



# Aerosol Modelling

*“for measurement people”*

**AeroCom Workshop 2010**

Oxford

**Philip Stier**

**Department of Physics**

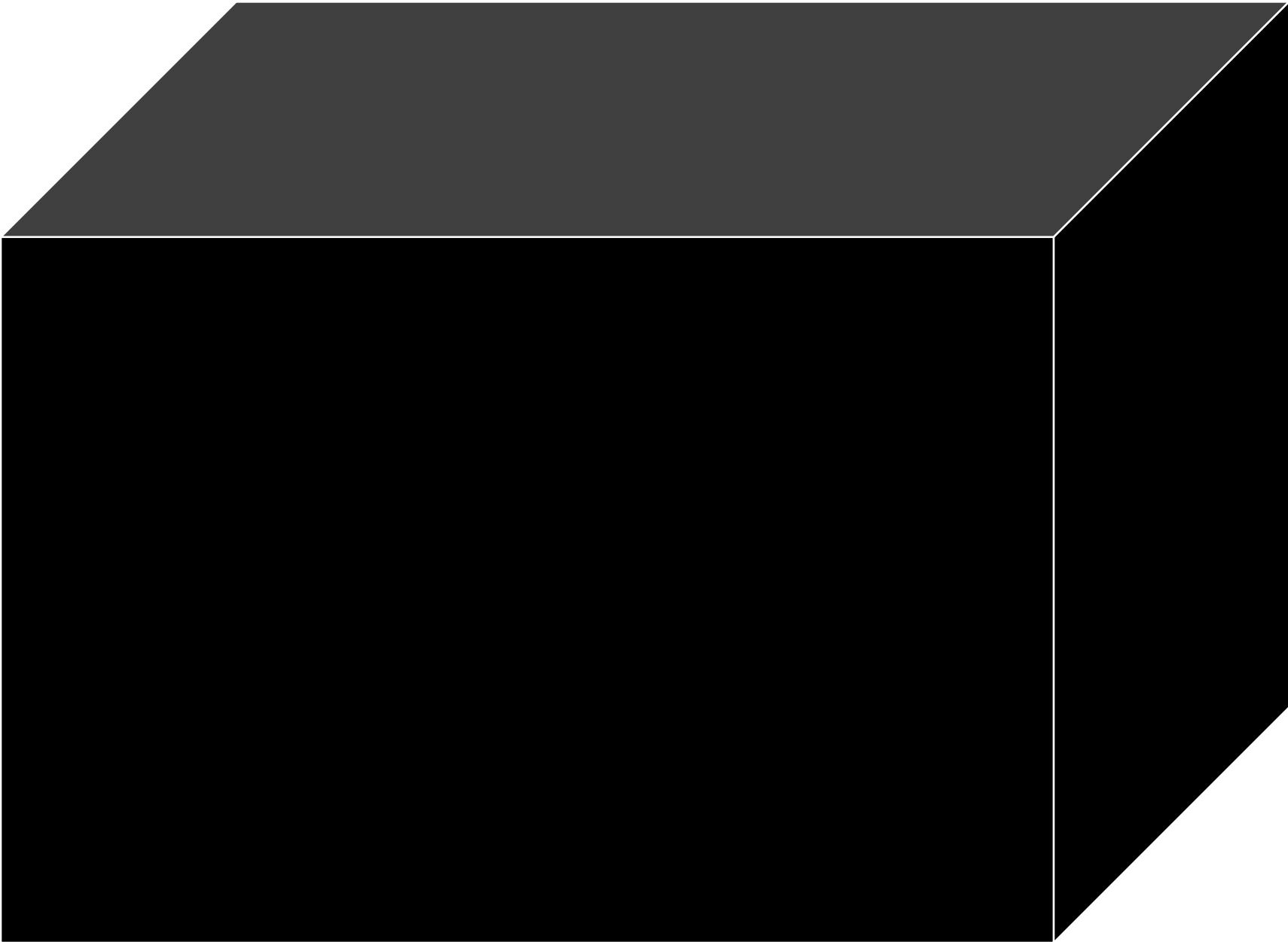
Atmospheric, Oceanic and Planetary Physics

**Oriel College**

**University of Oxford**



# Aerosol Models – A Black Box

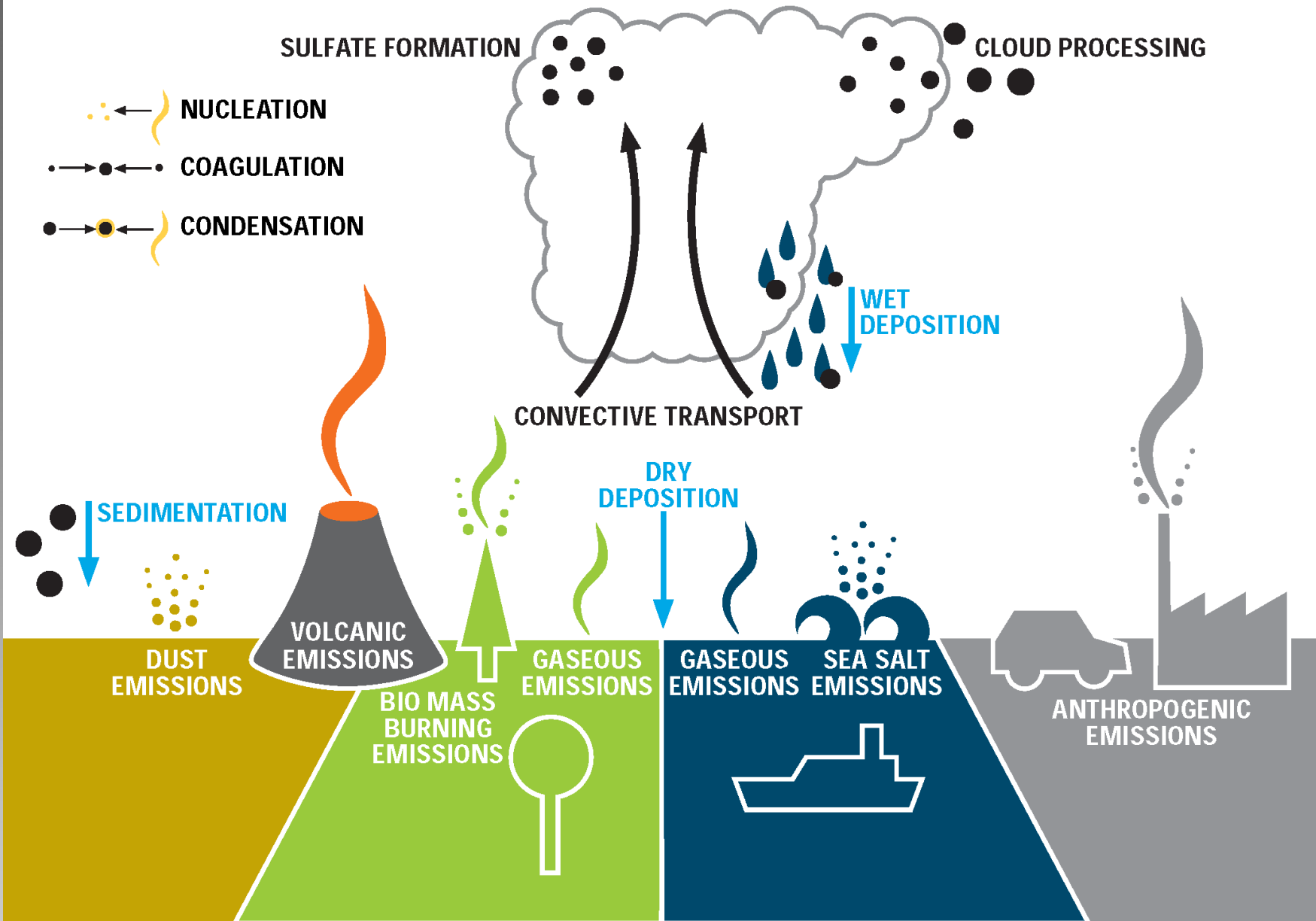


## Questions (by François-Marie Bréon):

- What is the typical resolution of models?
- How do models handle variability within grid box?
- How do models handle size distributions?
- What happens in a cloud?
- How are defined the sources?
- What is the lifetime of aerosol in models.  
Is it significantly different among aerosol types?
- How do you estimate injection heights?
- Are the aerosol well mixed within "mixing" layer?
- Is the mixing layer height well reproduced by transport models?
- How are the aerosol optical properties computed?
- What are the main sources of errors?

# Global Aerosol Cycles

Aerosol Modelling



## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

## Removal

- Dry deposition & sedimentation
- Scavenging

## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

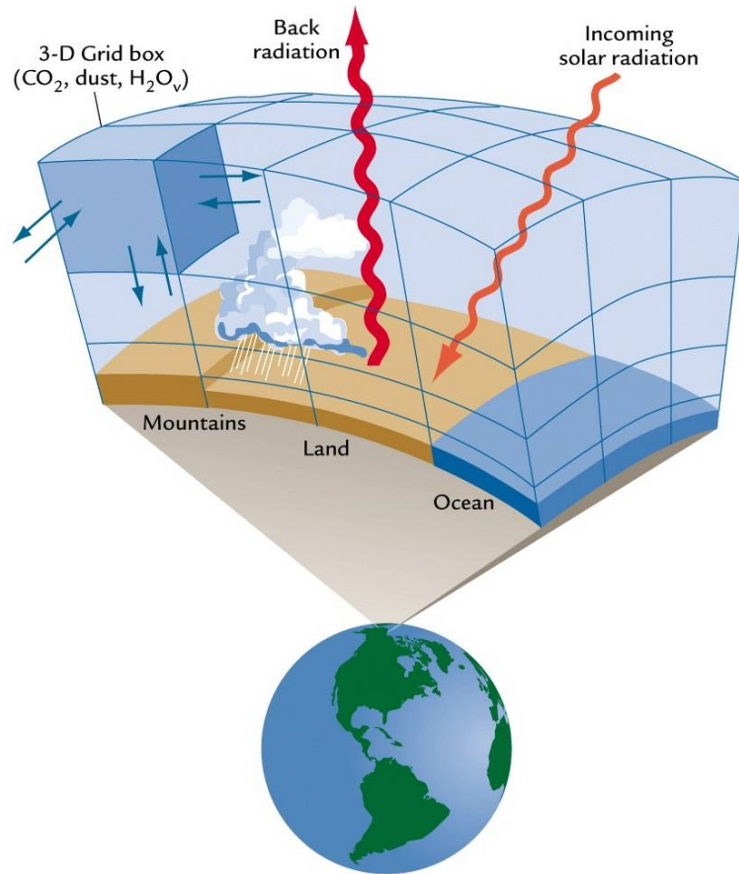
- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

## Removal

- Dry deposition & sedimentation
- Scavenging

# Atmospheric Models

Atmospheric circulation models are based on fundamental physics:



Numerical solution of fundamental physical equations:

- conservation of momentum
- conservation of mass
- conservation of energy
- equation of state

Additional sub-models for:

- **clouds cover**
- **cloud microphysics + precipitation**
- aerosols
- radiative transfer
- chemistry
- land surface processes
- vegetation
- carbon cycle
- cryosphere
- ....

# Dictionary of Atmospheric Models

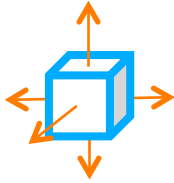
## Box Model

0D, no transport,  
no or external forcings



## Parcel Model

0D, moved by prescribed  
external forcings



## Single Column Model (SCM)

1D, vertical transport  
no or external forcings (e.g. campaign)



## Chemical Transport Model (CTM)

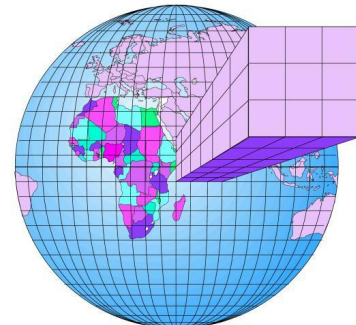
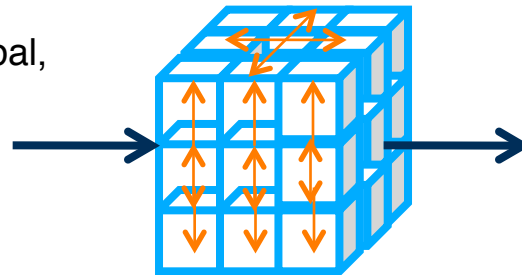
3D transport, regional (boundary conditions) or global,  
**met-fields diagnostic** from GCM

## Regional Circulation Model

3D transport, regional,  
**met-fields prognostic** but with boundary conditions from GCM

## Global Circulation Model (GCM)

3D transport, global, **met-fields prognostic**, potentially assimilated  
or “nudged” to assimilated meteorological analysis data

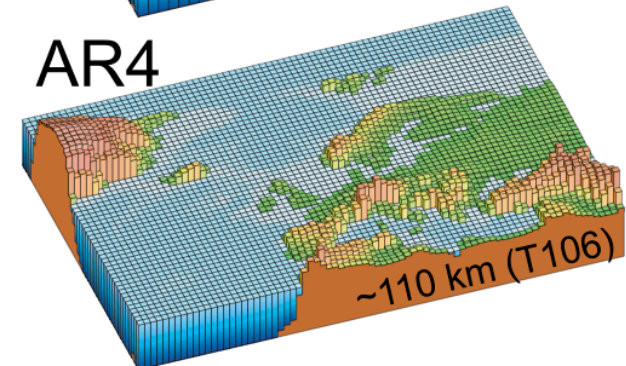
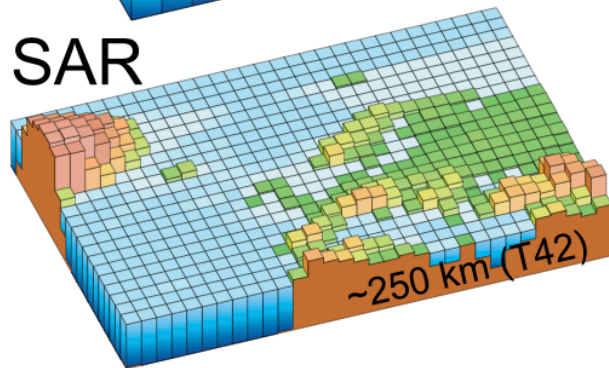
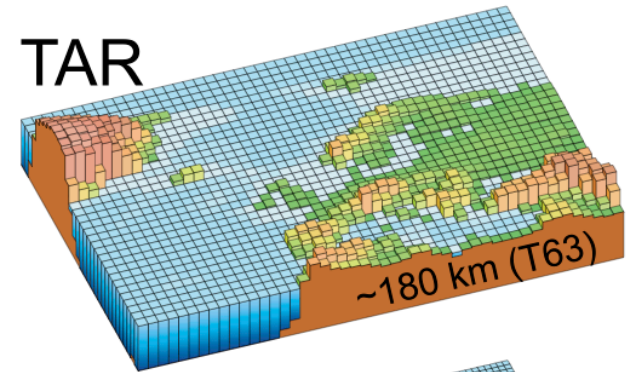
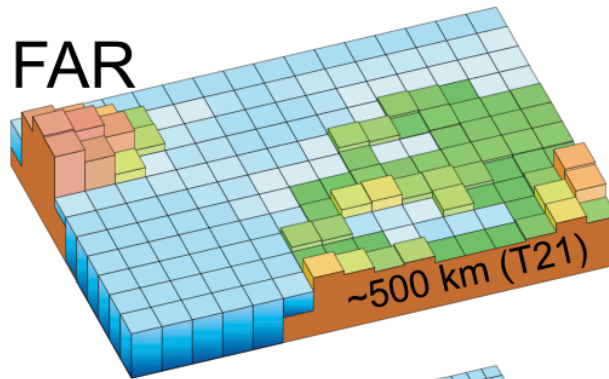
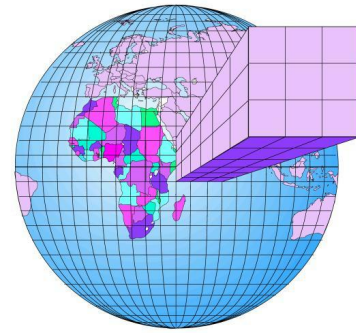




# Resolution of Atmospheric Models

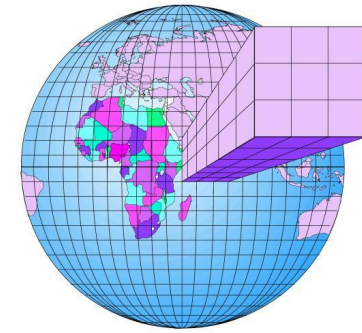
## Global Circulation Model (GCM)

Climate model resolution since IPCC FAR:



Typical AeroCom  
Aerosol Model Resolution

# Resolution of Atmospheric Models

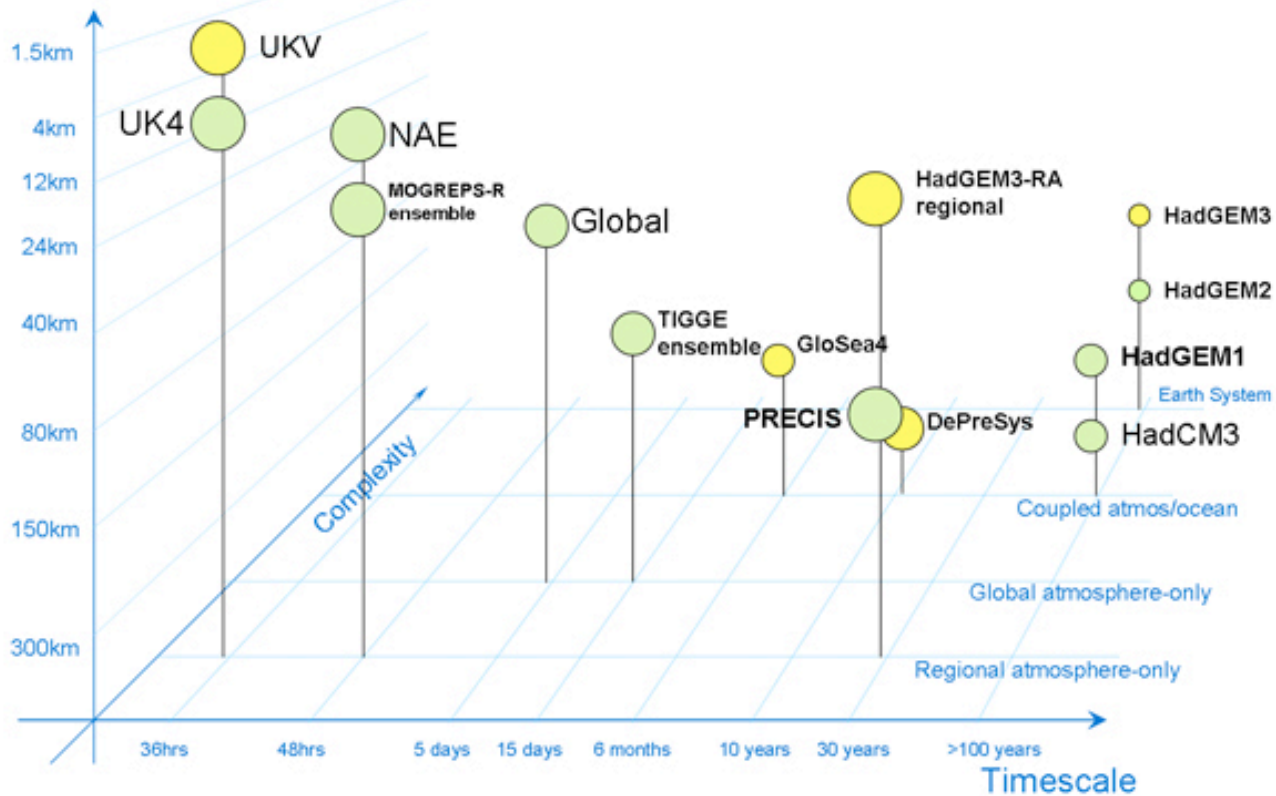


## Model Hierarchy

Resolution depends on complexity and temporal scales



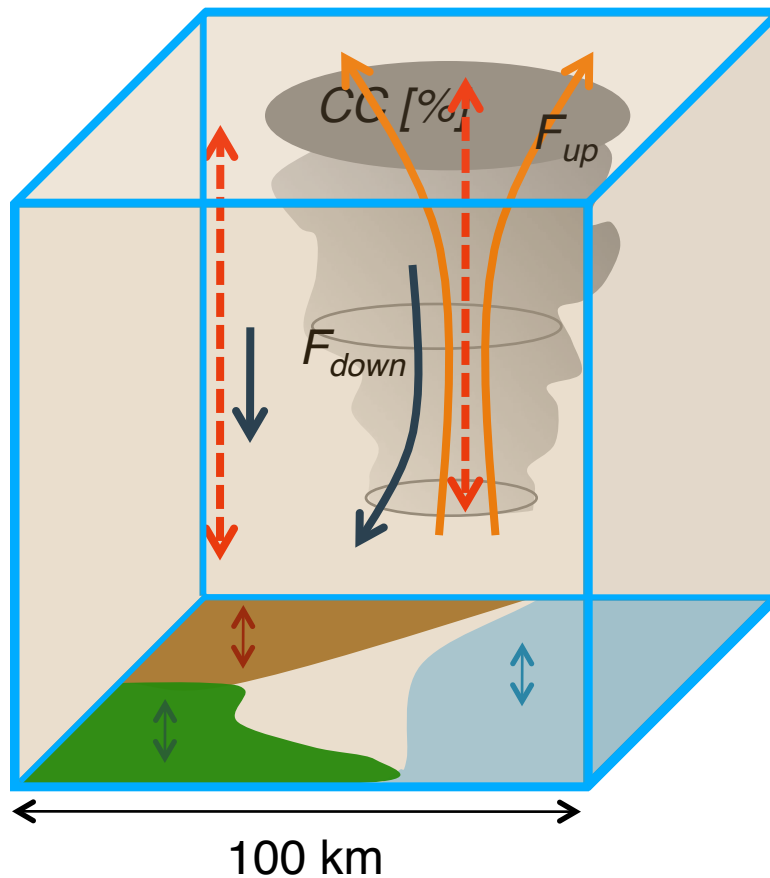
Atmospheric grid length



# Caveat: Unresolved Scales

**Within one model grid box:**

Tracers (mass or number) assumed homogeneously mixed



Parameterised fractional cloud cover

Mean In-cloud liquid-, ice-water (or sub-grid scale pdf)

Mean up- and down-drafts

Mean clear-sky and cloudy-sky radiative fluxes

Mosaic approach:  
Fractional surface cover

# Dictionary of Simulation Types

## Offline (CTM)

- Transport using prescribed met-fields from GCM or RCM

## Online (GCM)

- Transport solving the fundamental equations of motion

## Nudged (GCM)

- Transport solving the fundamental equations of motion
- Large scale prognostic variables relaxed to assimilated analysis data
- Sub-grid scales (e.g. clouds) not constrained

## “AMIP” (Atmospheric Model Intercomparison Project)

- Standardised simulation protocol
- Prescribed SST (“fixed SST run), Ozone, CO<sub>2</sub>, topography,...

## Climate

- Transport solving the fundamental equations of motion
- Simple ocean models (“slap”, “q-flux”, “mixed layer”) or
- Complex ocean general circulation models AtmosphereOceanGCMs

## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

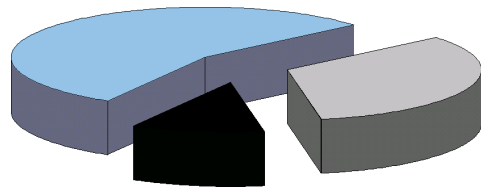
- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

## Removal

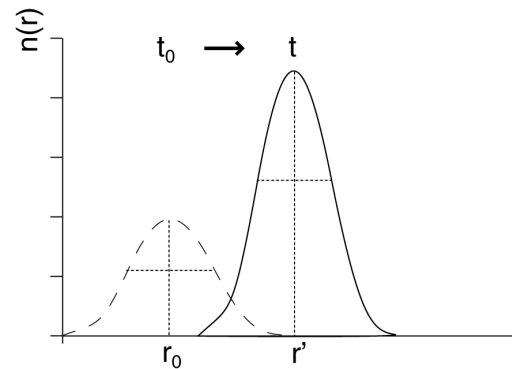
- Dry deposition & sedimentation
- Scavenging

# Aerosol Representation in Atmospheric Models

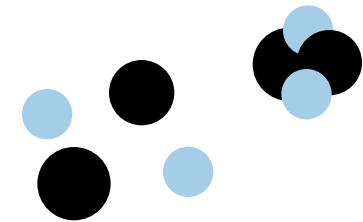
Aerosol microphysical state determined by:



composition



size distribution



mixing state

Caveat: models generally ignore the effects of non-spherical shapes...



Electron-microscopic image of black carbon aerosol (From Heintzenberg et al., 2003)

# Aerosol Representation in Atmospheric Models

## Key Model Types

### 1) Bulk (“mass based”)

Component masses only prognostic variable. Size and mixing assumed.

### 2) Moment based (“Modal”, “Log-Normal”, Quadrature of Moments)

Assume functional form of size distribution, predict evolution

Prognostic size, external mixing through several “moments”

Applied with/without microphysics, with various

### 3) Sectional (“bin”)

Split aerosol into bins and predict their evolution.

Assumptions, external mixing “expensive”.

Microphysics (e.g. dust models).

$$\frac{\partial n(v, t)}{\partial t} = \frac{1}{2} \int_0^v K(v-q, q)n(v-q, t)n(q, t)dq - n(v, t) \int_0^\infty K(q, v)n(q, t)dq - J_0(v)\delta(v-v_0) + S(v) - R(v)$$

General Aerosol Dynamic Equation...

Computational cost





## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

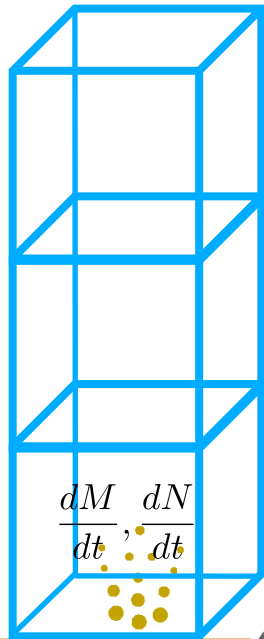
## Removal

- Dry deposition & sedimentation
- Scavenging

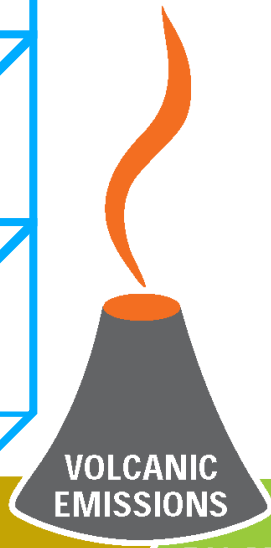
# Aerosol Sources in Modells

## Implementation of Primary Emissions

Apply tendency to mixing ratios in lowest grid box



DUST EMISSIONS



VOLCANIC EMISSIONS

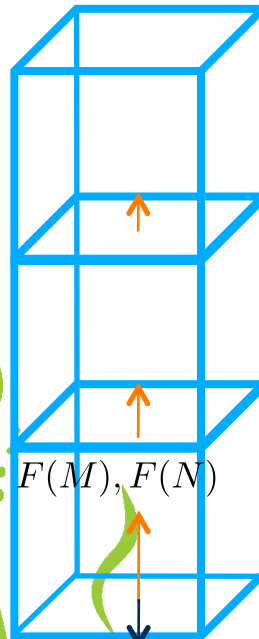
BIO MASS BURNING EMISSIONS



GASEOUS EMISSIONS

$F(M), F(N)$

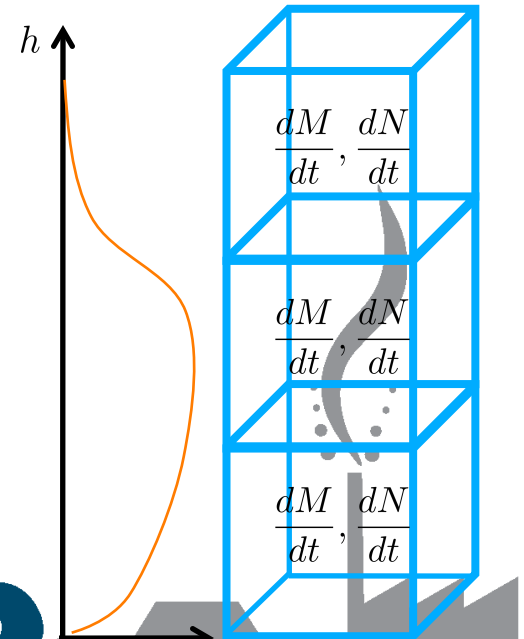
Apply (net) emission fluxes as boundary of vertical diffusion



GASEOUS EMISSIONS  
SEA SALT EMISSIONS



Apply **prescribed** injection height profile (or injection model)



ANTHROPOGENIC EMISSIONS

# Aerosol Sources in Modells

## Prognostic Emission Sub-Models

(Other emissions are generally prescribed from inventories)

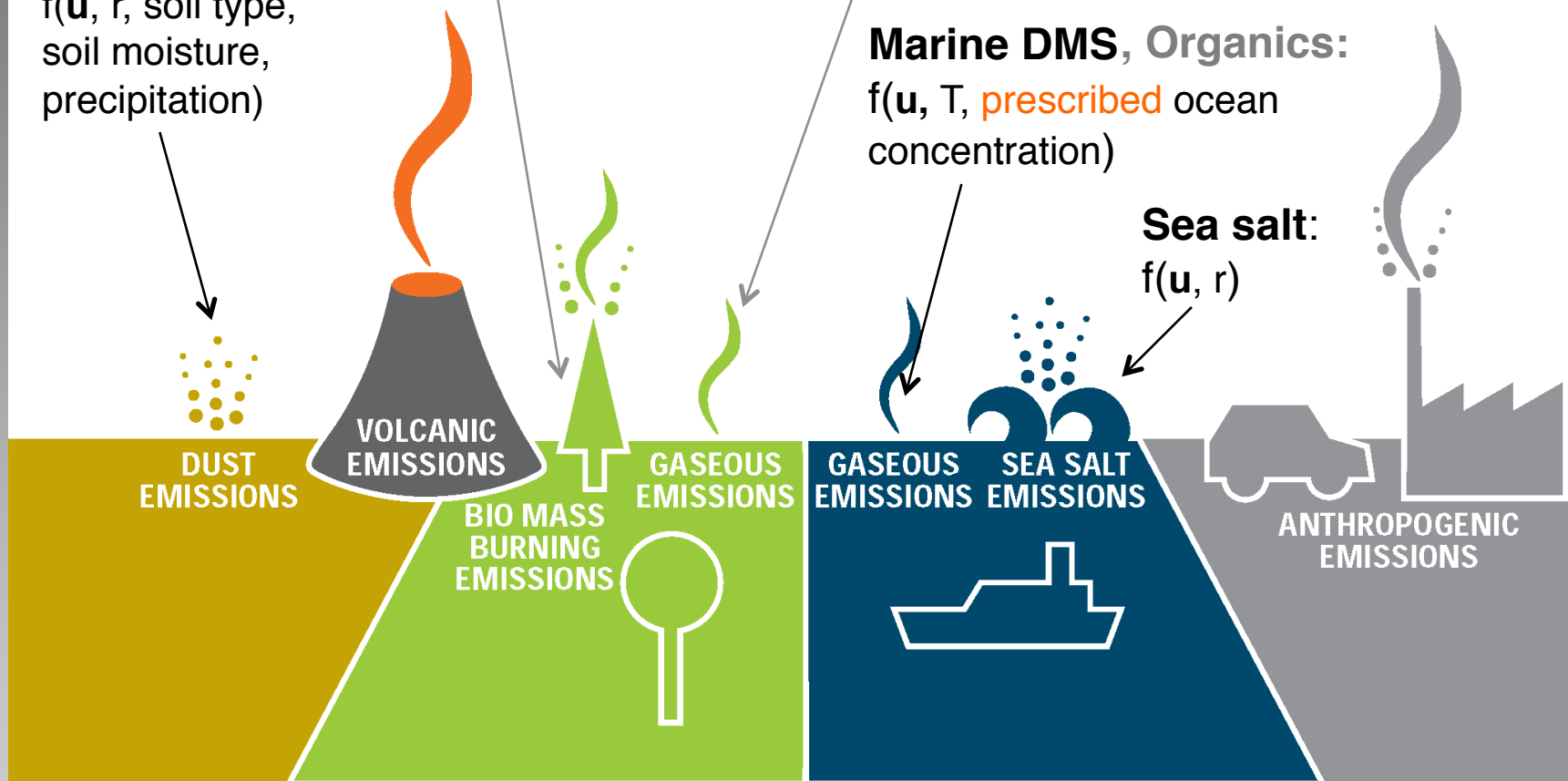
**Dust:**  
 $f(u, r, \text{soil type}, \text{soil moisture}, \text{precipitation})$

**Biomass burning:**  
 $f(u, T, P-E, \text{vegetation}, \text{climatology})$

**Biogenic:**  
 $f(u, T, \text{soil}, P-E, \dots)$

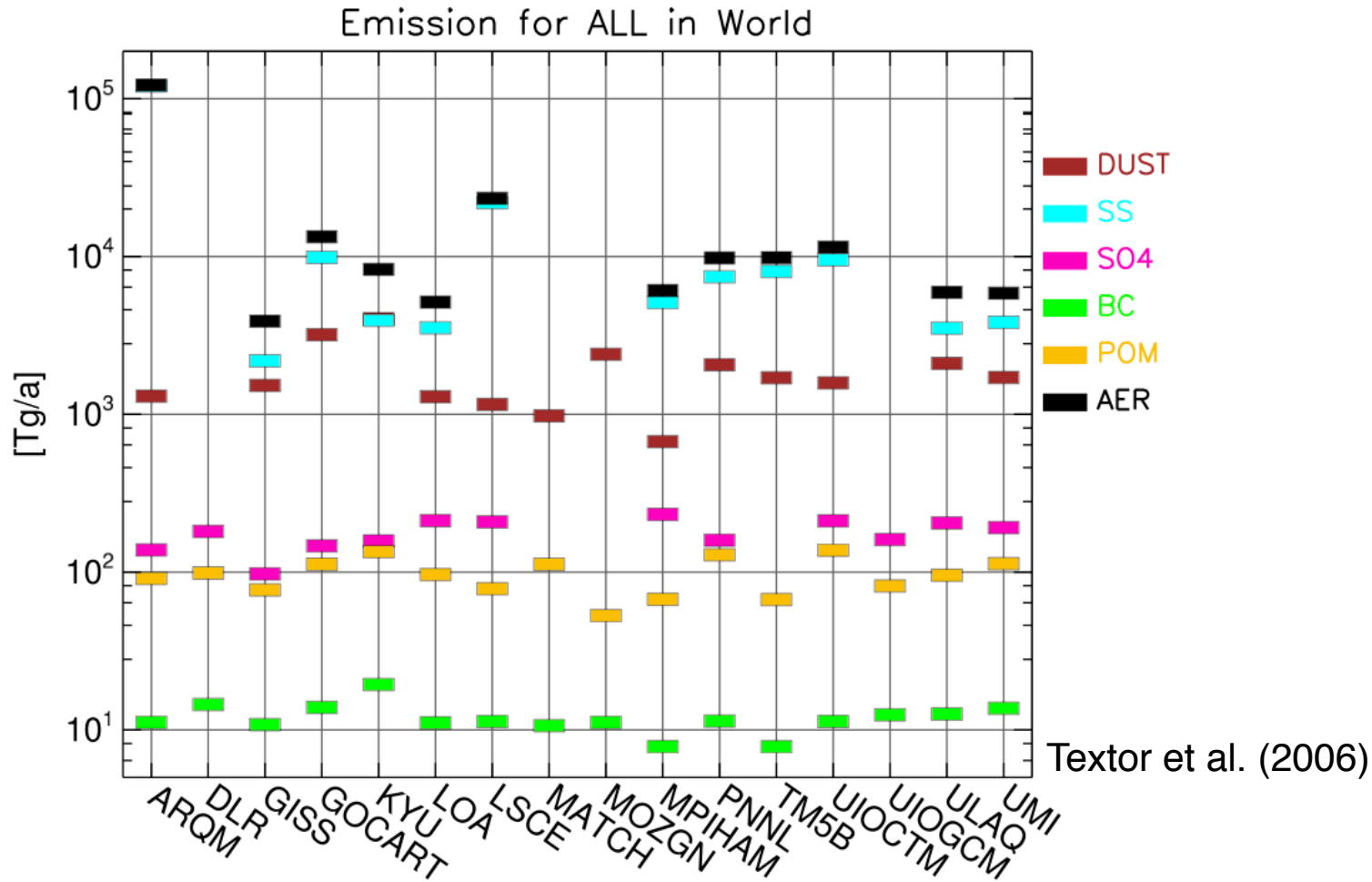
**Marine DMS, Organics:**  
 $f(u, T, \text{prescribed ocean concentration})$

**Sea salt:**  
 $f(u, r)$



# Aerosol Sources in Modells

## Emissions in AeroCom Phase I Experiment A:

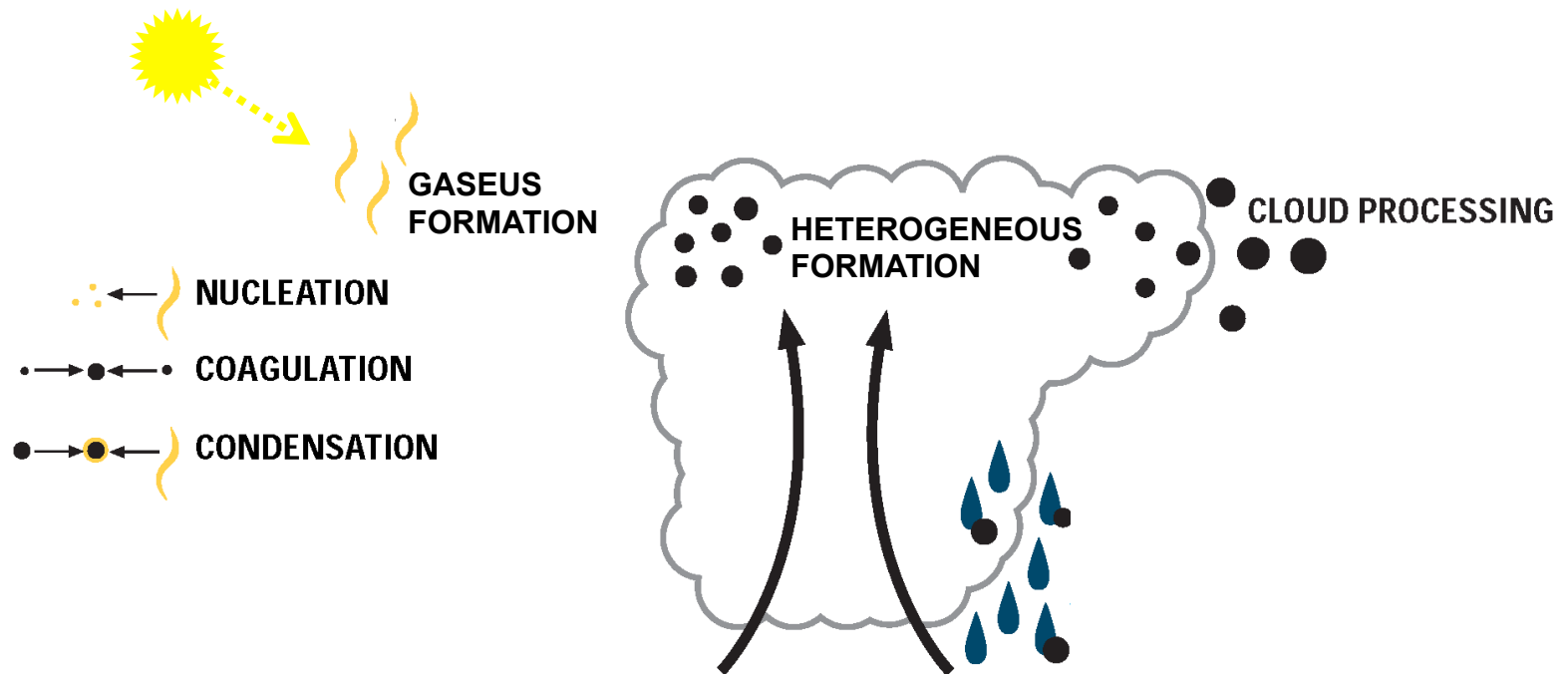


Caveat: Emission inventories currently provide only mass fluxes. Effective emission size distributions (at model scale) remain uncertain.

# Aerosol Sources in Modells

## Secondary formation in the atmosphere

Chemical formation of low-volatility products



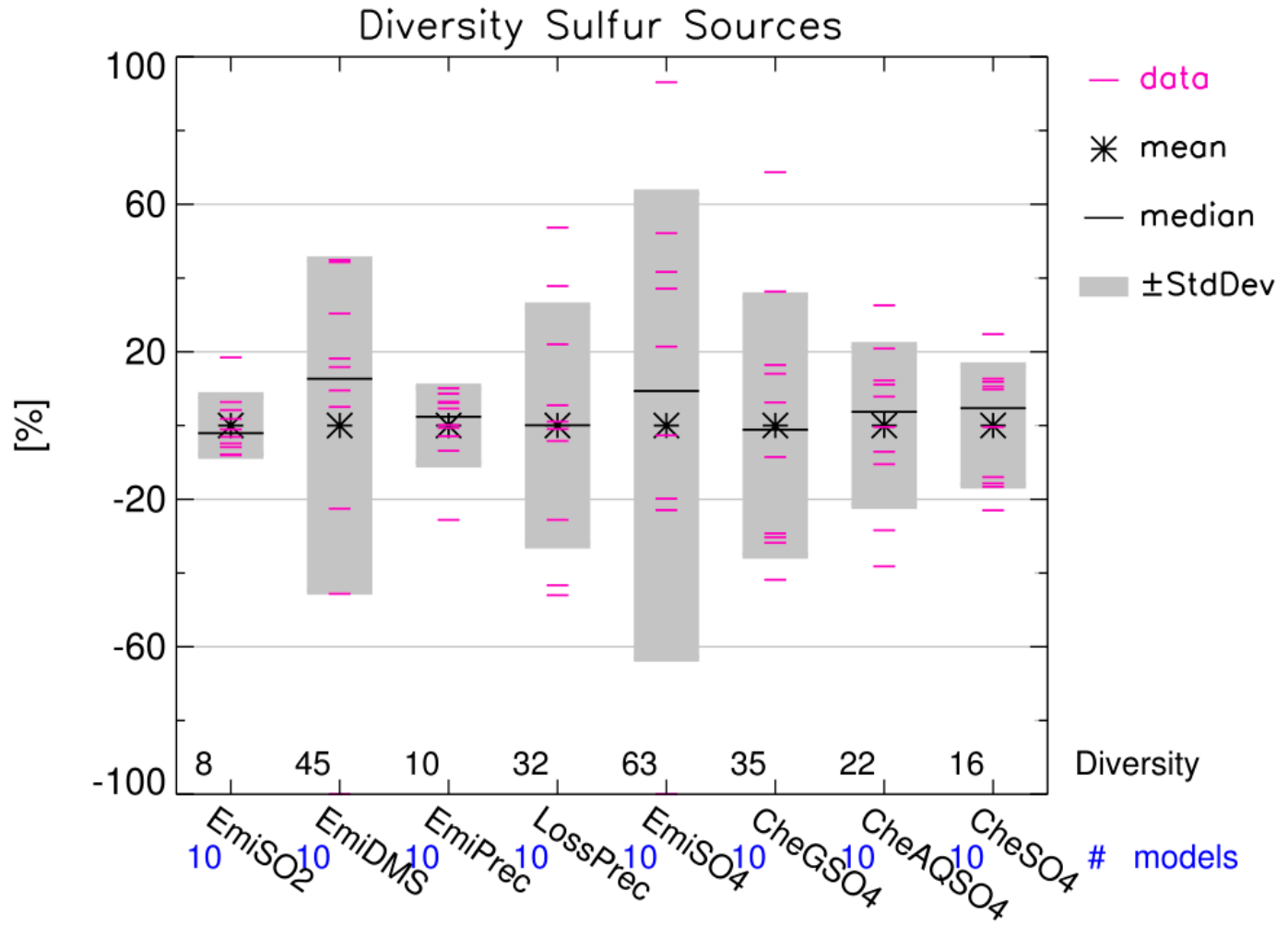
**All models:** sulfur cycle with homogeneous and heterogeneous chemistry

**Some models:** detailed inorganic chemistry, ammonium / nitrate system

**Few models:** secondary organic aerosol formation

# Aerosol Sources in Modells

## Sulfur cycle in AeroCom Phase I Experiment A:



## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

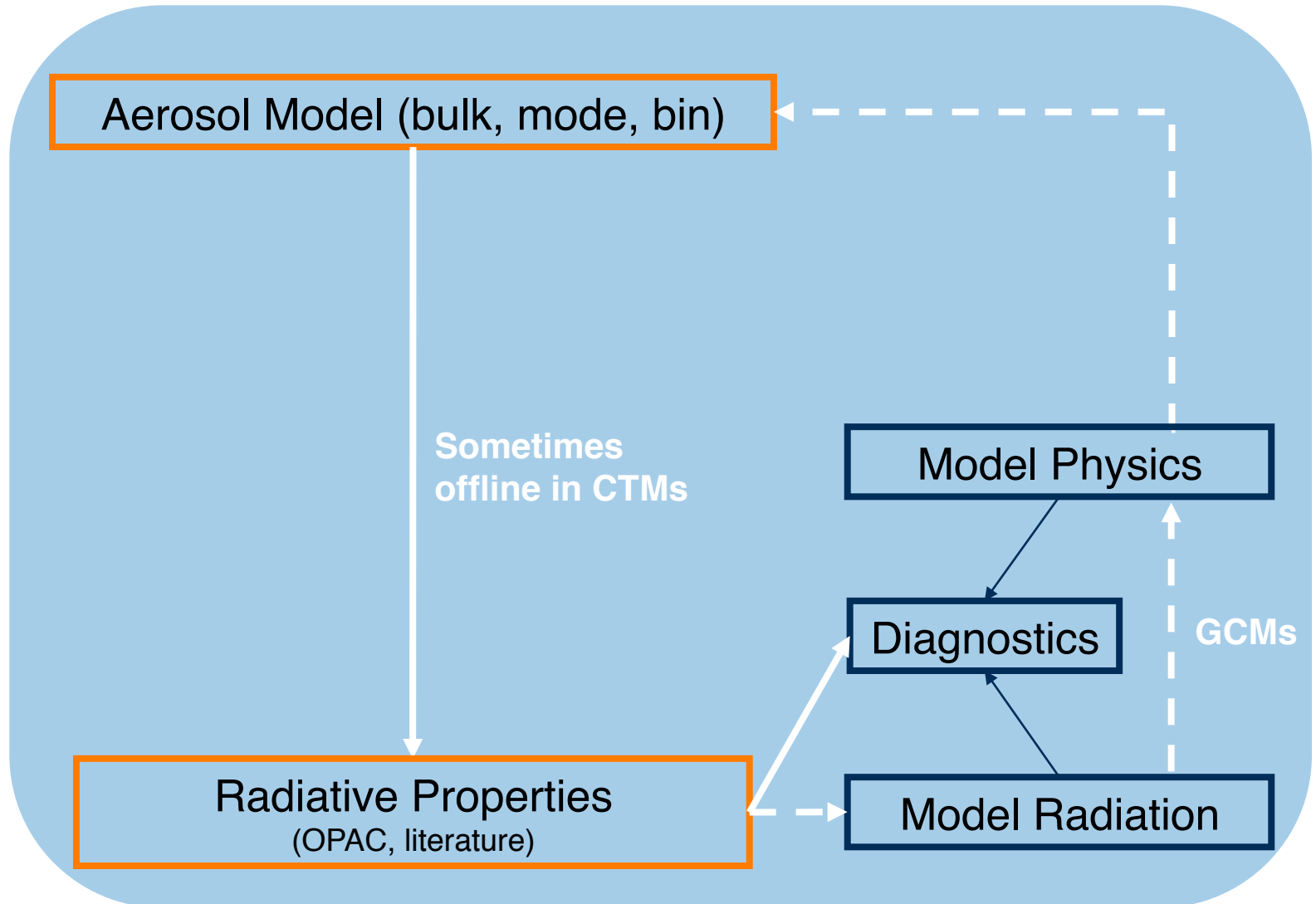
- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

## Removal

- Dry deposition & sedimentation
- Scavenging

# Aerosol Radiative Properties

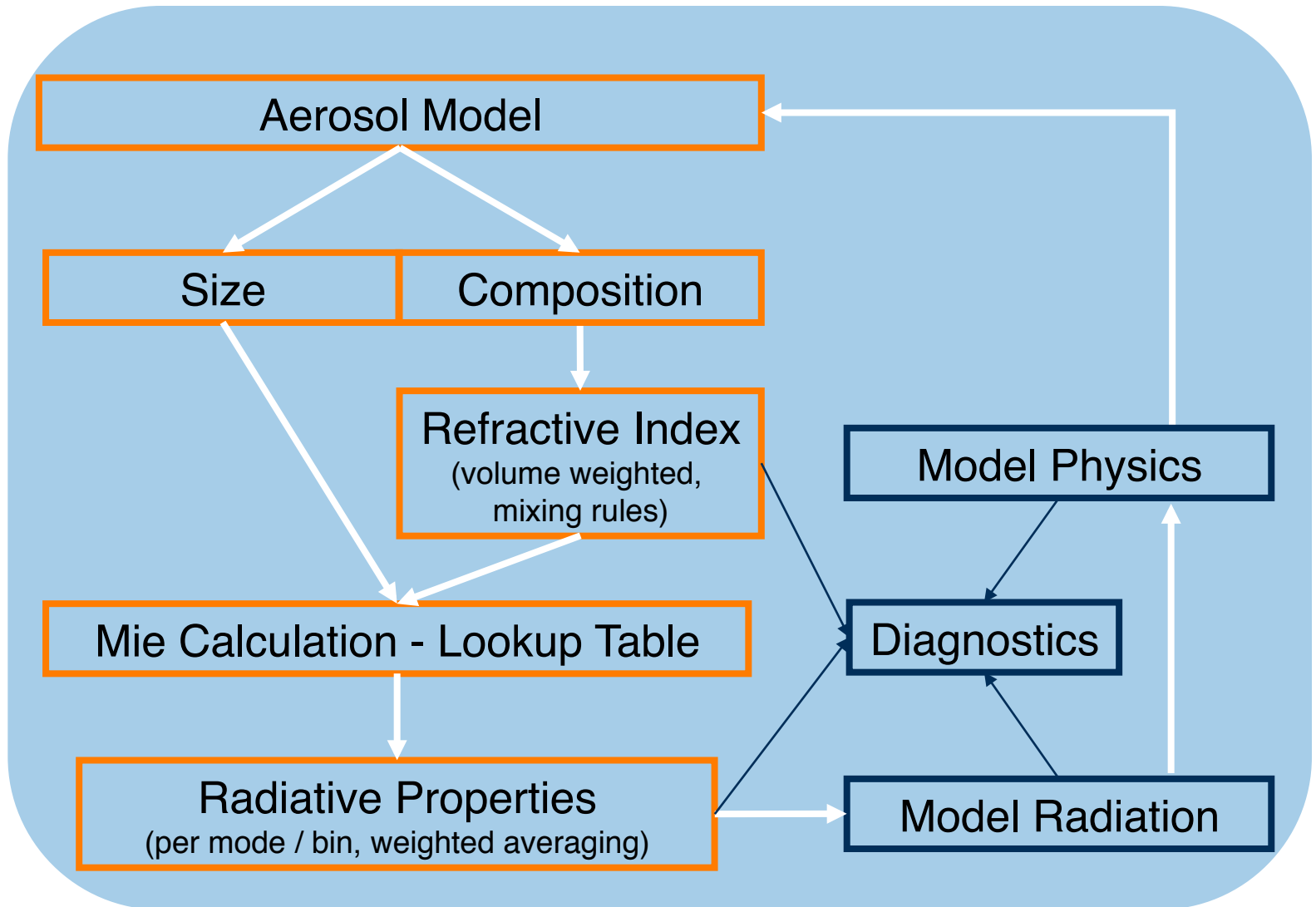
**Simple implementation** (not uncommon in CTMs and some GCMs):





# Aerosol Radiative Properties

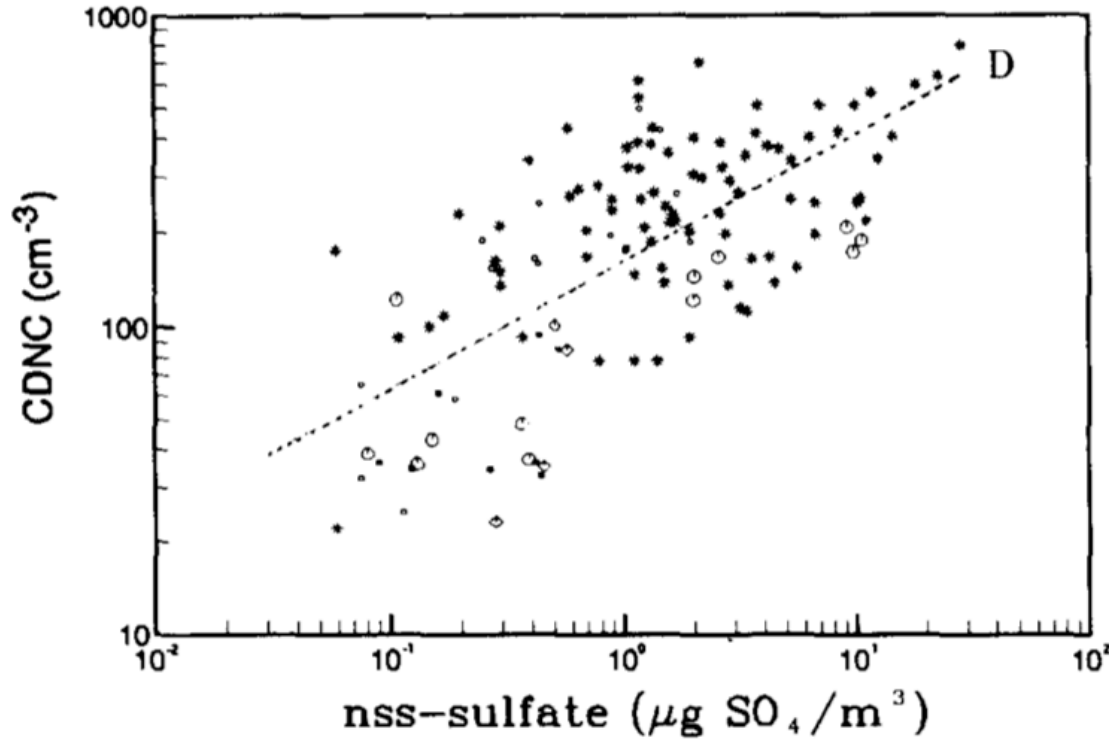
**Complex implementation** (or simplifications thereof):



# Aerosol-Cloud Coupling

## Aerosol activation

i) Highly empirical:



Boucher and Lohmann (1995)

# Aerosol-Cloud Coupling

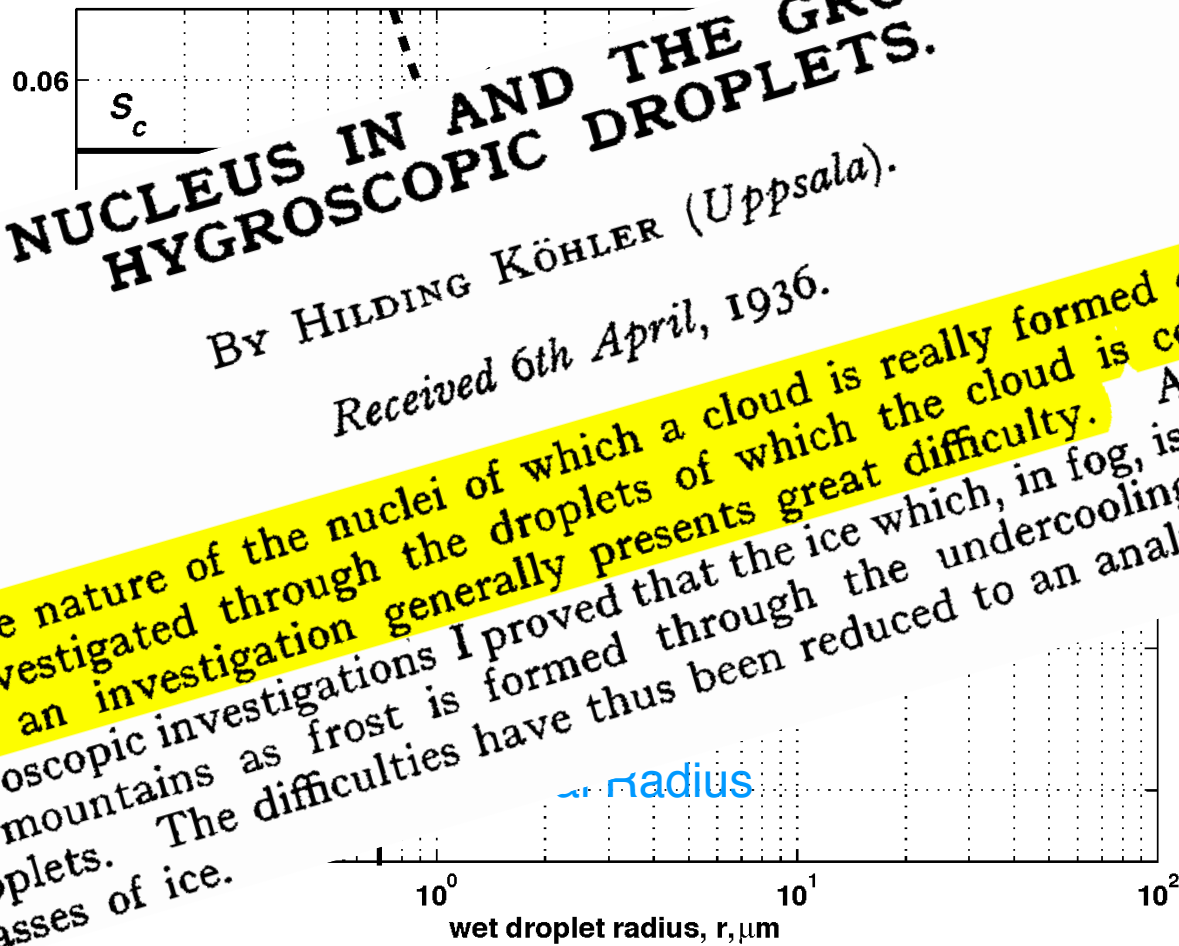
ii) Köhler (1936) based – Combining Raoult's Law and Kelvin Equation:

$$e_S^{sol}(r) = e_S(\infty) \left( 1 - \frac{B}{r^3} \right) \left( e^{\frac{A}{r}} \right)$$

**THE NUCLEUS IN AND THE GROWTH OF HYGROSCOPIC DROPLETS.**

BY HILDING KÖHLER (Uppsala).  
Received 6th April, 1936.

The nature of the nuclei of which a cloud is really formed can best be investigated through the droplets of which the cloud is composed. Such an investigation generally presents great difficulty. After long microscopic investigations I proved that the ice which, in fog, is deposited on mountains as frost is formed through the undercooling of water droplets. The difficulties have thus been reduced to an analysis of such masses of ice.



# Aerosol-Cloud Coupling

## Difficulty?

Caveat: Estimation of maximum supersaturation

$$\frac{dS}{dt} = \alpha V - \gamma \frac{dW}{dt} \quad \text{where}$$

$$\frac{dW}{dt} = 4\pi\rho_w GS \int \left( r^2(\tau) + 2G \int_{\tau}^{t_{max}} S(t) dt \right)^{1/2} n(S') dS'$$

## Solutions to supersaturation balance equation:

- i) Empirical fit to detailed parcel model (Abdul-Razzak and Ghan, 2000)
- ii) Population splitting allows to minimise empirical contributions:  
(Nenes & Seinfeld, 2003; Barahona et al., 2010)

Caveats: updraft velocity is sub-grid scale and not prognostic in mass-flux based convection schemes. Diagnosed from prognostic variables e.g. via TKE.

Interested? Posters by Rosalind West and Steve Ghan

# Aerosol-Cloud Coupling

## Coupling to cloud microphysics:

i) Two moment cloud microphysics schemes:

$$\frac{\partial N}{\partial t} = \frac{DN^{act}}{Dt} + \left(\frac{\partial N}{\partial t}\right)^{Transport} + \left(\frac{\partial N}{\partial t}\right)^{Sources} + \left(\frac{\partial N}{\partial t}\right)^{Sinks}$$

$$\frac{\partial M}{\partial t} = \frac{DM^{cond}}{Dt} + \left(\frac{\partial M}{\partial t}\right)^{Transport} + \left(\frac{\partial M}{\partial t}\right)^{Sources} + \left(\frac{\partial M}{\partial t}\right)^{Sinks}$$

directly coupled to cloud radiative properties and precipitation scheme

ii) Single moment (bulk) cloud microphysics schemes

**Caveat:**

Diagnostic calculation of  $r_{eff}$  from  $N^{act}$  and M

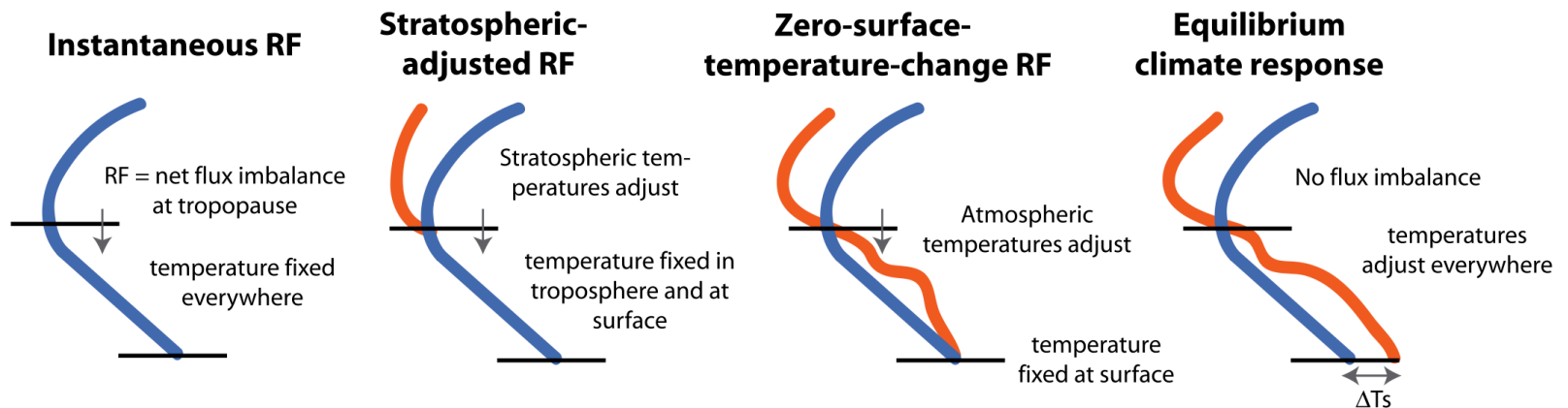
No or highly parameterised effects on precipitation

Lack of reliable evaluation data...

# Aerosol Radiative Effects

## Radiative Forcing

“the change in net (down minus up) irradiance (solar plus longwave; in  $W m^{-2}$ ) at the tropopause after allowing for stratospheric temperatures to readjust to radiative equilibrium, but with surface and tropospheric temperatures and state held fixed at the unperturbed values”



(IPCC, Forster et al., 2007)

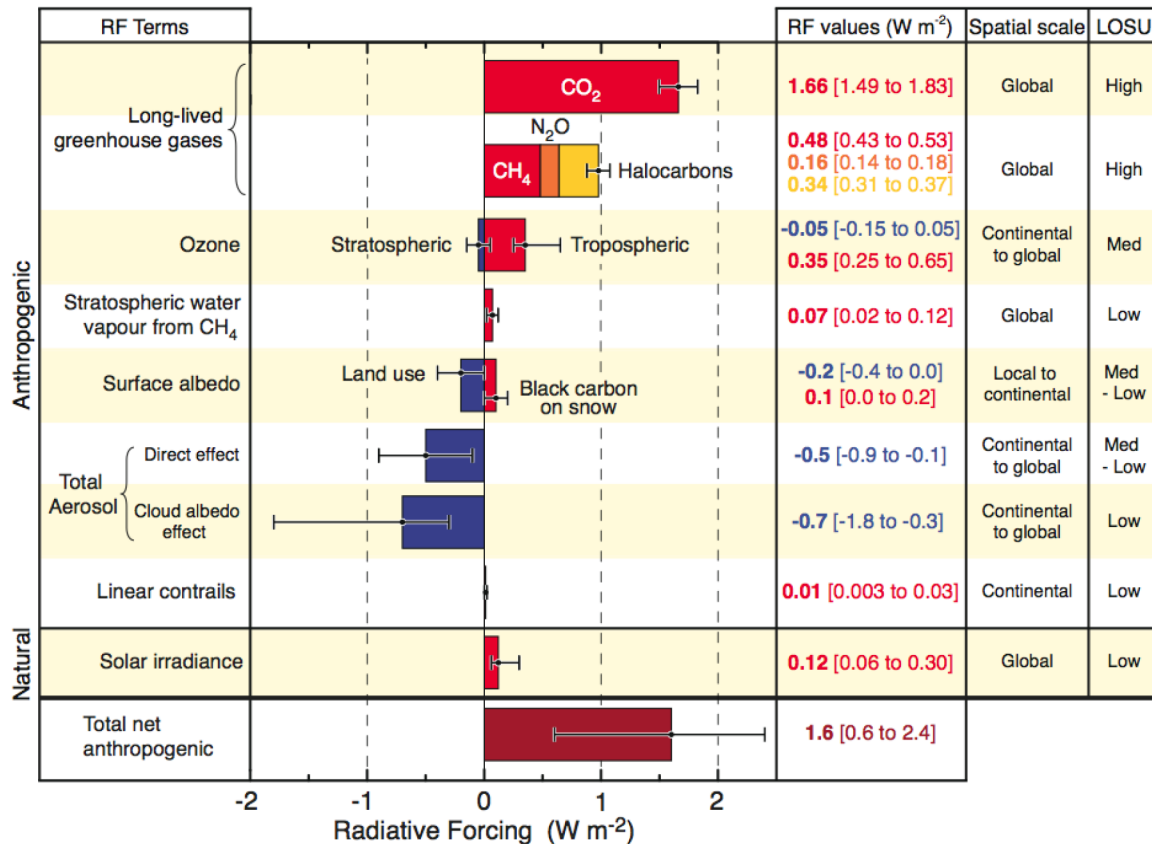
**Caveat:**

Instantaneous definition excludes (fast) cloud-lifetime and dynamical effects

# Anthropogenic Perturbations to the Climate System

Current best estimate of anthropogenic radiative forcing:

Radiative Forcing Components



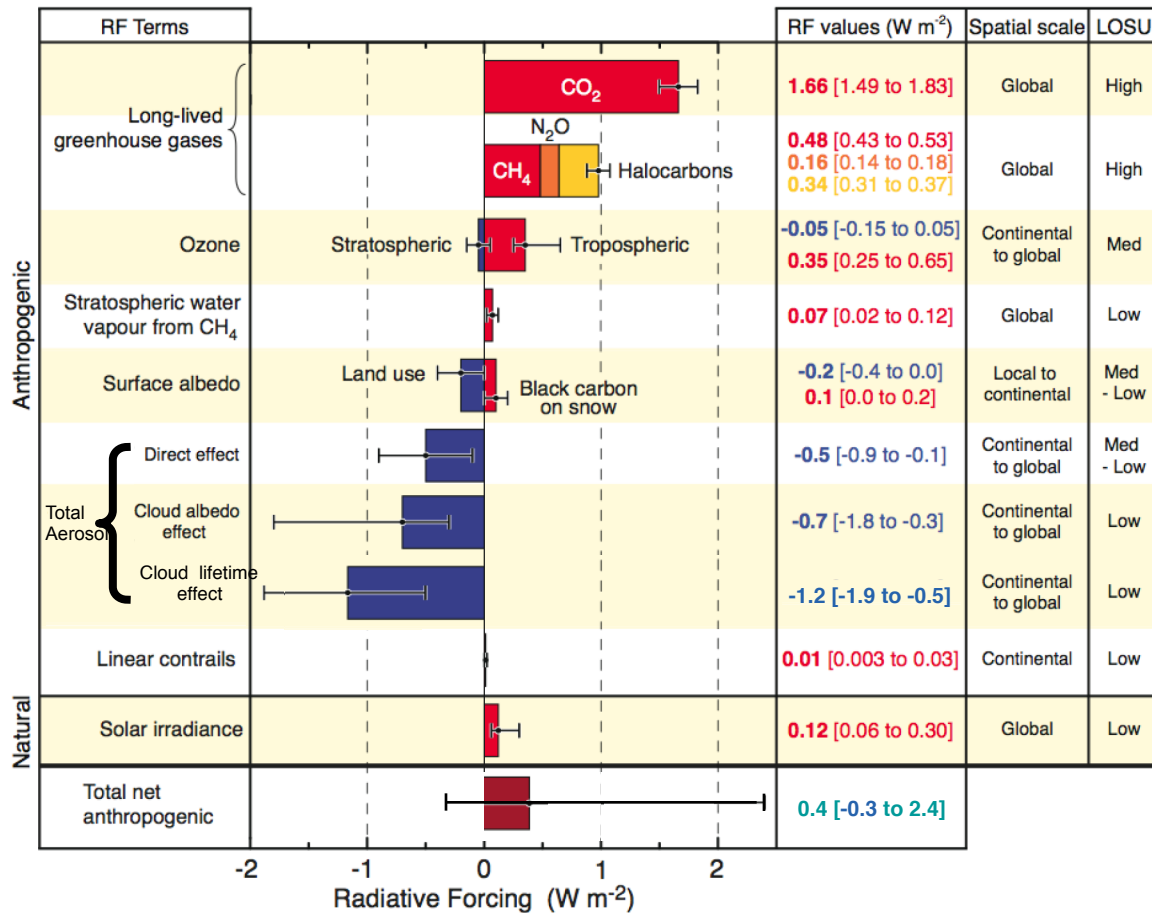
©IPCC 2007: WG1-AR4

Intergovernmental Panel on Climate Change estimate of present day global annual mean anthropogenic radiative forcings (Solomon et al., 2007)

# Anthropogenic Perturbations to the Climate System

Including (fast) cloud-lifetime effect:

## Radiative Forcing Components



Lohmann & Feichter (2005)



## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

## Removal

- Dry deposition & sedimentation
- Scavenging

# Aerosol Removal Processes

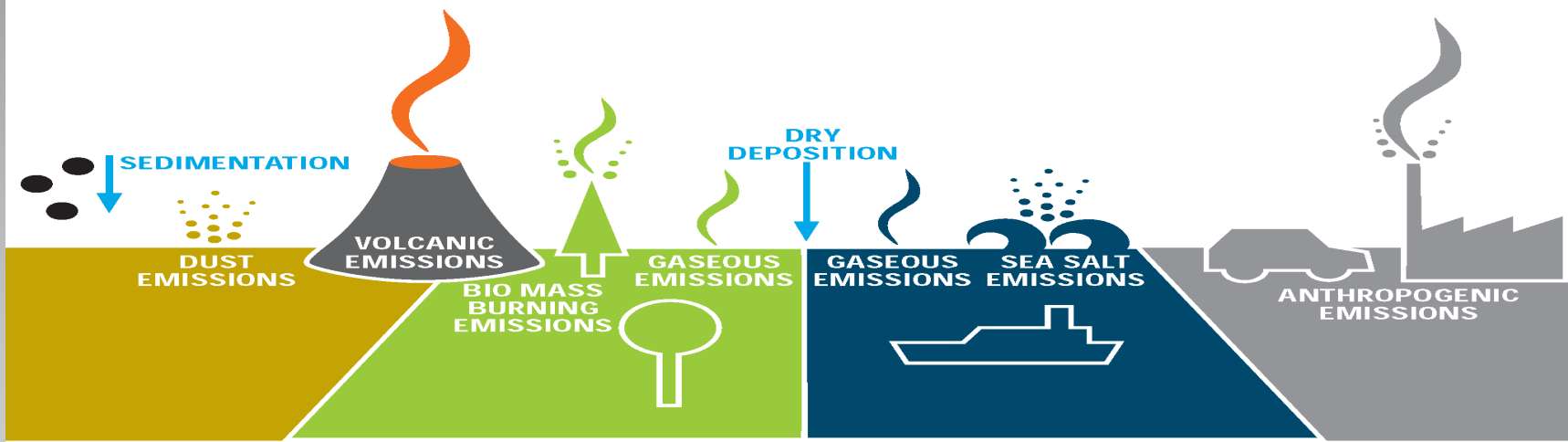
## Dry Deposition

Most models use classical serial resistance approach:

$$F_d = C \rho_{air} v_d \quad v_d = v_g + \frac{1}{(r_a + r_s)}$$

Caveats:

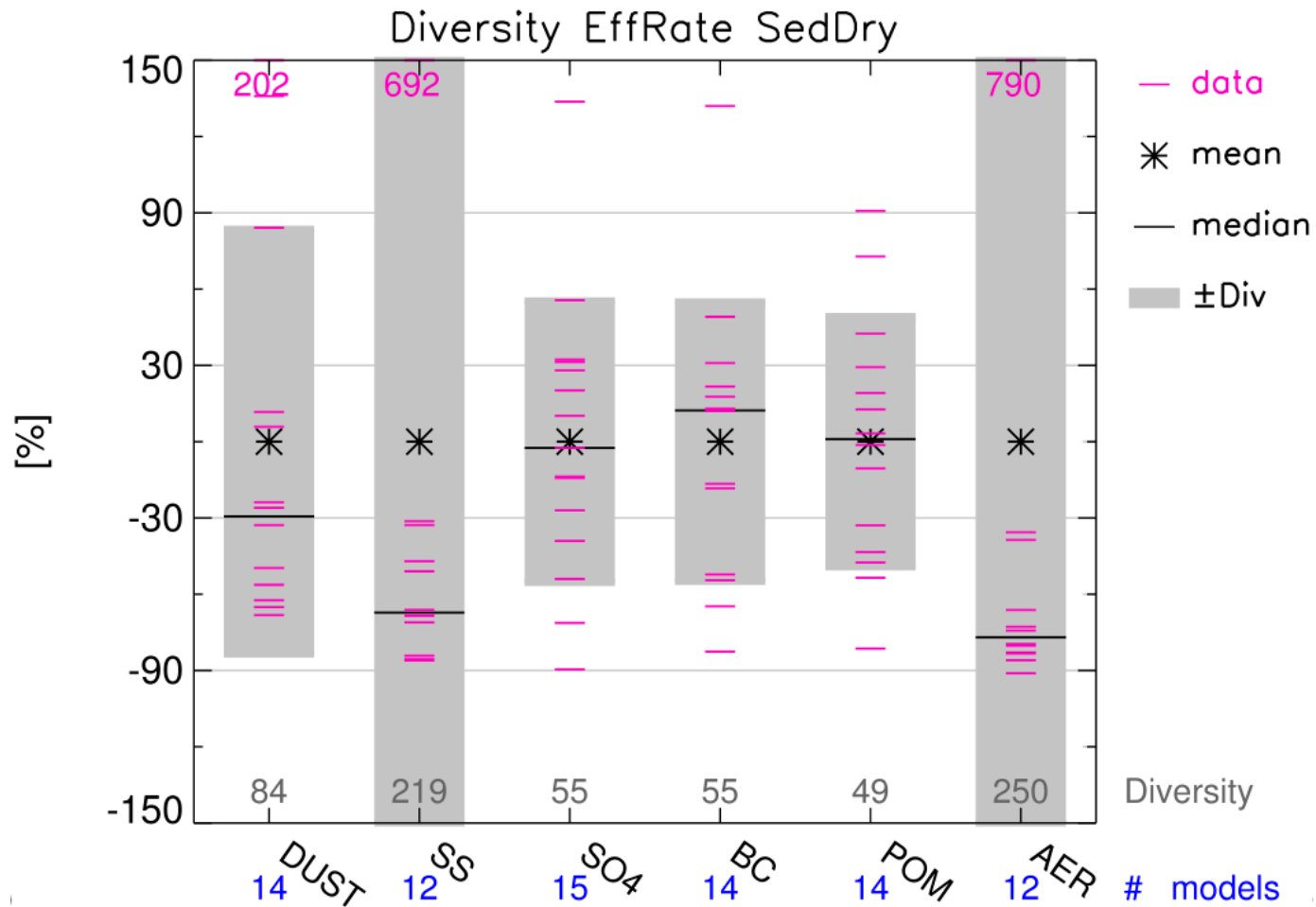
- i) Surface resistance terms are uncertain and land-type specific. Only few models consider explicit mosaic approach.
- ii) Aerodynamic resistance is dependent on turbulent transport in the boundary layer – difficult to simulate with few layers, expensive with many layers



# Aerosol Removal Processes

## Dry Deposition

Diversity of effective total dry deposition rate coefficients in AeroCom Phase I:

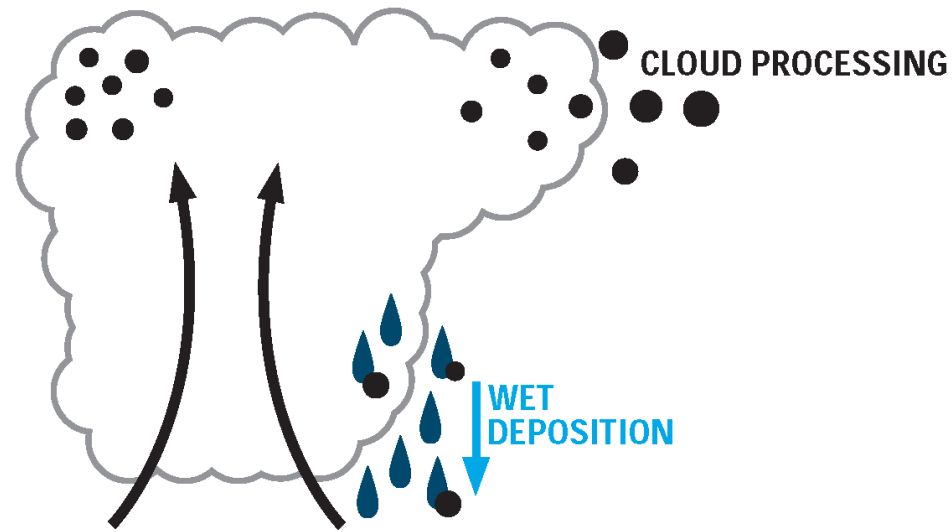


# Aerosol Removal Processes

## Caveat: Wet Deposition

Convolution of difficult (sub-grid scale) processes:

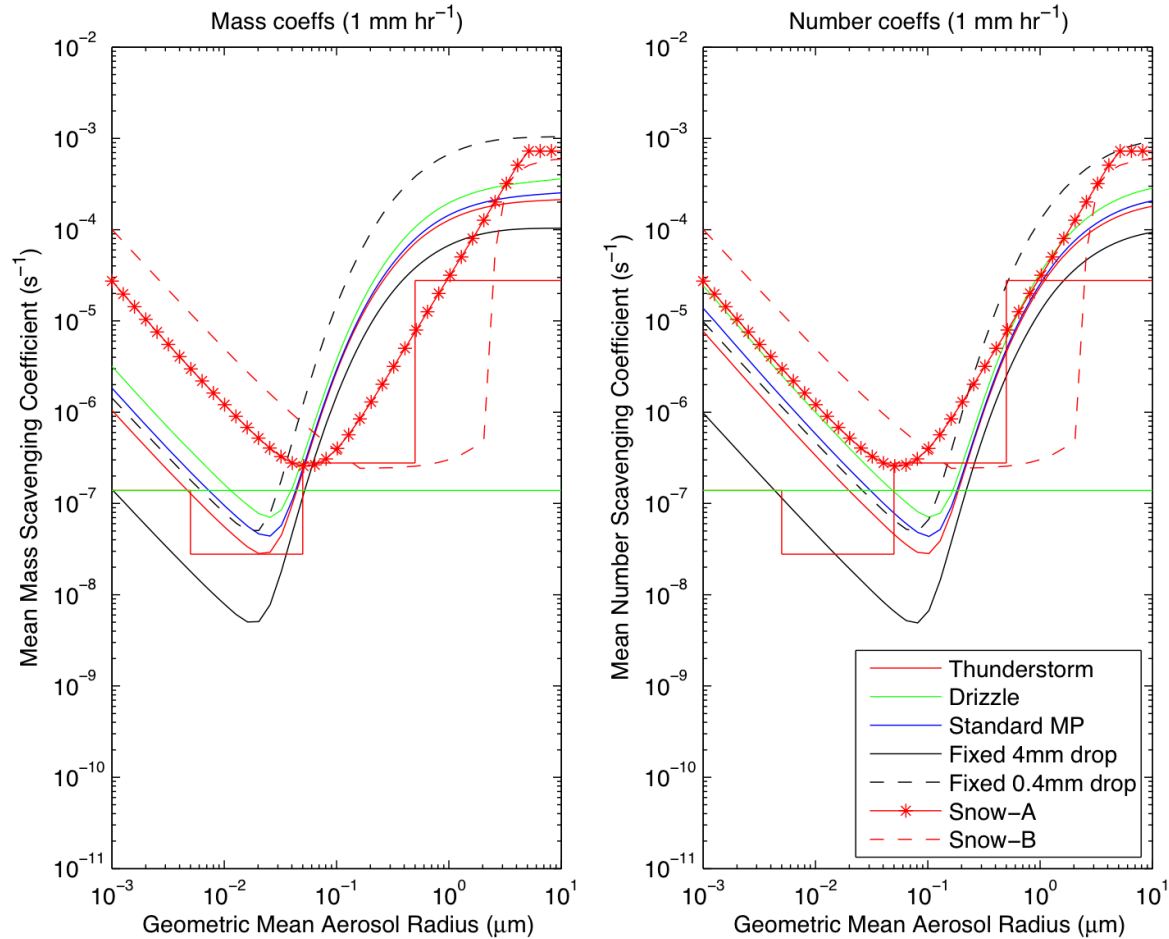
- i) Cloud microphysics not existent (CTMs) or of limited complexity (GCMs)
- ii) Simulated precipitation in GCMs is imperfect
- iii) Uptake processes are difficult (water) or insufficiently (ice) understood
- iv) Cloud cycling and evaporation often ignored



# Aerosol Removal Processes

## Caveat: Wet Deposition

Impaction scavenging coefficients from explicit calculation

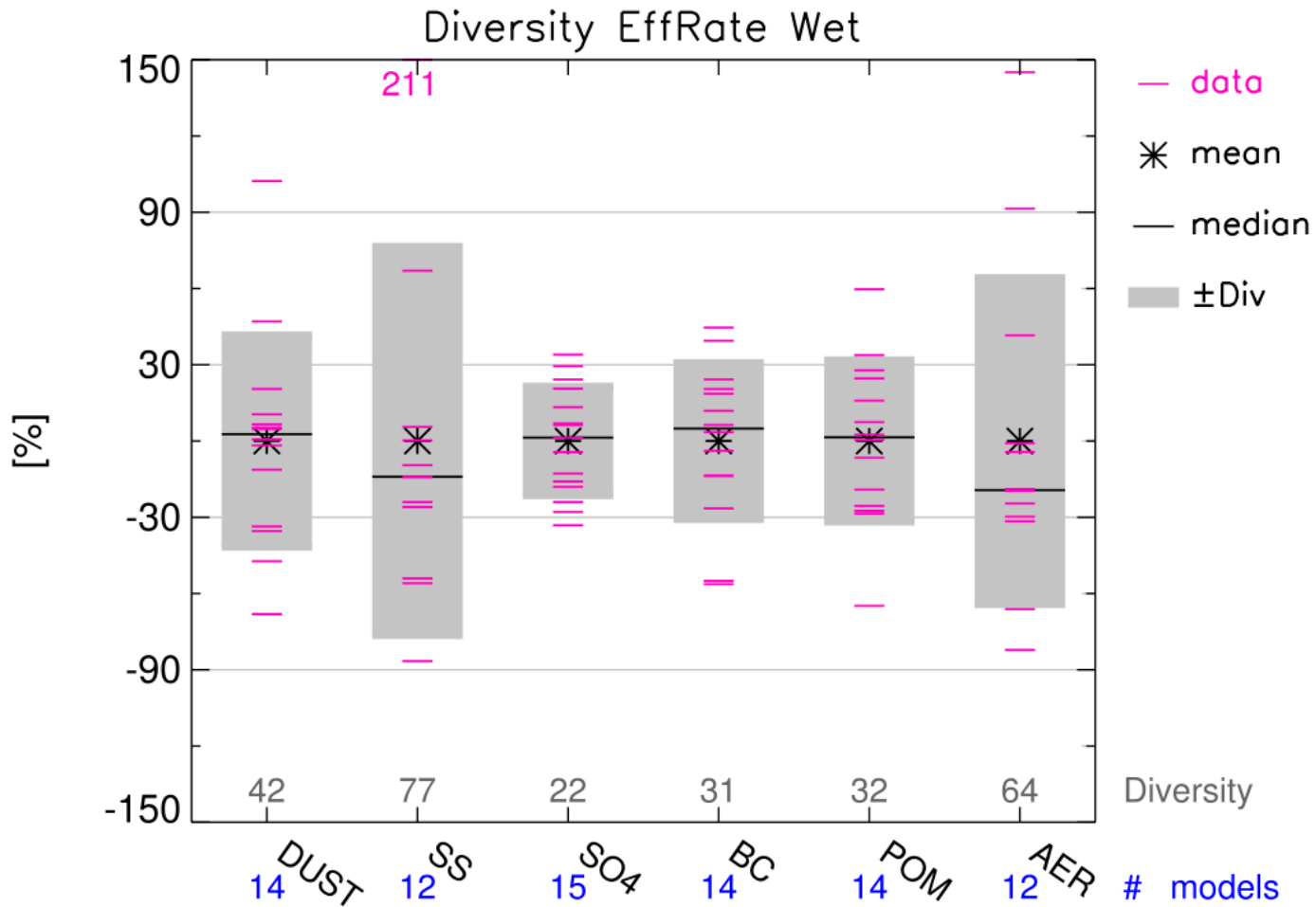


Croft et al,  
(2009)

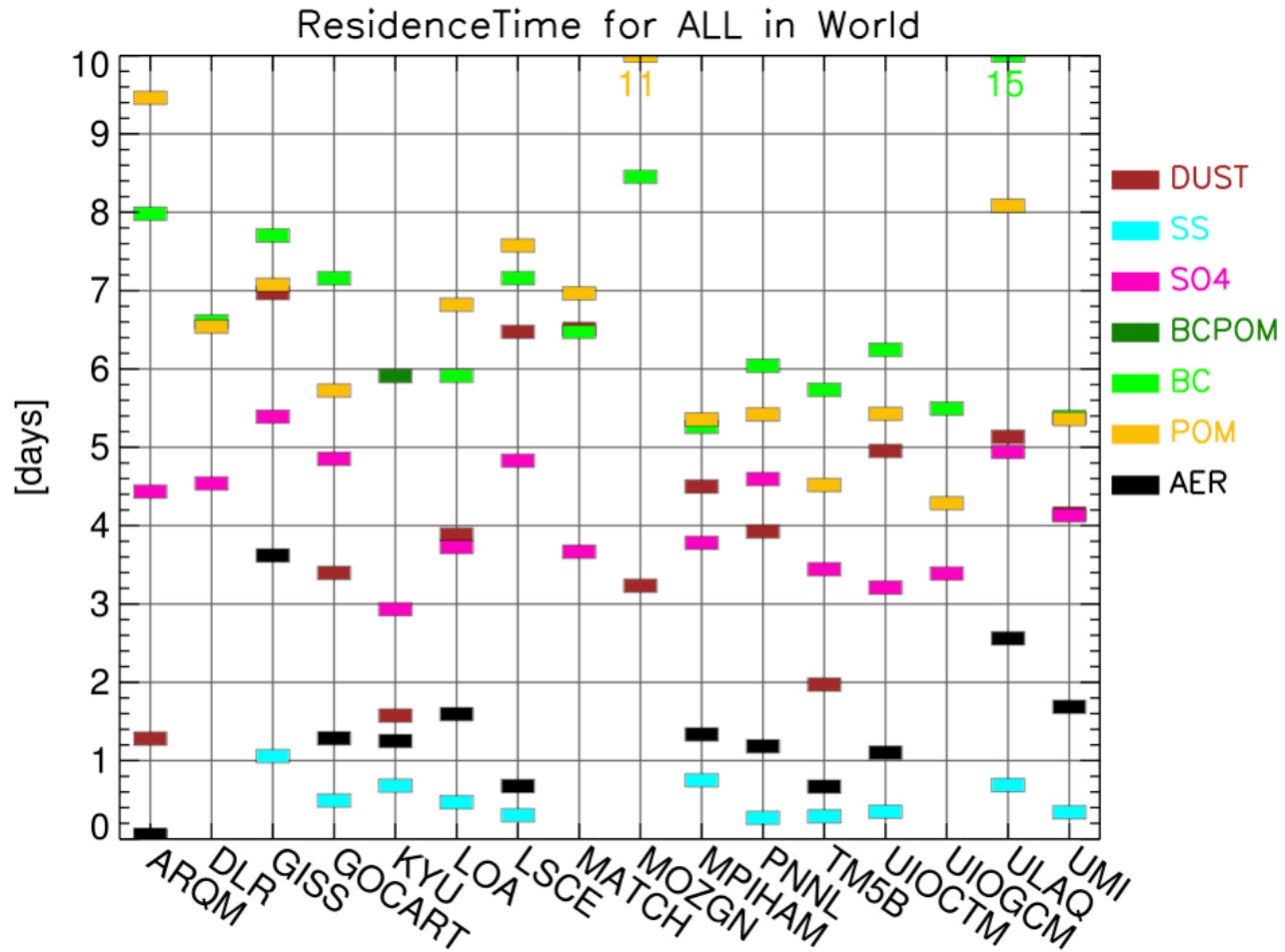
Difficult to approximate with simple aerosol representations

# Aerosol Removal Processes

## Caveat: Wet Deposition



# Aerosol Residence Time



Textor et al. (2006)

## Host Models

- Box-, Parcel-, Single Column-, Chemical Transport-, Regional Circulation-, Global Circulation Models
- Offline, Online, Nudged, AMIP, Climate Simulations
- Resolution, resolved and unresolved processes – parameterisations

## Aerosol Models

- Bulk Models
- Moment-Based
- Sectional Models

## Sources

- Primary emission
- Secondary formation

## Transport

- Advection, Turbulence, Convection

## Effects

- Radiative Properties
- Aerosol activation and ice nucleation
- Radiative “effect”, “forcing”, “feedback”

## Removal

- Dry deposition & sedimentation
- Scavenging