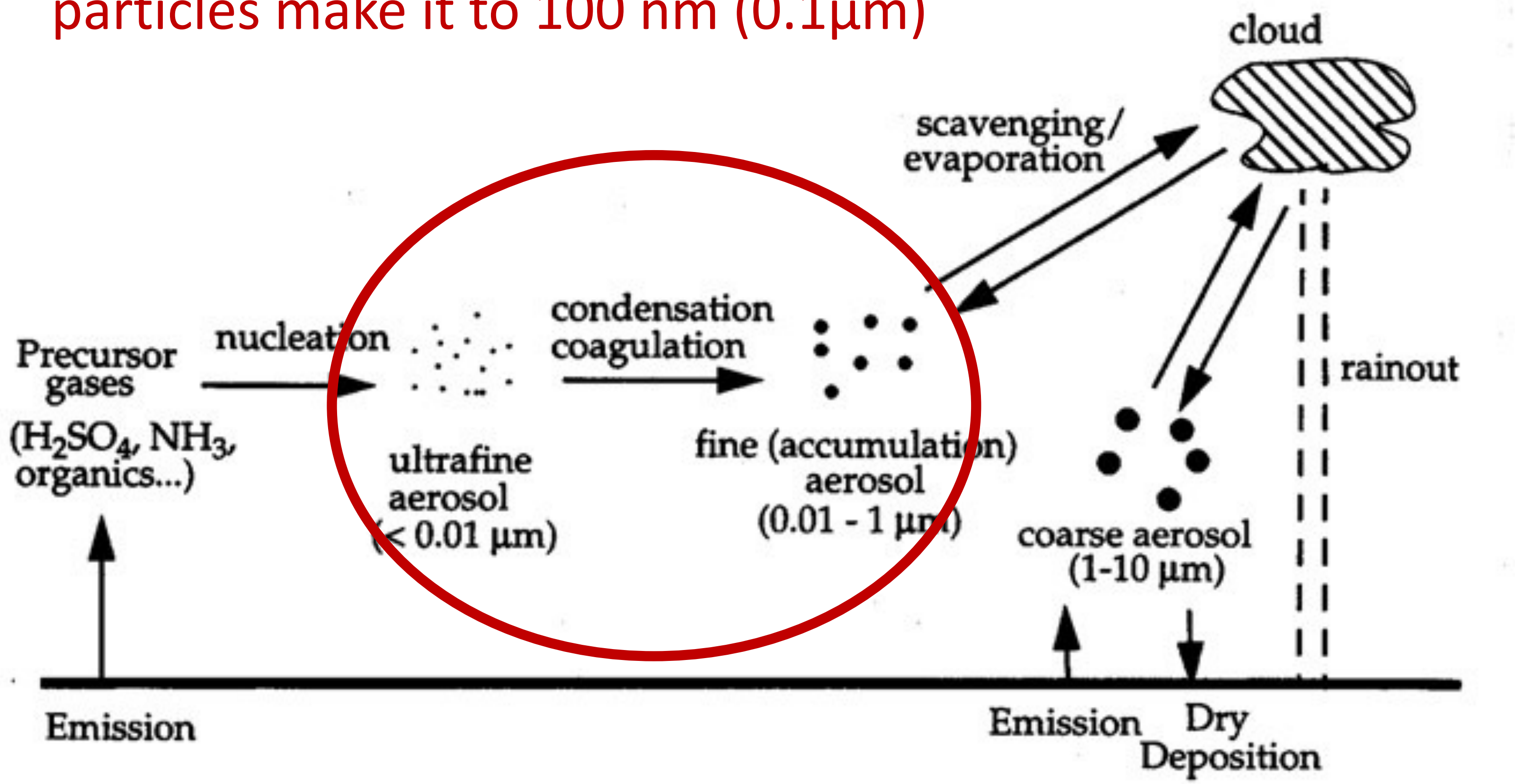




Kerminen 2018

Processes controlling and shaping the size distribution

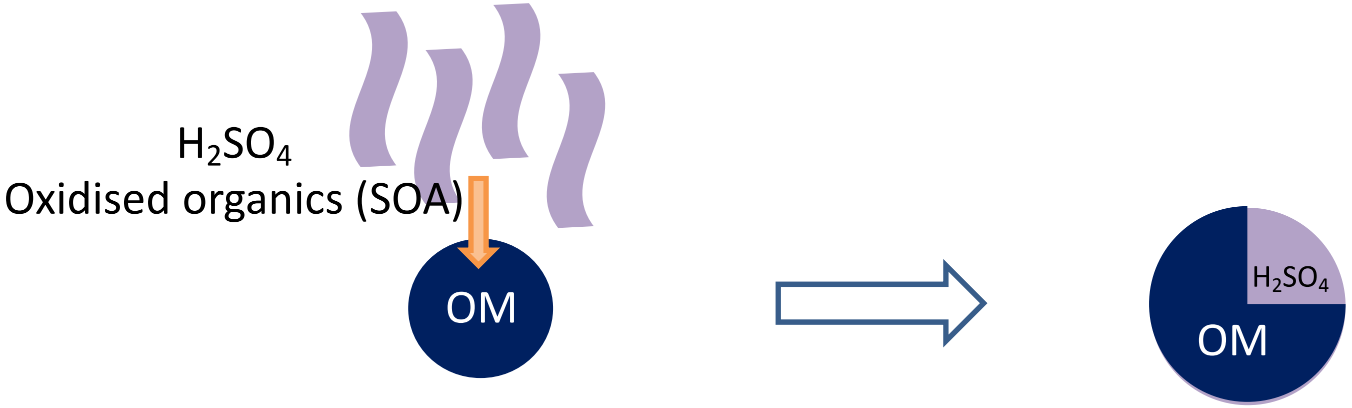
Only ~ 10% of newly formed particles make it to 100 nm (0.1µm)



Jacob, Introduction to Atmospheric Chemistry, 2000.

Growth: Condensation

- **Condensation**
- Low-volatility gas phase compounds preferentially condense onto the surface of pre-existing aerosol particles.
- Doesn't increase particle number, but does **increase particle size**.
- As modes grow some of the particles may get passed upwards to the larger size modes.

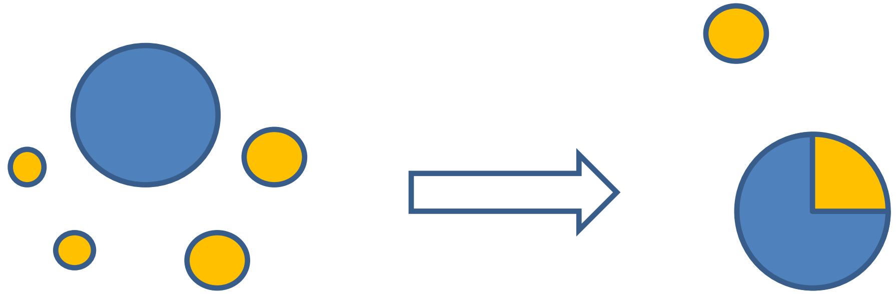


Condensational growth changes the aerosol composition.

Can move aerosol from the insoluble to the soluble distributions.

Growth: Coagulation

- **Coagulation:**
- Reduces the number of aerosol; forms **fewer, larger particles**.
- Mainly due to Brownian motion (collisions with air molecules) of small aerosol particles.
- Particularly important when have large numbers of small particles (e.g, plumes).
- Can have coagulation both **within** a mode and **between** modes.



- Coagulation can also change the aerosol composition.
- Can move aerosol from the insoluble to the soluble distribution.

Processes controlling and shaping the size distribution

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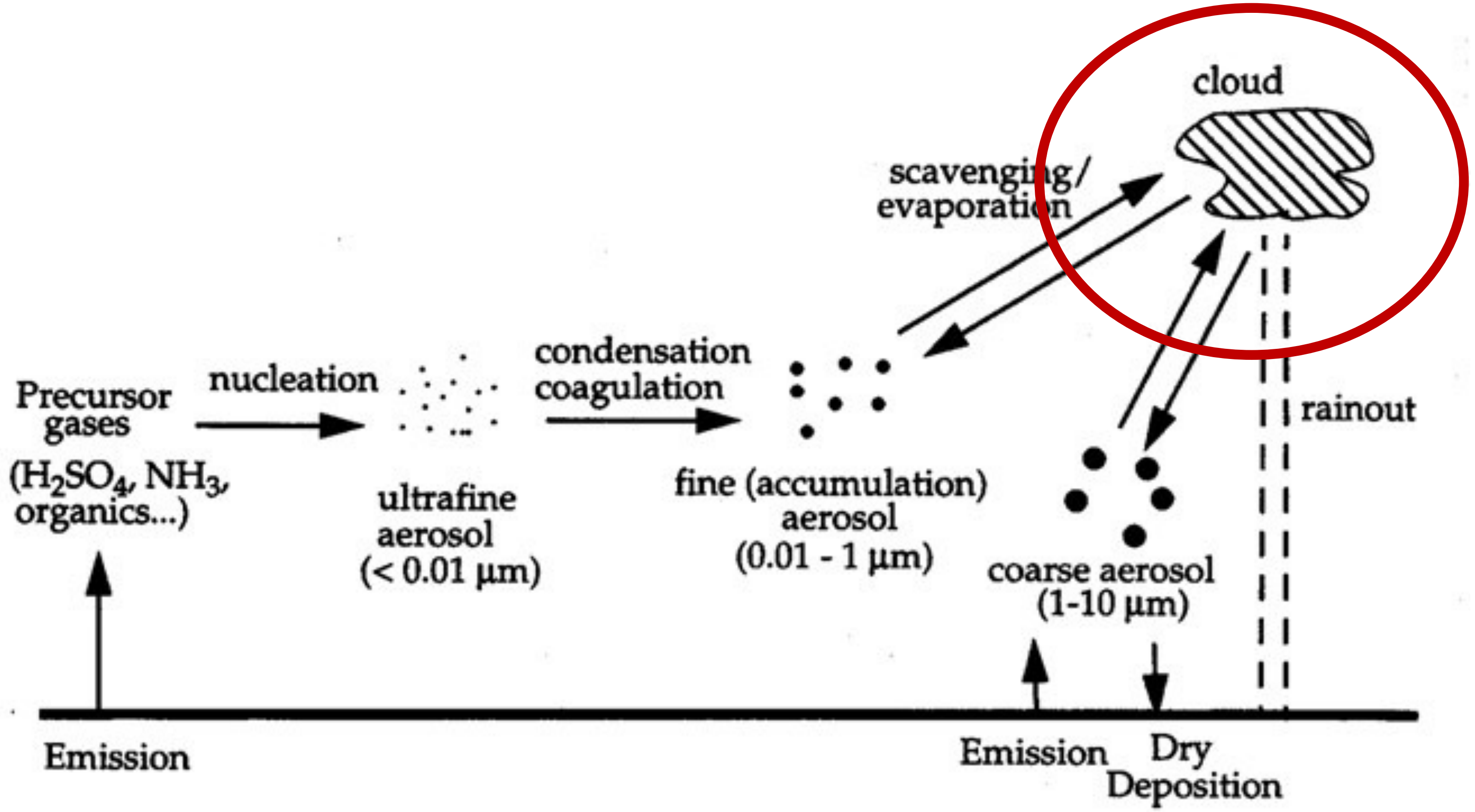
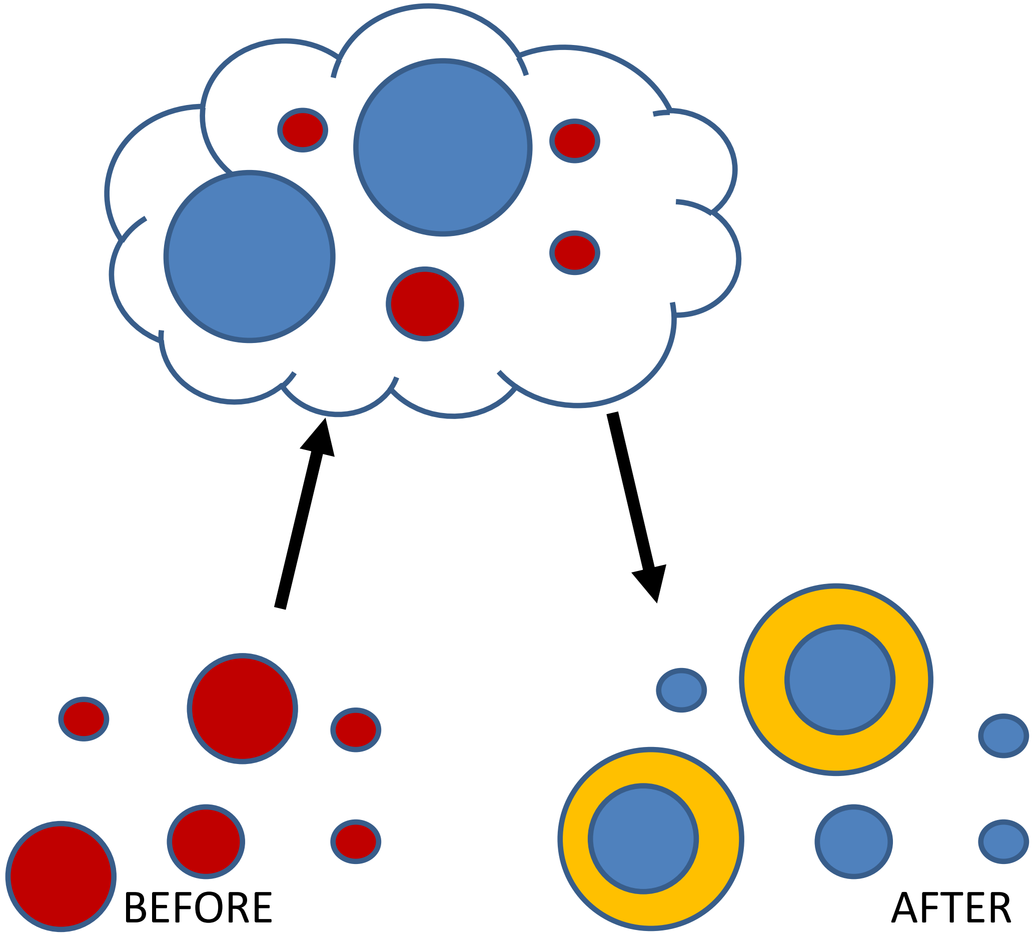


Jacob, Introduction to Atmospheric Chemistry, 2000.

In-cloud processing

Only large hydrophilic aerosol can activate (form cloud droplets).



- Aerosol particles can grow in size as a result of chemical processing in non-precipitating clouds.
- Soluble species (e.g. SO_2) can dissolve in liquid cloud water, undergo chemical reactions (e.g., to H_2SO_4), which increases the mass of the aerosol species.
- When the cloud evaporates the aerosol will be released into the particulate phase.
- Can see the effect of this process in the bimodal size distribution in marine areas.

Deposition

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NAME	LOCATION	DEPENDS ON	NOTES
Dry deposition	Model layer closest to Earth's surface.	Particle size Surface type (e.g. forest / ocean).	
Sedimentation / gravitational settling	*All model levels*	*Particle size (gravity)*	*Only removes aerosol from the lowest altitude level.*
In cloud / nucleation scavenging	Within a raining cloud	Particle size Particle composition	
Below cloud / impaction scavenging	In model levels below a raining cloud	Particle size (smallest and largest most affected)	

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Challenge 2: Particles vary in composition – different species mix together.

Challenge 3: Microphysical processes change the aerosol size distribution.

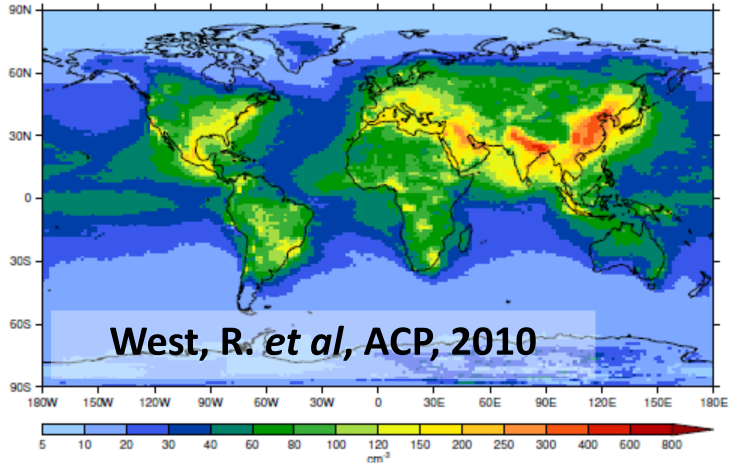
Challenge 4: Link it to the other parts of the model!

Edited Call Sequence

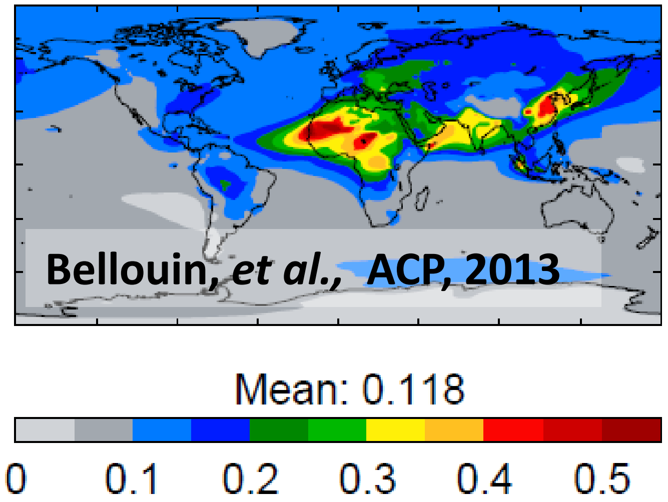
- UKCA_EMISSION_CTL – Emit gases
- UKCA_CHEMISTY_CTL – Chemistry routines
- UKCA_AERO_CTL – Aerosol routines
- UKCA_AERO_STEP
- UKCA_CALCDRYDIAM & UKCA_CALC_DRYDIAM
- UKCA_PRIM_SU (and CAR, SS and DU)
- UKCA_IMPC_SCAV & UKCA_RAINOUT
- UKCA_WETOX
- UKCA_CLOUDPROC
- UKAC_DDEPAER_INCL_SEDI
- UKCA_REMODE
- UKCA_CALC_COAG_KERNAL
- UKCA_CONDEN
- UKCA_CALCNUCRATE
- UKCA_COAGWITHNUCL
- UKCA_AGEING
- UKCA_CALCDRYDIAM & UKCA_VOLUME_MODE
- UKCA_REMODE
- UKCA_ACTIVATE – Cloud droplet number

Links to other parts of the model

Cloud droplet number



GLOMAP-mode AOD



UKCA_ACTIVATE (R. West, P. Stier)

Calculates the number of cloud droplets formed at cloud base.

Based on aerosol number, size, composition and updraft speed.

This number is replicated vertically throughout cloud layers.

(Because UKCA does not have an advected tracer for droplet number – it is re-calculated each timestep).

UKCA_RADAER (N. Bellouin)

Calculates the aerosol optical properties (e.g. scattering and absorption of radiative fluxes)

Conclusions

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1. UKCA-Mode is a global aerosol model in which the aerosol size distribution is represented using (normally 5) interacting lognormal modes.

2. The standard model treats 4 species: sulphate, black carbon, organic carbon and sea spray. Dust is also possible. With the nitrate scheme, also: ammonium (NH4), nitrate (NO3), sodium nitrate (NN).

3. The model setup can be altered to use more / fewer modes and species.

4. Treats the main microphysical processes that control the size distribution – emission, nucleation, coagulation, condensation, in-cloud processing and dry and wet deposition.

5. Is coupled to (some) other parts of the model.

6. UKCA-Mode is a working model that compares well with observations.

Useful references

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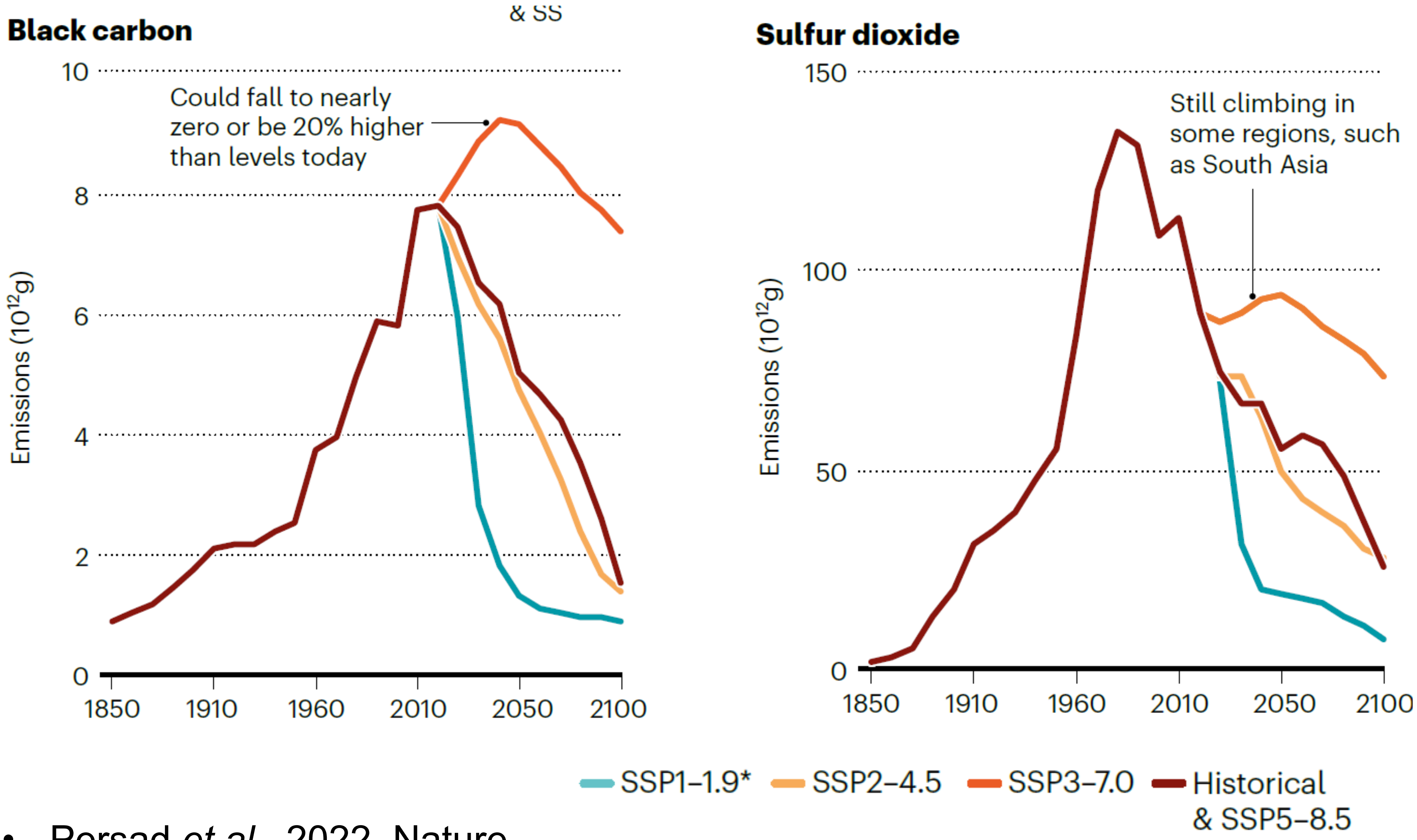
1. GLOMAP-Mode model description paper (Mann et al., 2010): https://gmd.copernicus.org/articles/3/519/2010/

2. Description and evaluation of aerosol in UKESM (Mulcahy et al., 2020): https://gmd.copernicus.org/articles/13/6383/2020/

3. “Aerosols and Climate” textbook (Carslaw, 2022, Elsevier): https://www.sciencedirect.com/book/9780128197660/aerosols-and-climate

4. UM documentation (doc number 84 for UKCA) :- https://code.metoffice.gov.uk/doc/um/vn13.4/umdp.html

Future emissions very uncertain



- Persad *et al*., 2022, Nature.