Introduction to aerosol modelling with UKCA

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Based (with thanks!) on slides from **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

The Global Aerosol Distribution

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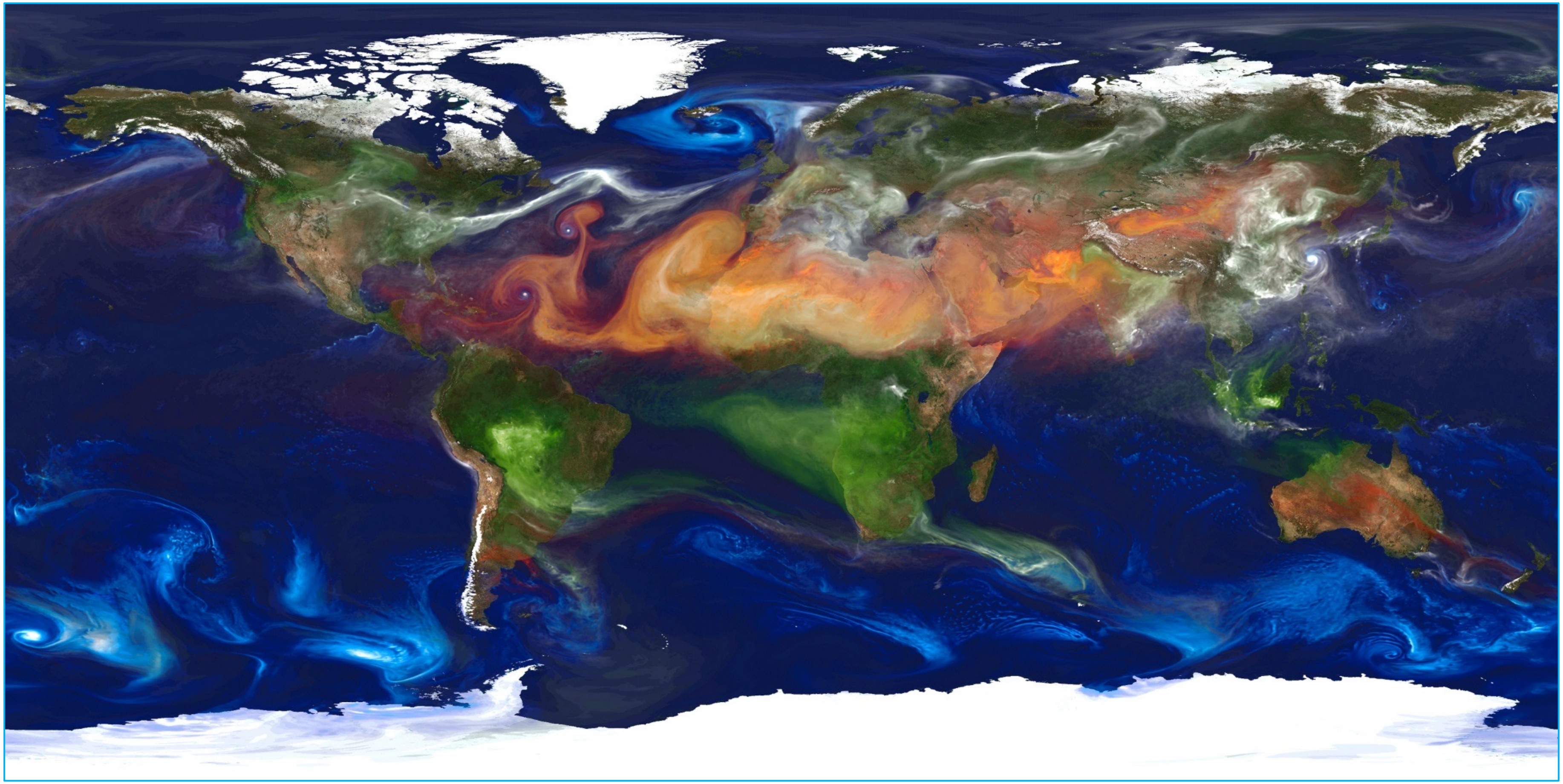


NASA: A portrait of global aerosol.
Composite of satellite and model data.

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

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

Why model aerosol?

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

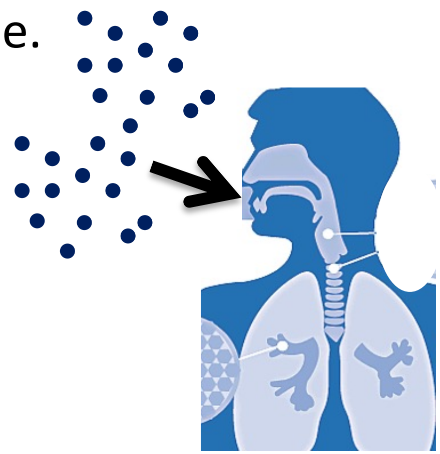
- Aerosol provide a surface area for chemical reactions.

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 cancer and heart disease.



Big uncertainty in climate impact

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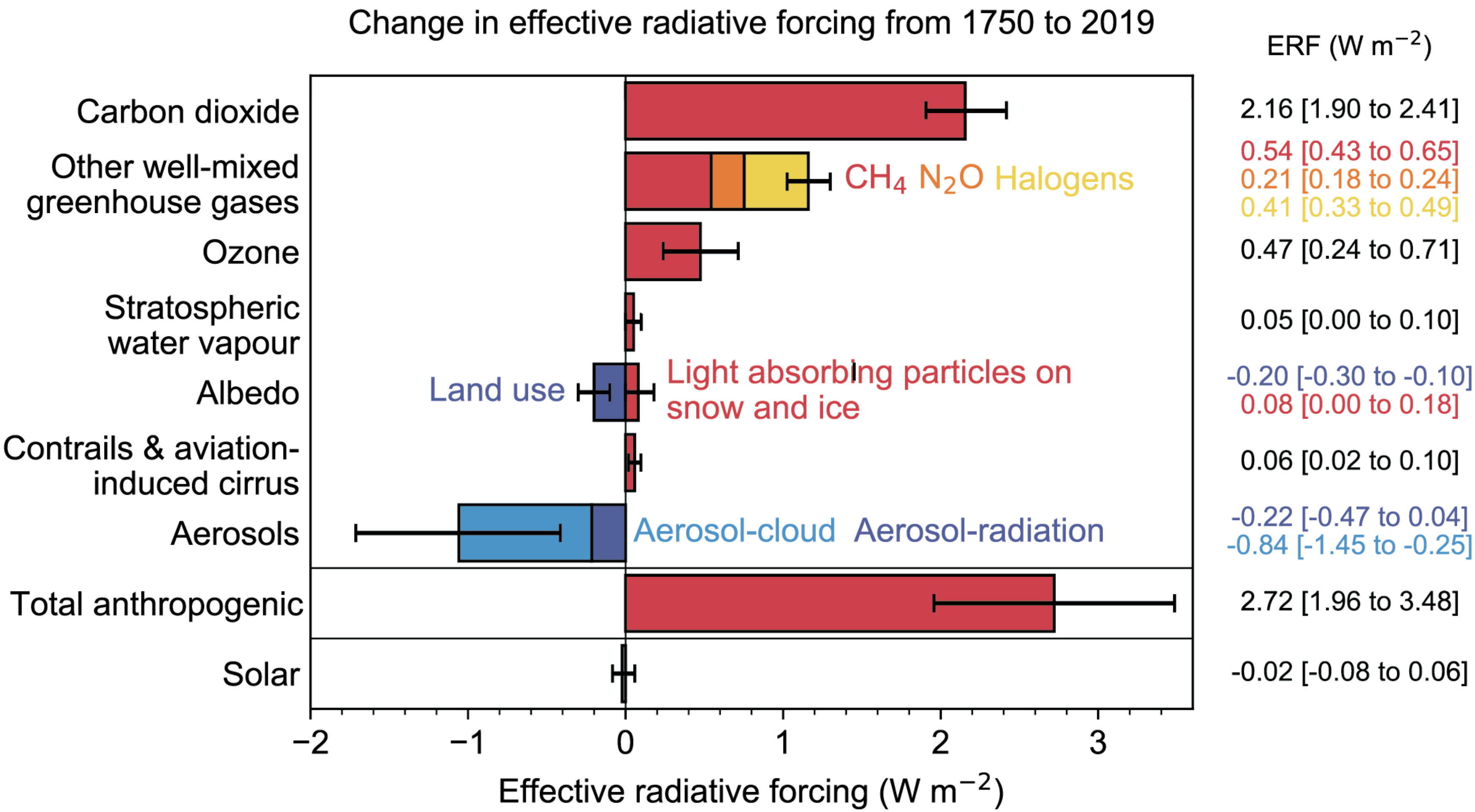

Figure 7.6, WGI, AR6, IPCC (2021)

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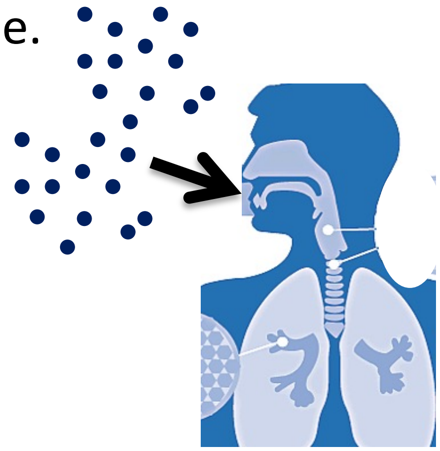

Model design needs to consider the degree of representation necessary to represent this complexity with **sufficient** accuracy.

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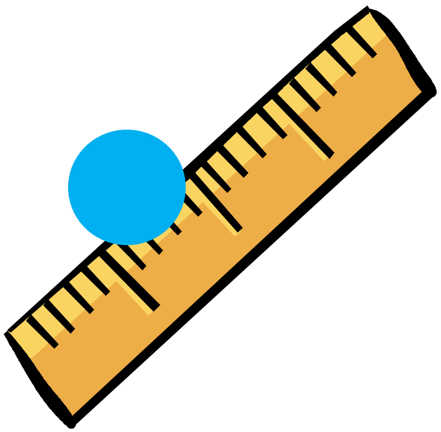

Typical size distributions can vary regionally

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Measured size distributions at locations around the world:

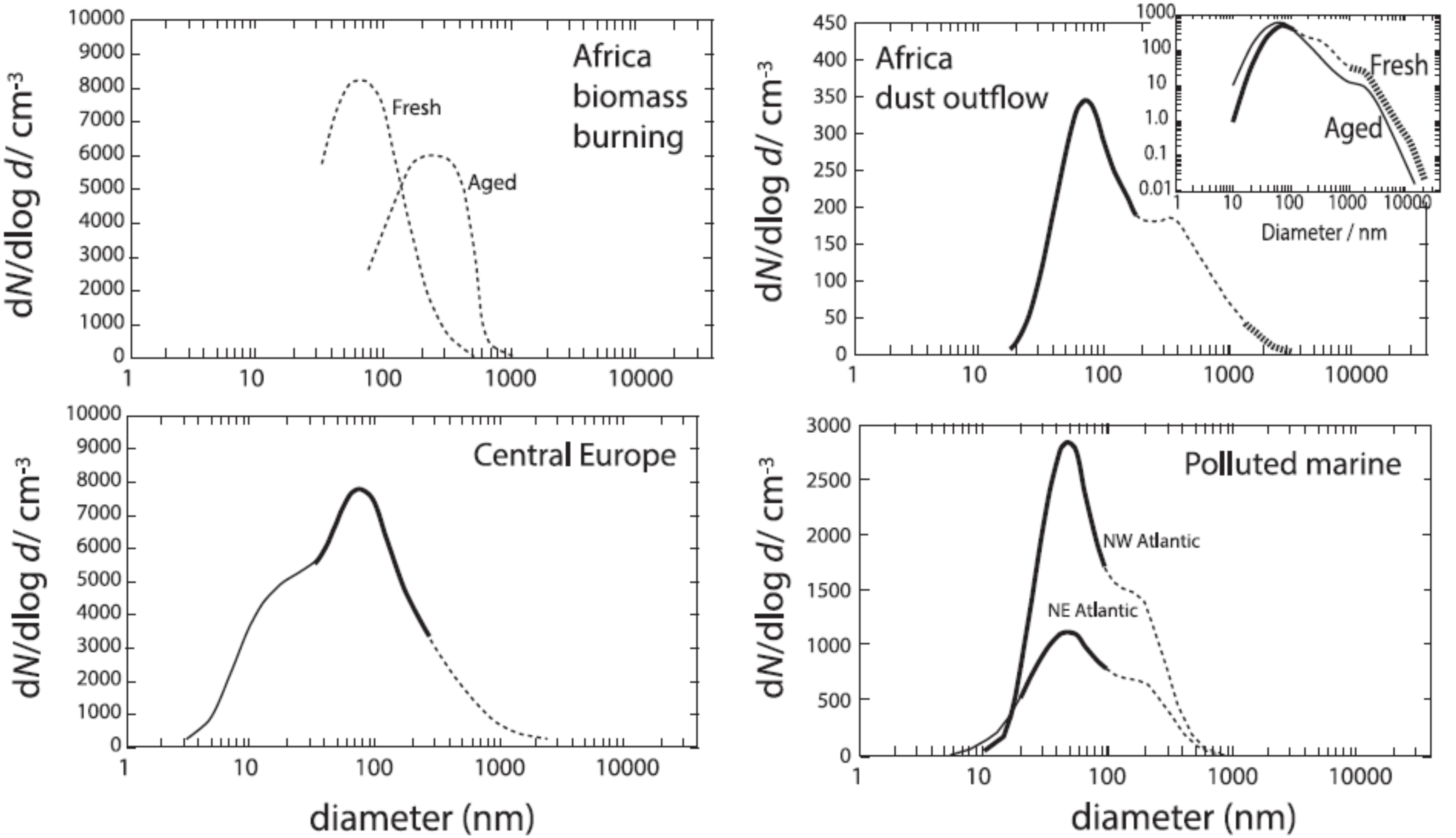

Fig 4.9 from Chapter 4 by Carslaw & Pringle, in “Aerosols and Climate”, 2022, Elsevier

….but also seasonally in the same location

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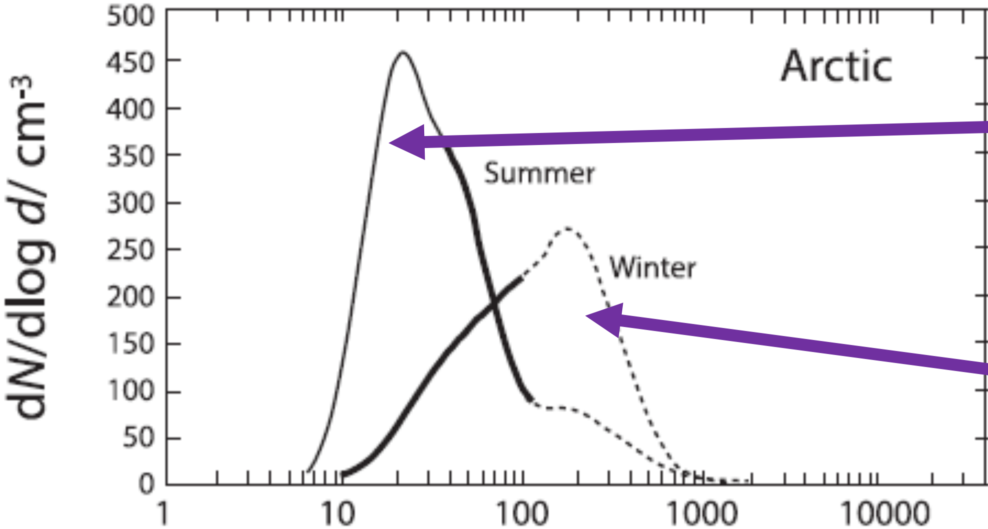


Local formation of new particles during summer

Winter / spring see effective transport from mid-latitudes

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

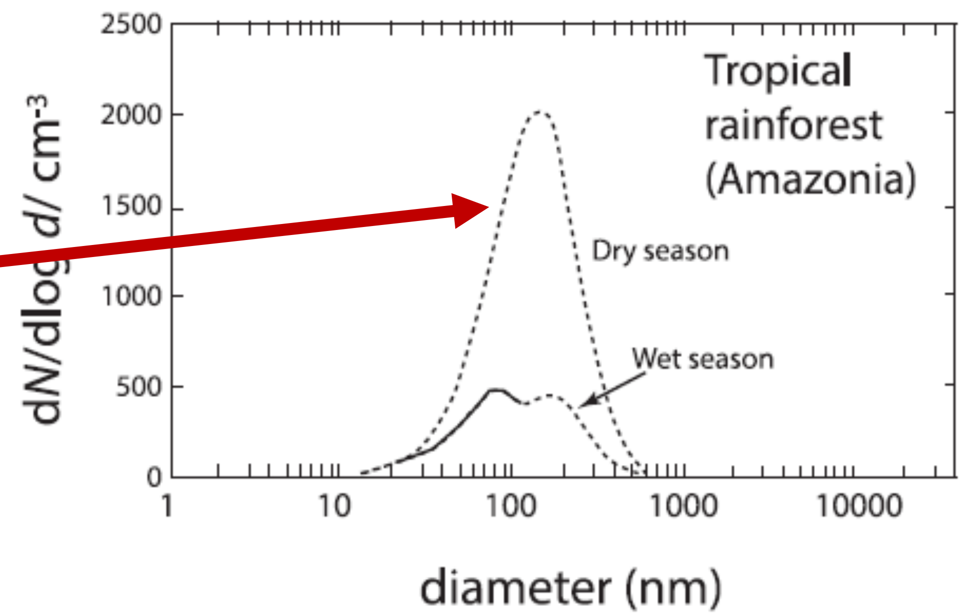
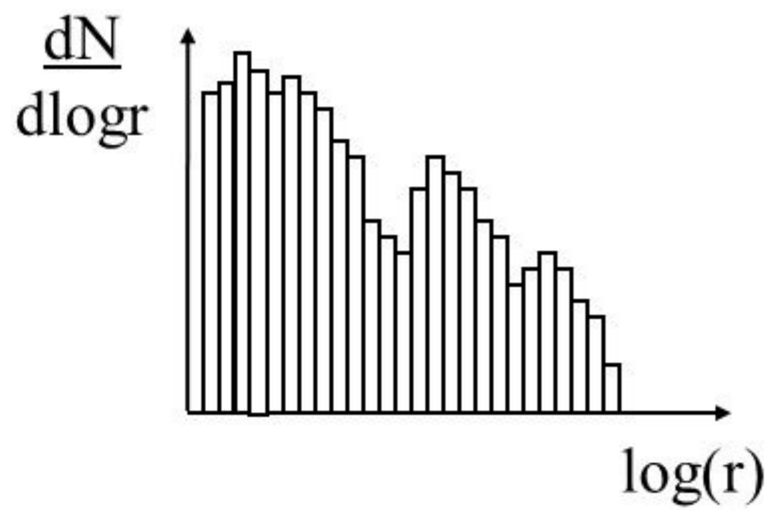


Fig 4.9 from Chapter 4 by Carslaw & Pringle, in "Aerosols and Climate", 2022, Elsevier

Representing the aerosol size distribution in models

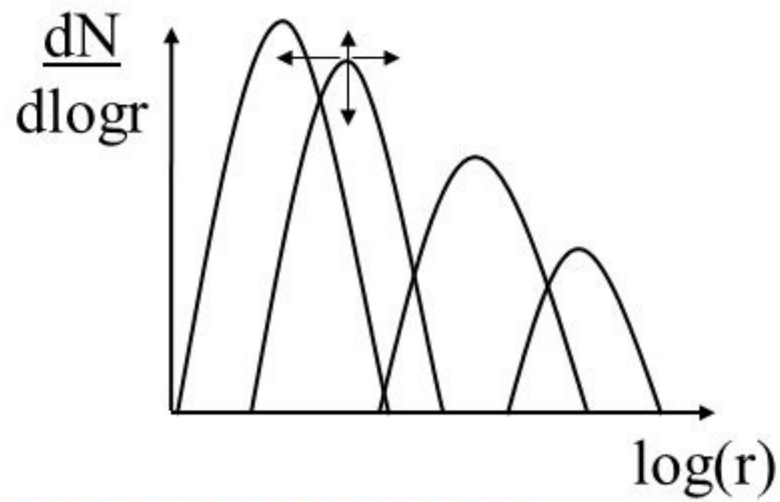
Sectional or Bin Schemes

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



Modal Schemes

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



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.

Particle composition varies regionally

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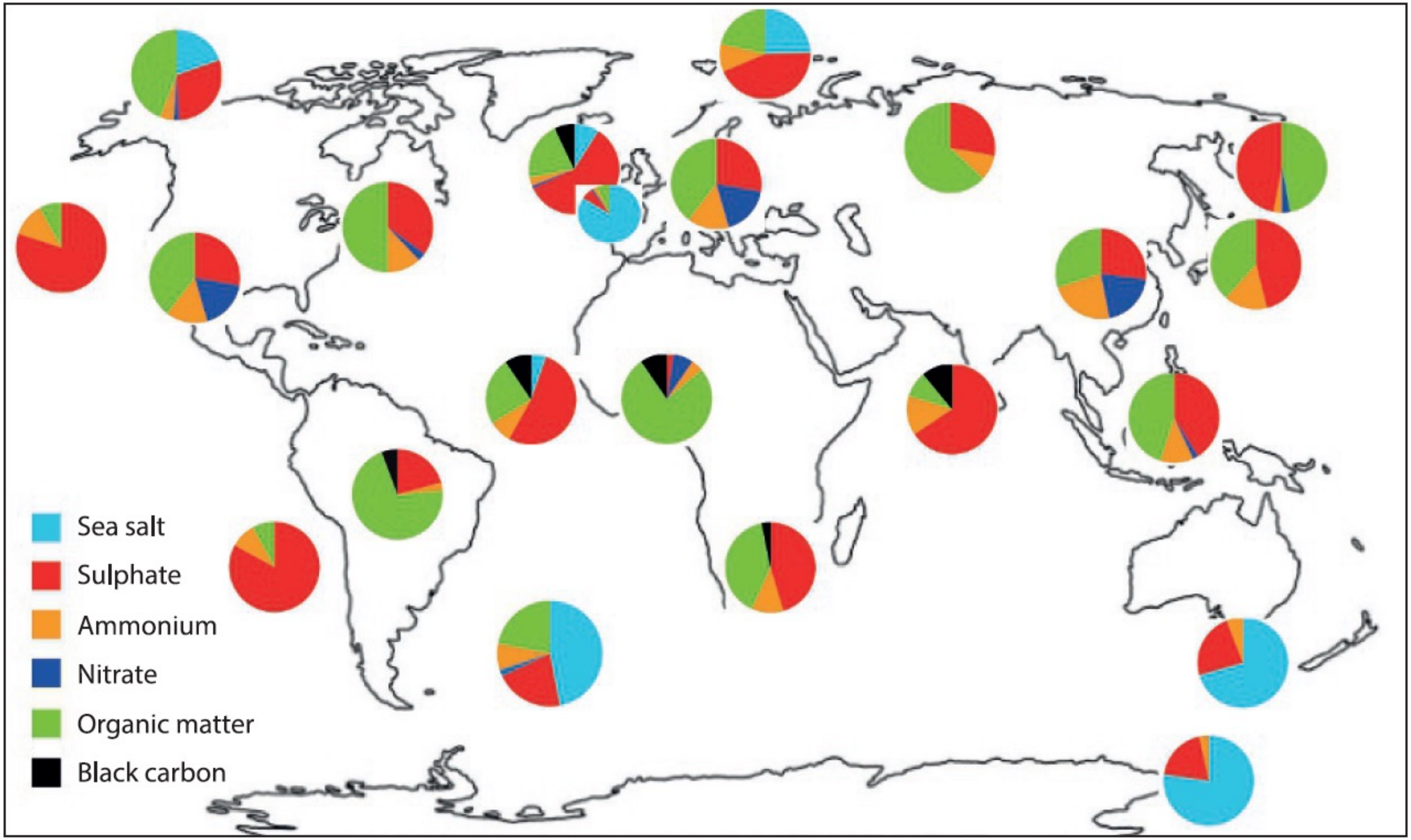

Fig 4.8 from Chapter 4 by Carslaw & Pringle, in “Aerosols and Climate”, 2022, Elsevier

Modelling the aerosol size distribution

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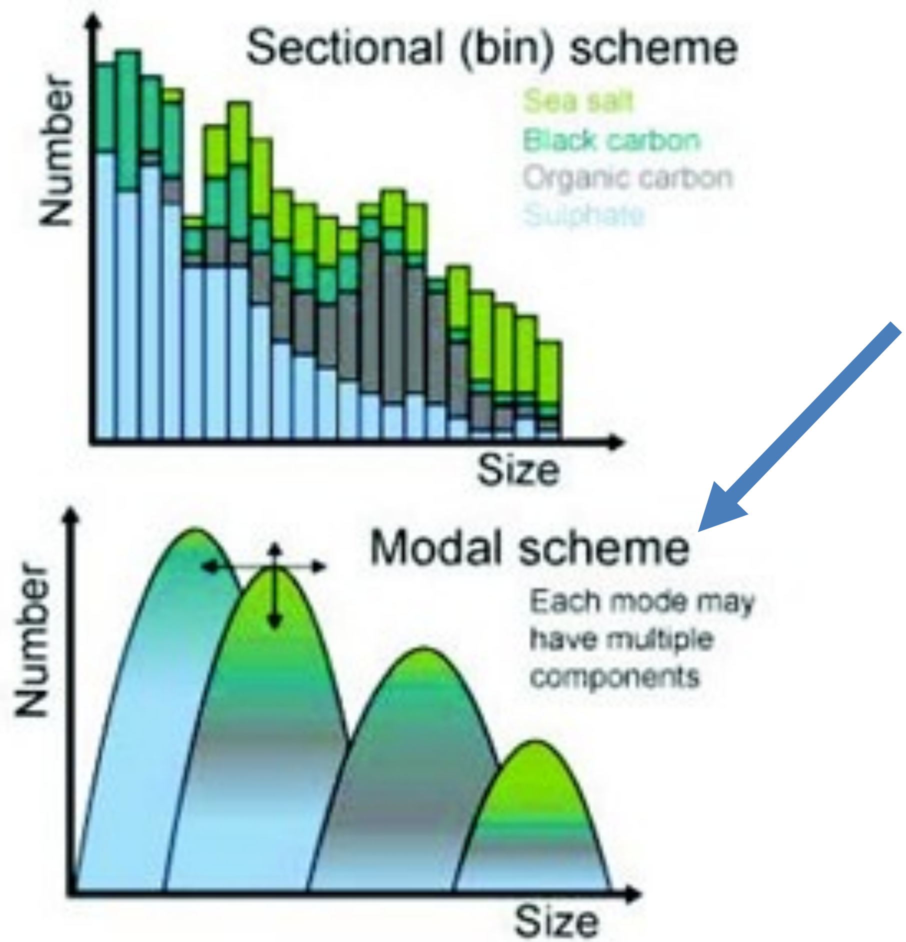

UKCA: Uses GLOMAP-Mode aerosol.

- 7 interacting lognormal modes
- 2 distributions (hydrophilic and hydrophobic)
- Composition can vary between modes.
- Composition is uniform within a mode.
- Some rules about species permitted in each mode.

Limitations:

- Cannot account for different composition within a species.
- Assumes a degree of instantaneous mixing.
- Mode width is fixed.

Schematic GLOMAP-Mode size distribution

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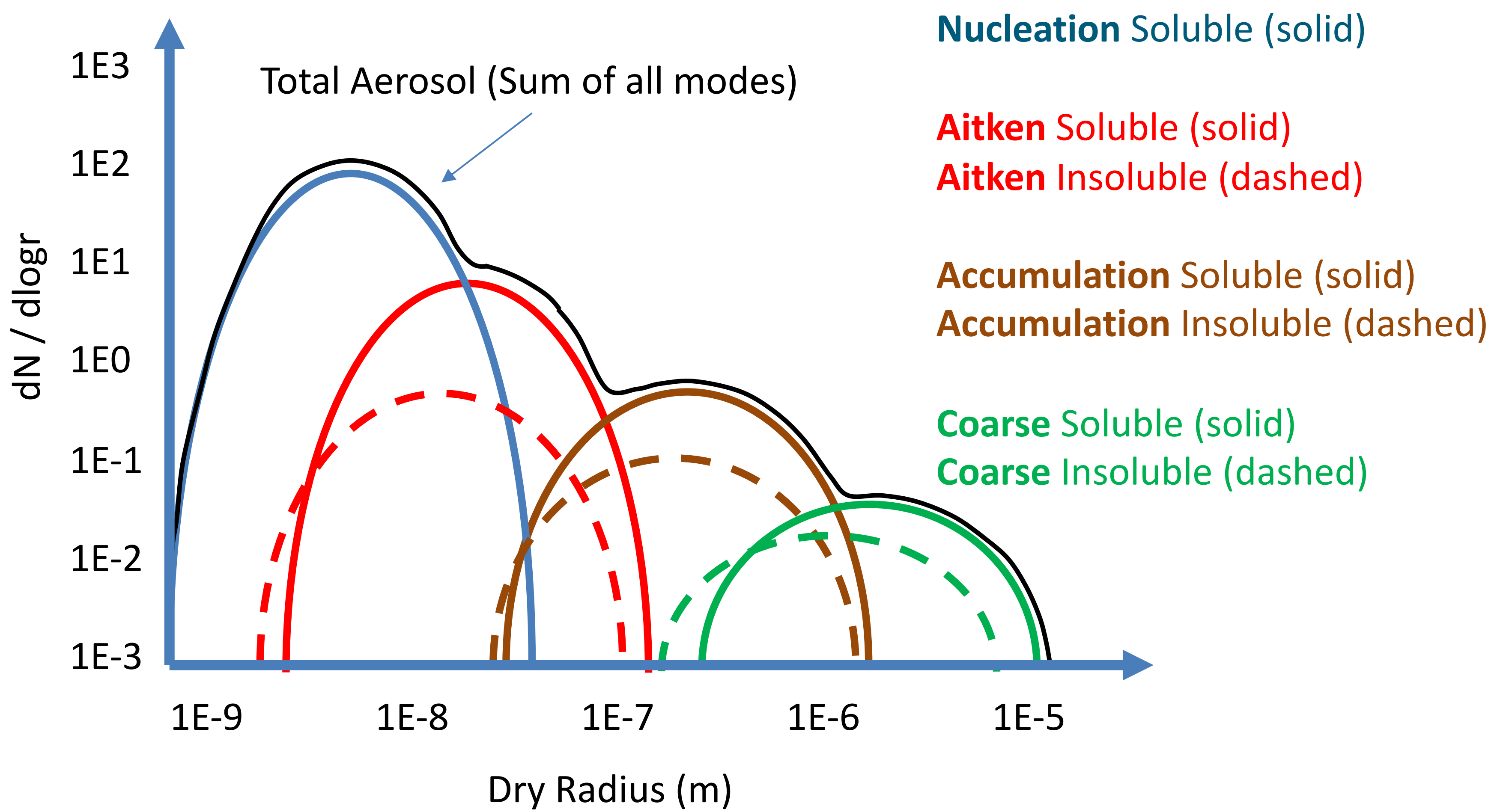

Each gridbox contains information on the mass, radius and composition of each of the 7 modes; can recreate an simulated aerosol size distribution.

Chemical Species Simulated

Standard setup of UKCA treats 5 chemical species:

1. Sulfate aerosol (SO_4 or SU)

2. Organic matter (OM)

3. Black carbon (BC)

4. Sea salt (SS)

5. Dust (DU; treated separately in UKESM)

“Standard” UKCA Aerosol Scheme

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Mode name	Mean rad range nm	Species Permitted in Mode	Production / Emission
Nucleation Soluble	< 5	SO_4, OM	SO_4: Nucleation
Aitken Soluble	5 -50	SO_4, BC, OM	BC, OM: Primary Emission
Accumulation Soluble	50 – 500	SO_4, BC, OM, SS, DU	SS: Primary Emission
Coarse Soluble	> 500	SO_4, BC, OM, SS, DU	SS: Primary Emission
Aitken Insoluble	5 – 50	BC, OM	BC, OM: Primary Emission
Accumulation Insoluble	50 – 500	BC, OM, DU	DU: Primary Emission
Coarse Insoluble	> 500	BC, OM, DU	DU: Primary Emission

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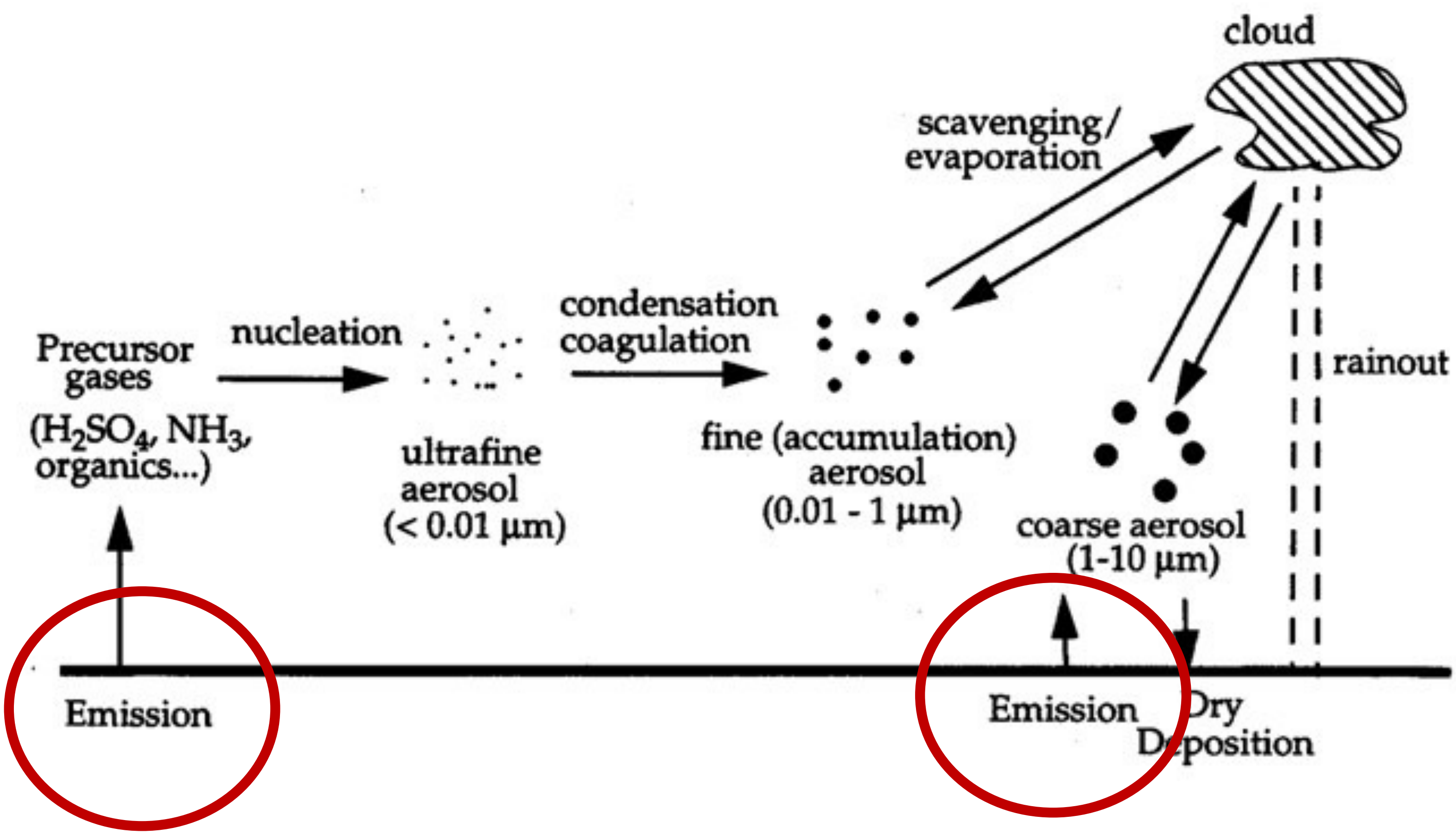
Challenge 2: Particles vary in composition – different species mix together.

Challenge 3: Microphysical processes change the aerosol size distribution.

Processes controlling and shaping the size distribution



Jacob, Introduction to Atmospheric Chemistry, 2000.

Primary Emission

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

- Gas phase sulfur 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
- BC / OC emitted into Aitken mode. Sensitivity of results to assumed size.
- Developing offline emissions inventories:

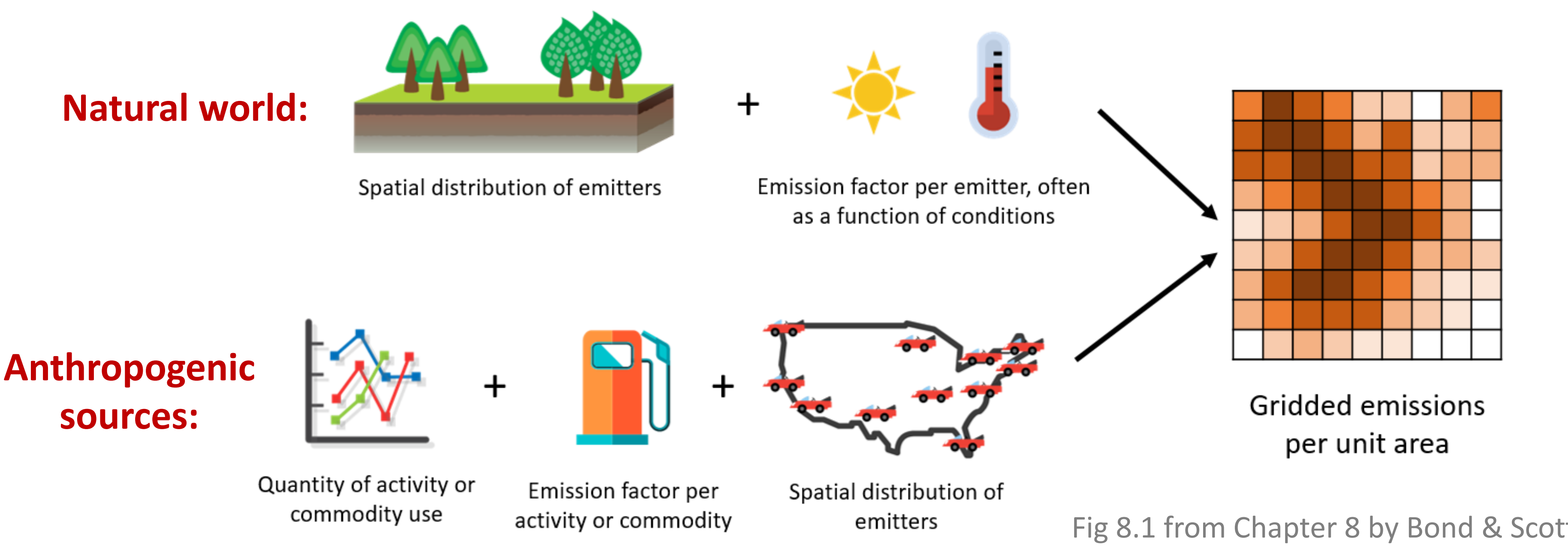


Fig 8.1 from Chapter 8 by Bond & Scott, in "Aerosols and Climate", 2022, Elsevier

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

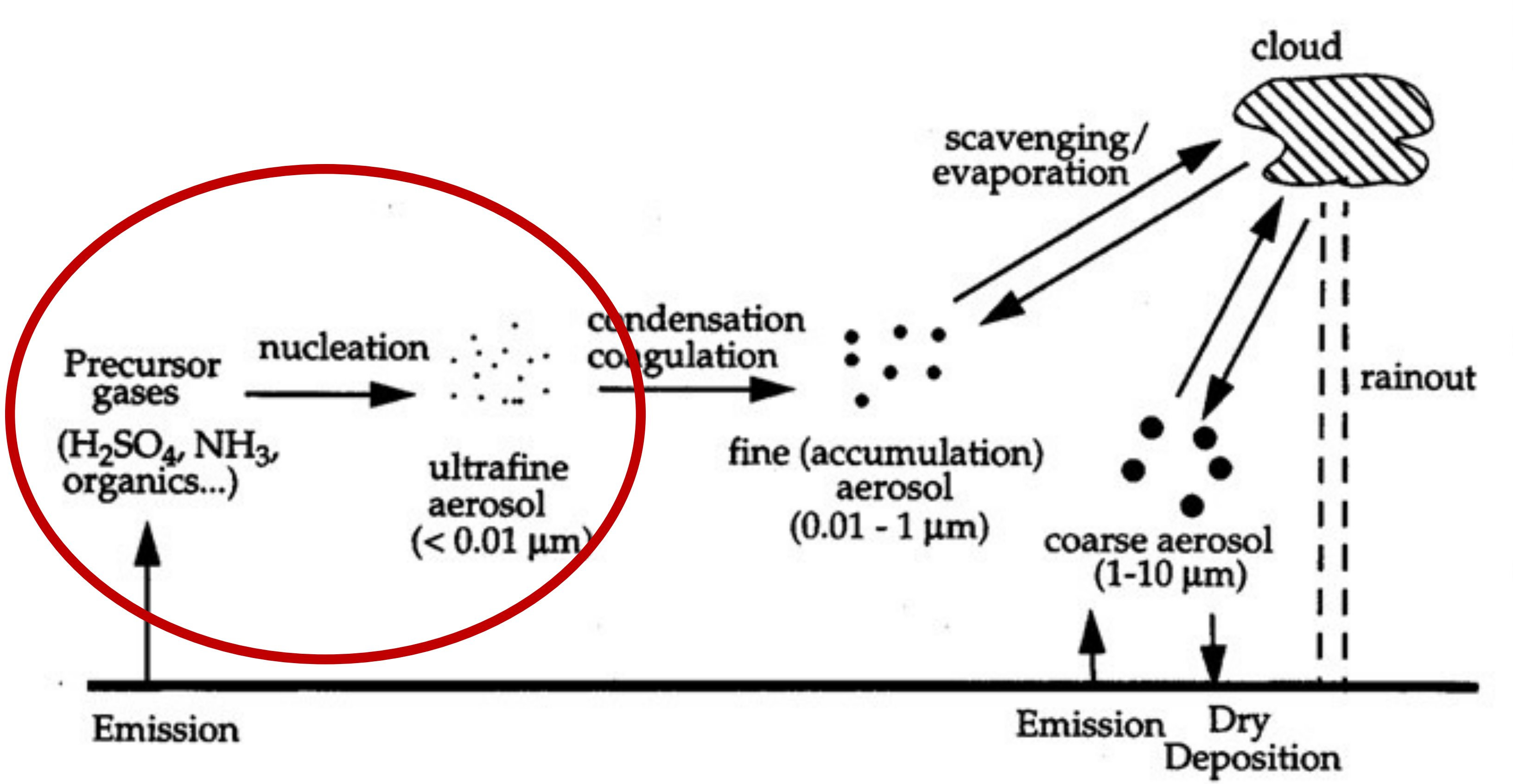
Sea spray:

- 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.

Processes controlling and shaping the size distribution



Jacob, Introduction to Atmospheric Chemistry, 2000.

Nucleation (new particle formation)

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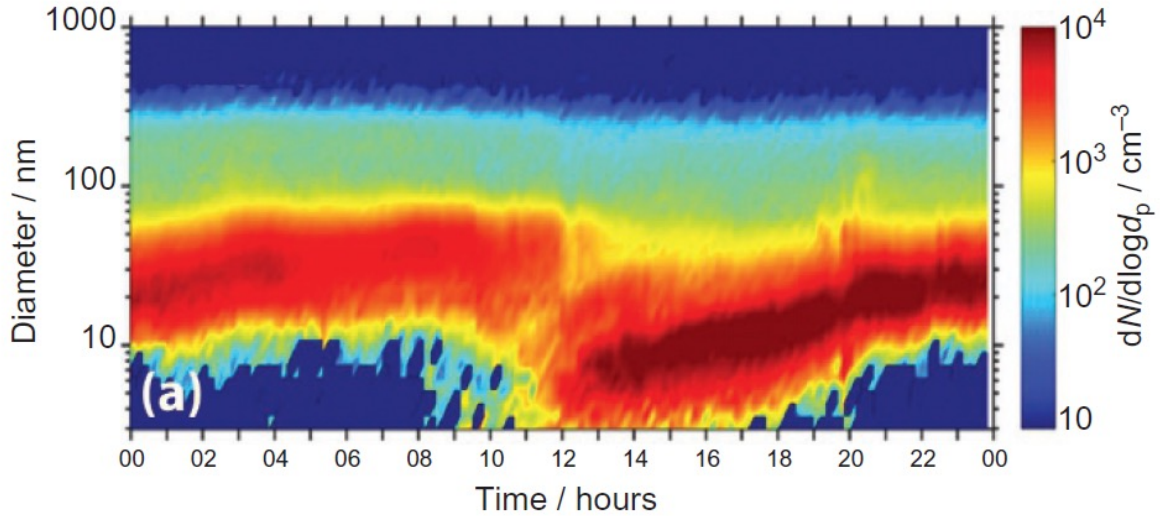
Upper Tropospheric Nucleation

- 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 and or ammonia.
- Metzger (2010), Riccobono (2014), Kirkby (2016)

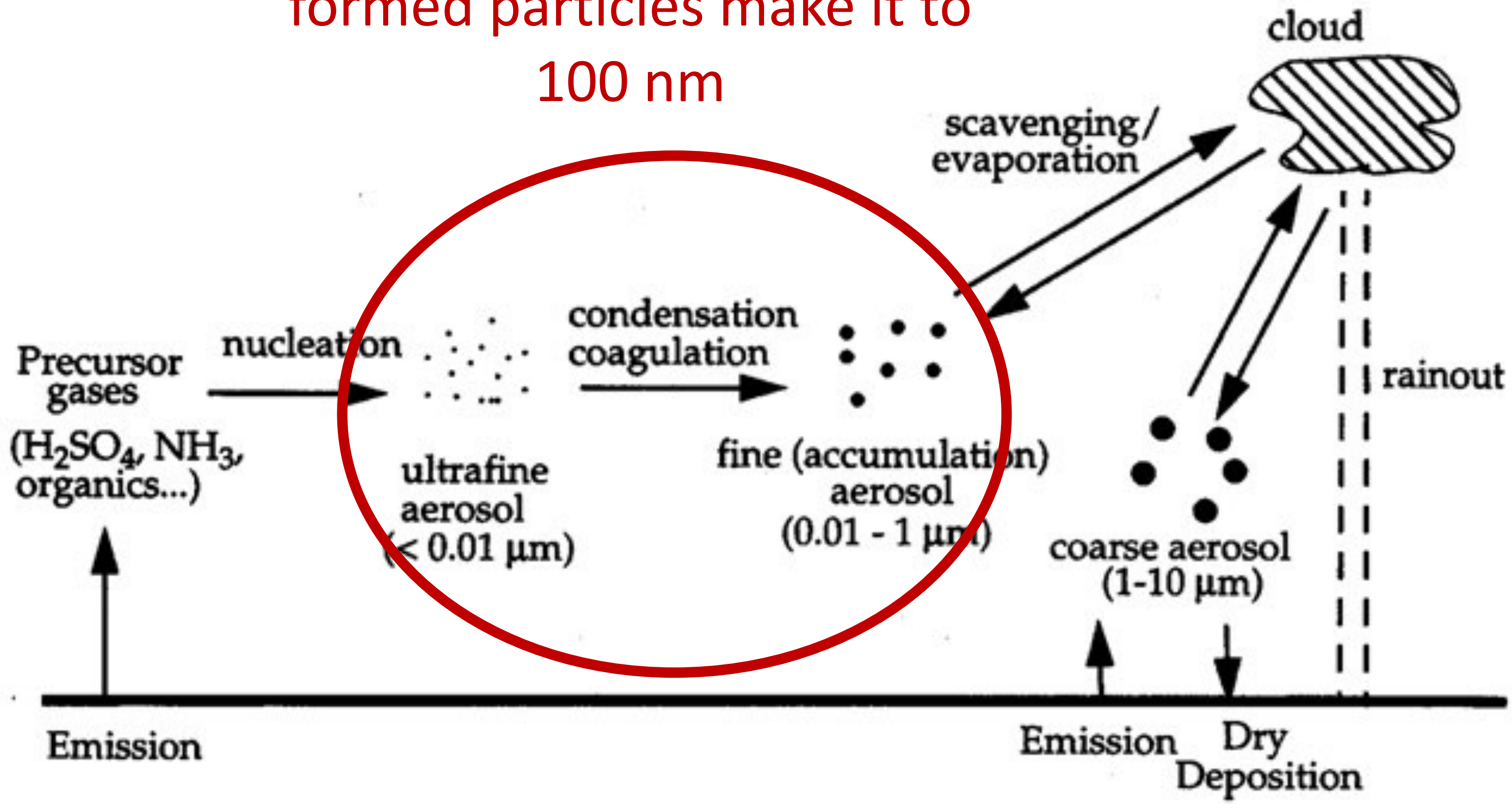


Kerminen 2018

UKCA: logical switches are used to choose / combine nucleation parameterisations.

Processes controlling and shaping the size distribution

Only ~ 10% of newly formed particles make it to 100 nm



Jacob, Introduction to Atmospheric Chemistry, 2000.

Growth: Condensation

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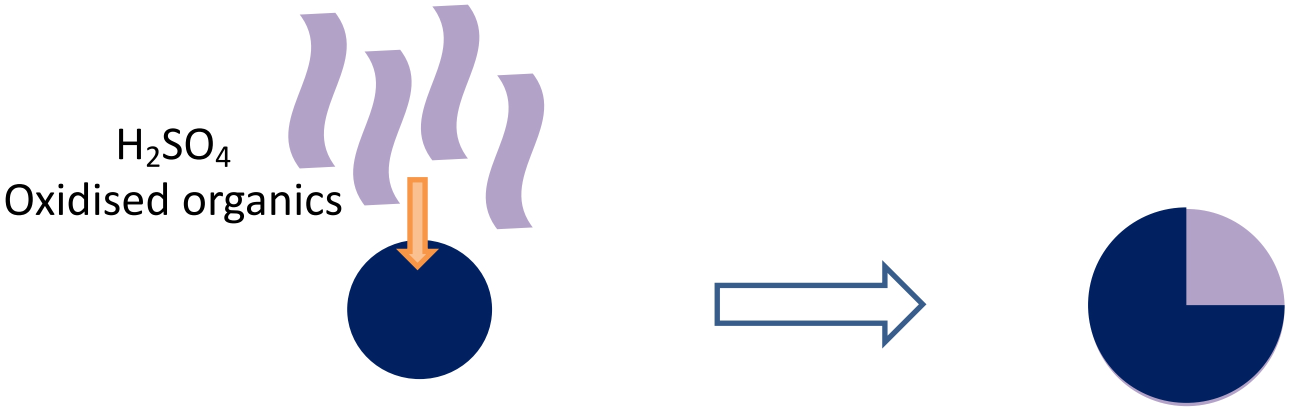
Condensation

- 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**.



Coagulation and condensational growth also change the aerosol composition; can move aerosol from the insoluble to the soluble distribution.

Growth: Coagulation

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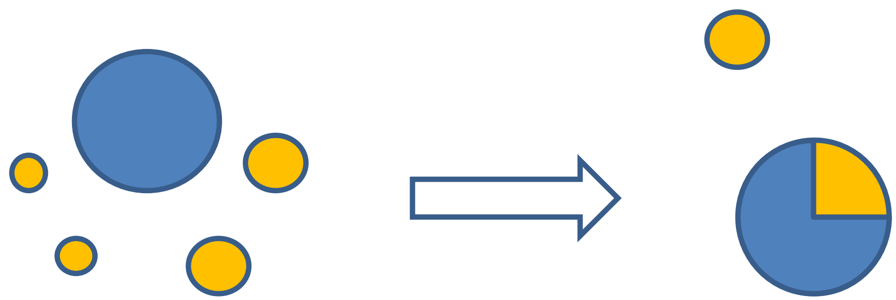
Coagulation:

- Reduces the number of aerosol; forms **fewer, larger particles**.
- Can be represented numerically, modal scheme makes assumptions about mixing state.



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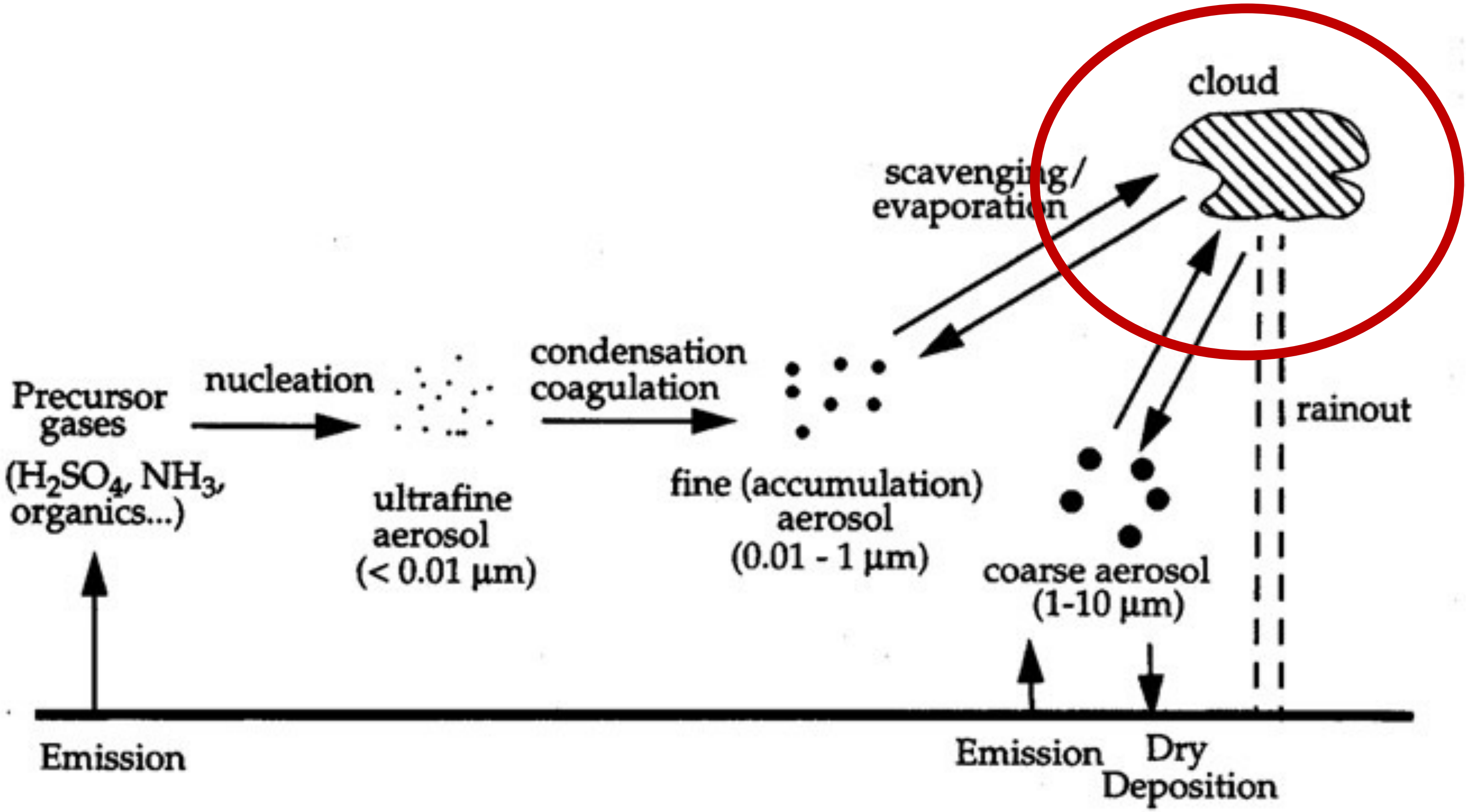
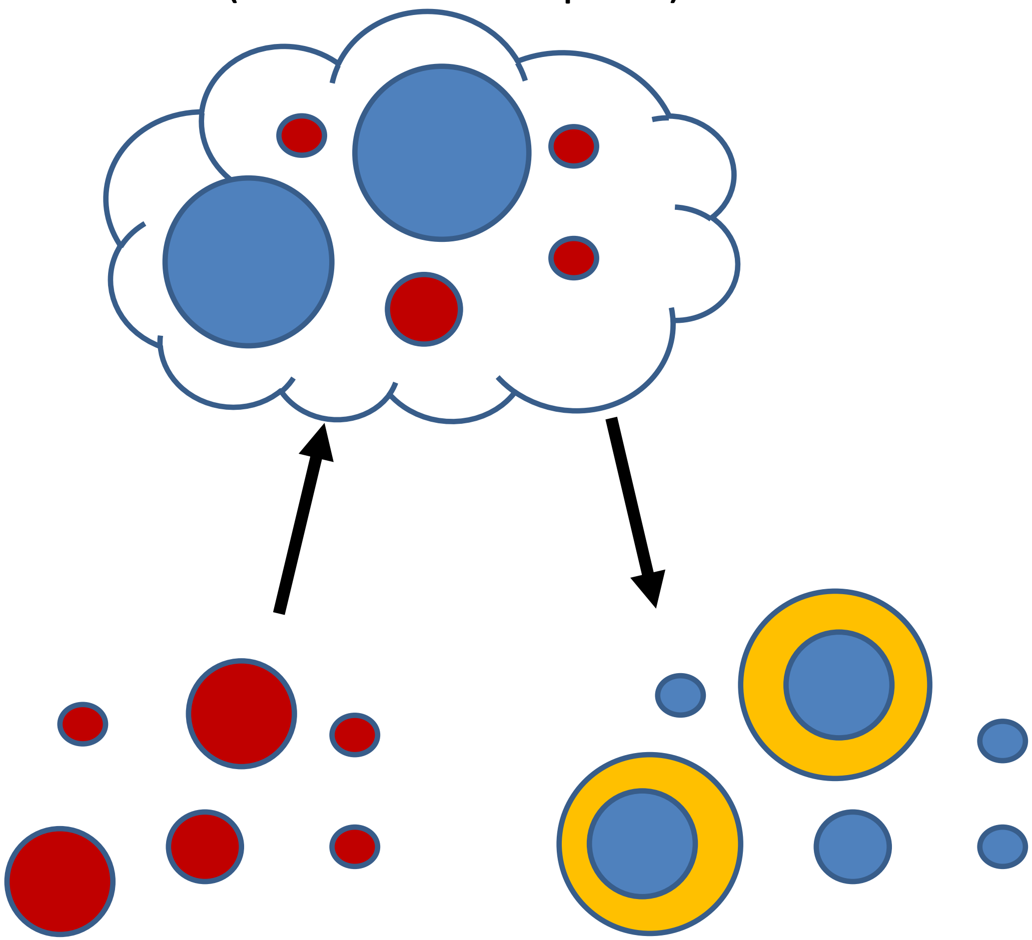
Processes controlling and shaping the size distribution



Jacob, Introduction to Atmospheric Chemistry, 2000.

In-cloud processing

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



BEFORE

AFTER

Aerosol particles can grow in size as a result of chemical processing in non-precipitating clouds.

Soluble species can dissolve in liquid cloud water, undergo chemical reactions and, when the cloud evaporates, 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 in the lowest 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)	

Build Your Own Global Aerosol Model

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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

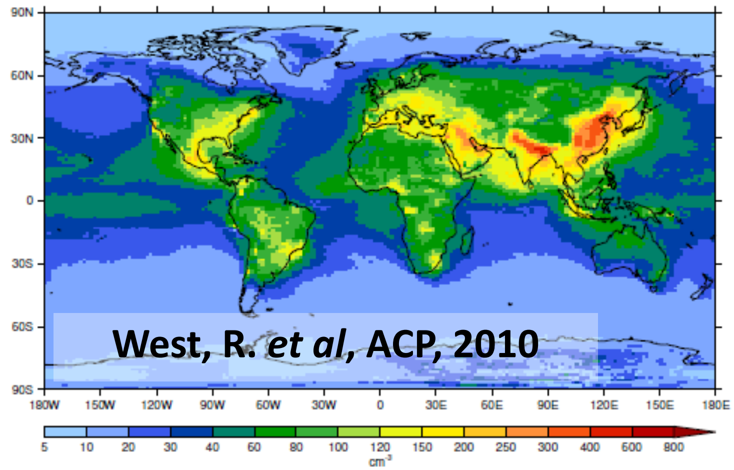
UKCA_AERO_CTL – Aerosol routines

- 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

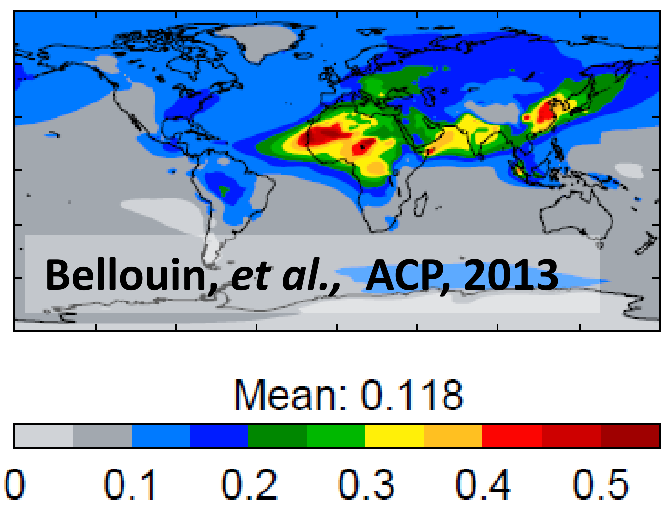
Cloud droplet number



UKCA_ACTIVATE (R. West, P. Stier)

Calculates the number of cloud droplets formed at cloud base. Dependent on the number, size and composition of the aerosol.

GLOMAP-mode AOD



UKCA_RADAER (N. Bellouin)

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

Big uncertainty in climate impact

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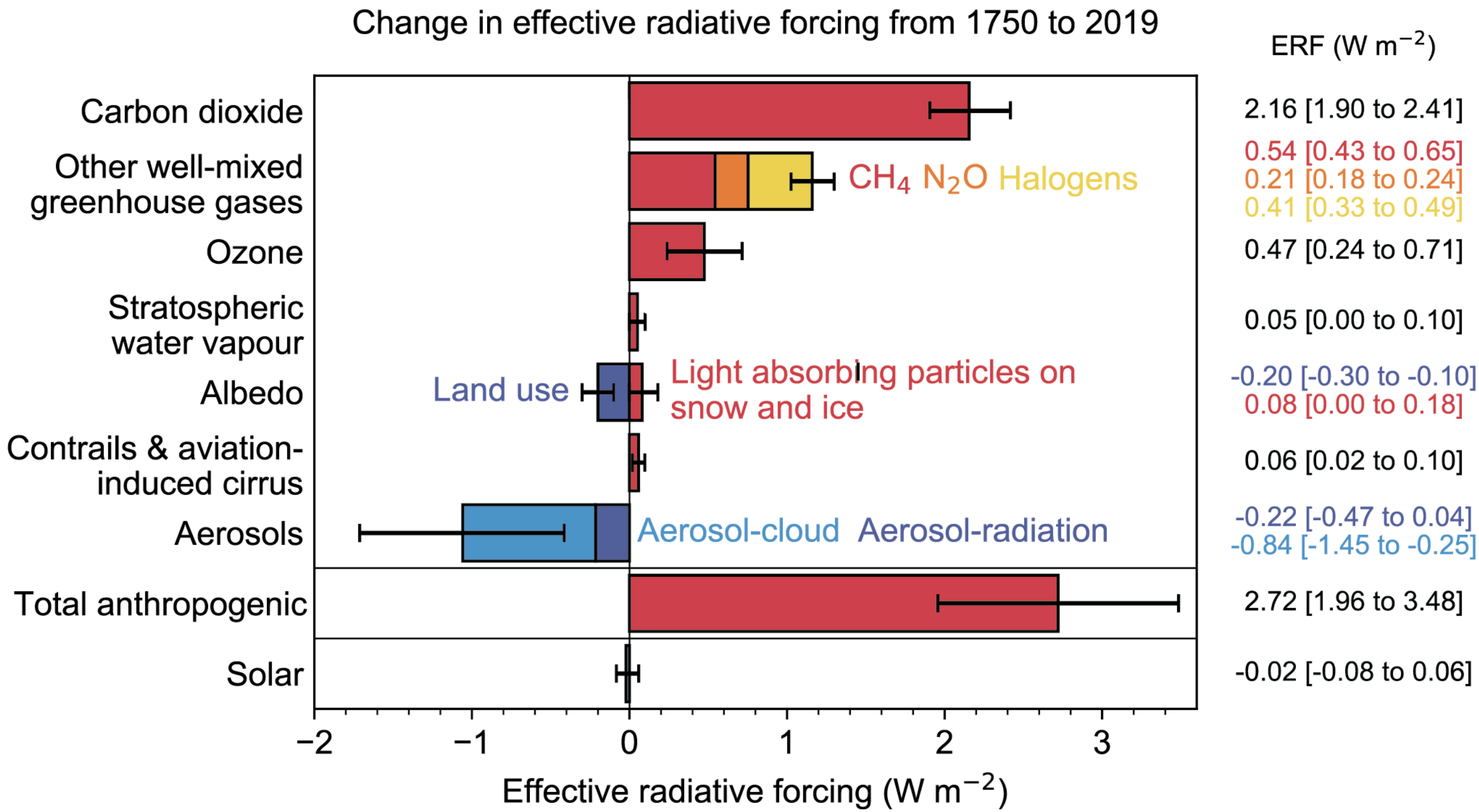

Figure 7.6, WGI, AR6, IPCC (2021)

Future emissions very uncertain

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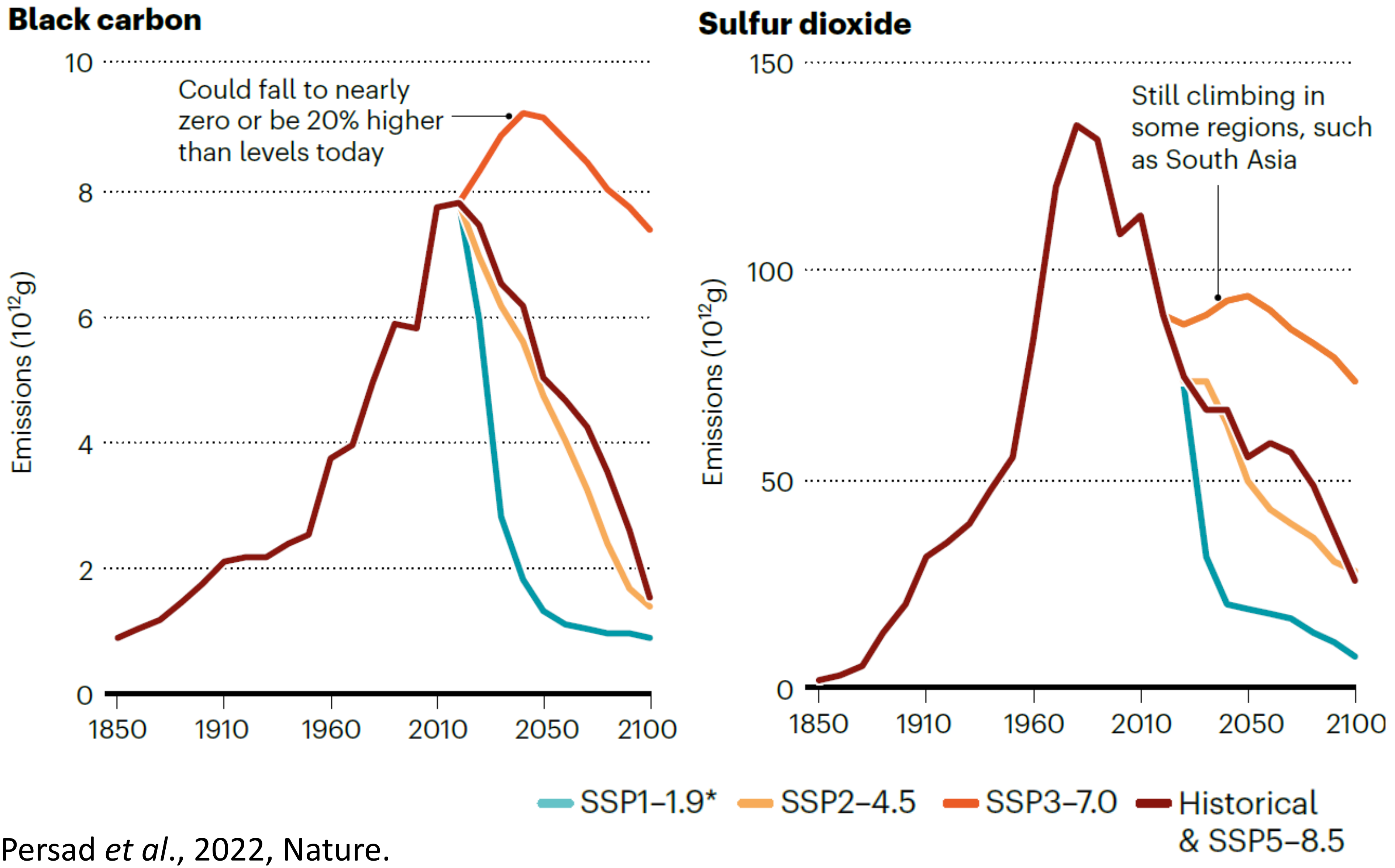

Persad *et al.*, 2022, Nature.

Conclusions

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1. UKCA-Mode is a global aerosol model in which the aerosol size distribution is represented using (normally 7) interacting lognormal modes.

2. The model treats 5 species: sulfate, black carbon, organic carbon, sea spray and dust.

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