

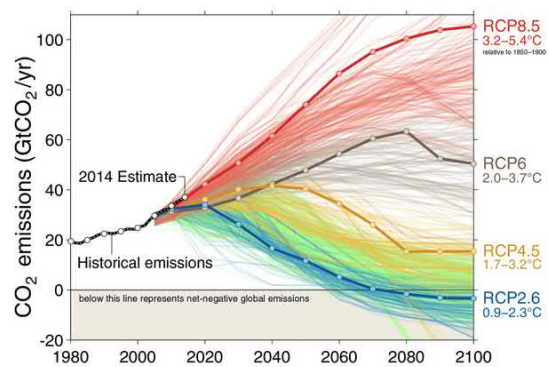
# Earth System Modelling and specific challenges

**Risto Makkonen**  
Finnish Meteorological Institute  
and University of Helsinki

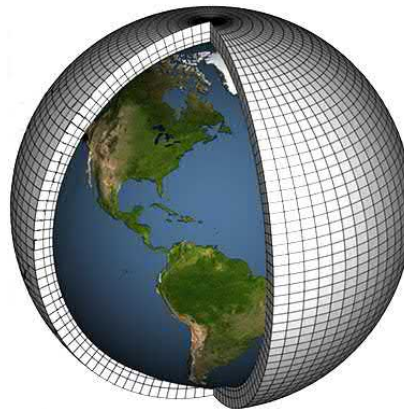
MEGAPOLIS 2021



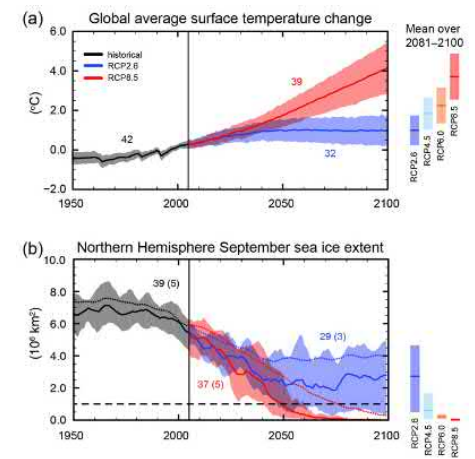
## Input (e.g. greenhouse gas emission)



## Earth System Model



## Climate prediction

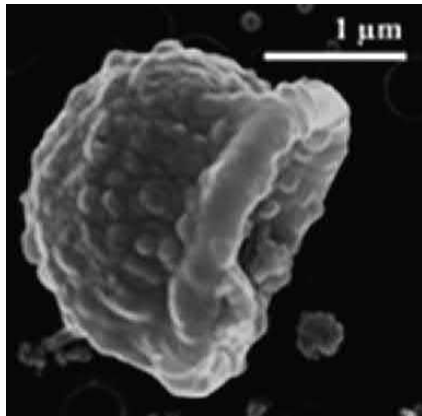




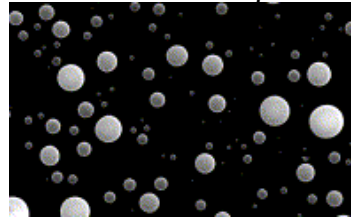
# What are atmospheric aerosols?

*Solid or liquid particles suspended in air*

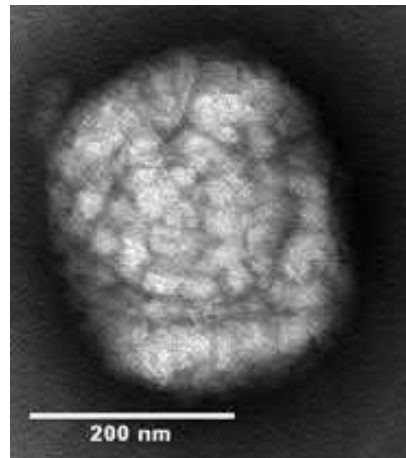
Spores



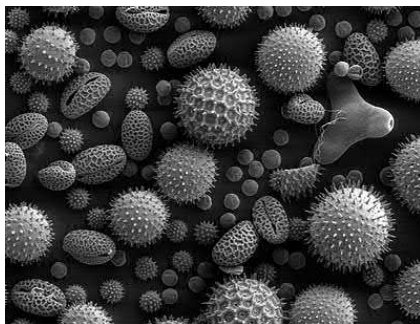
$\text{NaNO}_3$



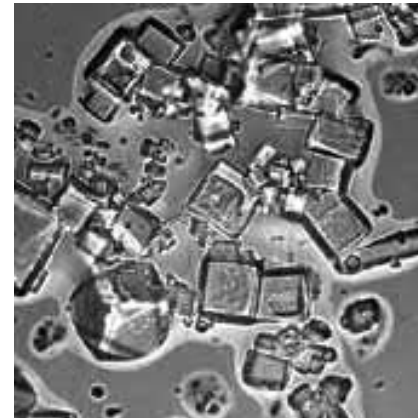
Virus



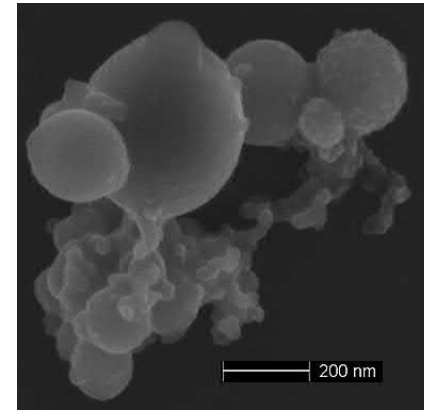
Pollen



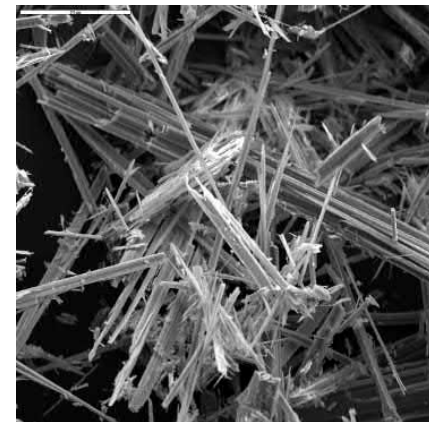
Sea salt



Wood smoke

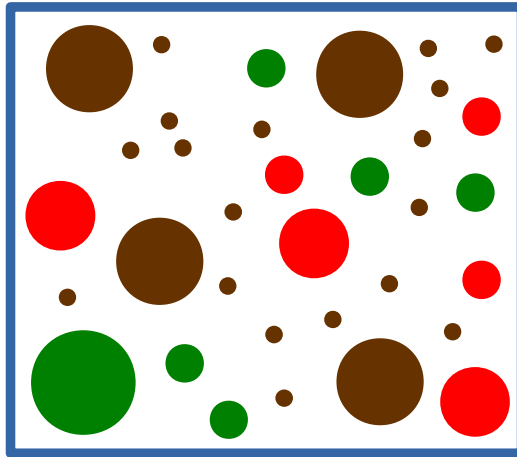


Fibres



**Urban  
atmosphere**

Aerosol number conc.  $10^4$ - $10^8$  # /cm<sup>3</sup>  
Aerosol mass 10-200  $\mu\text{g} / \text{m}^3$

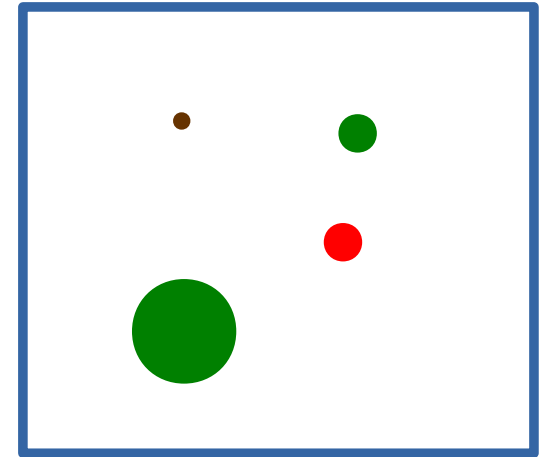


Aerosols  
reduce  
visibility



**Remote  
atmosphere**

even  $< 50$  # /cm<sup>3</sup>  
 $< 1 \mu\text{g} / \text{m}^3$



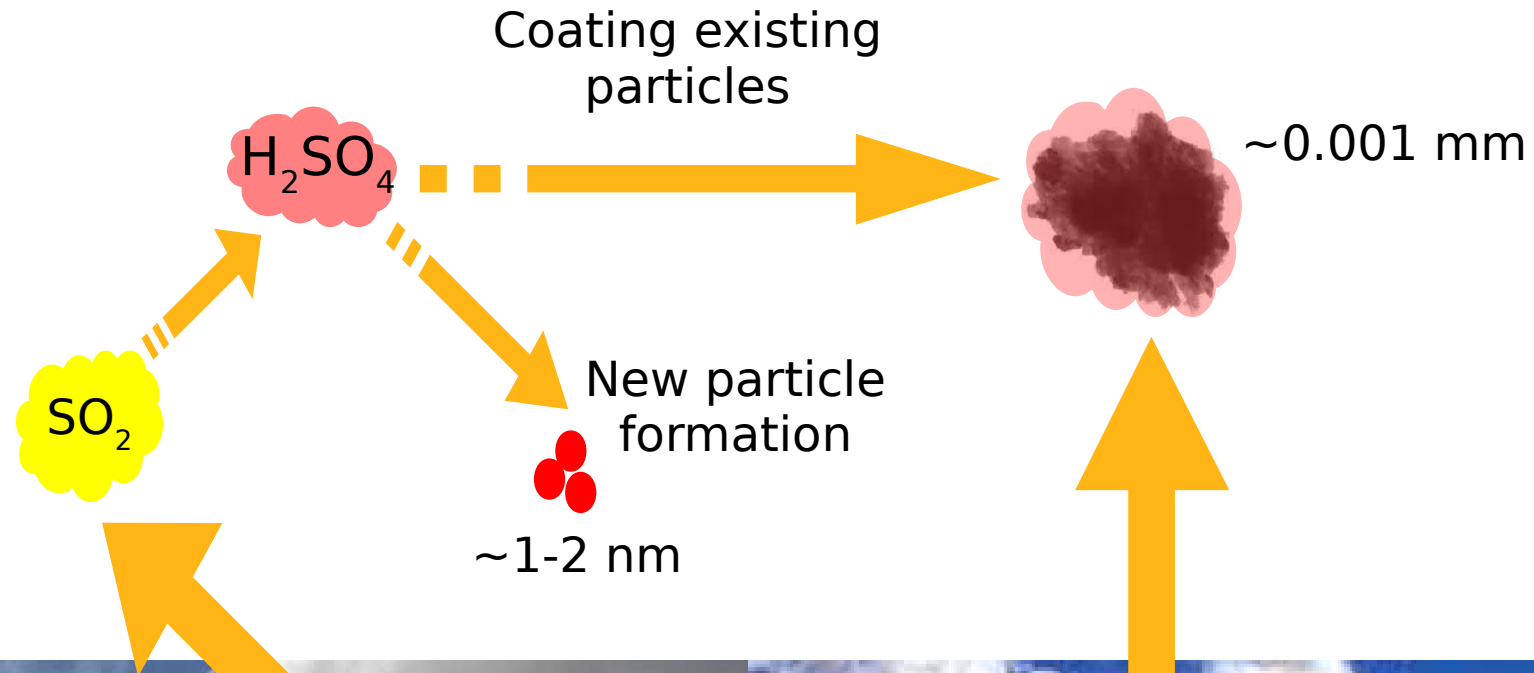
# How do aerosols enter the atmosphere?

Example: wind-blown dust



# How do aerosols enter the atmosphere?

Example: wind-blown dust and secondary formation from sulfur dioxide

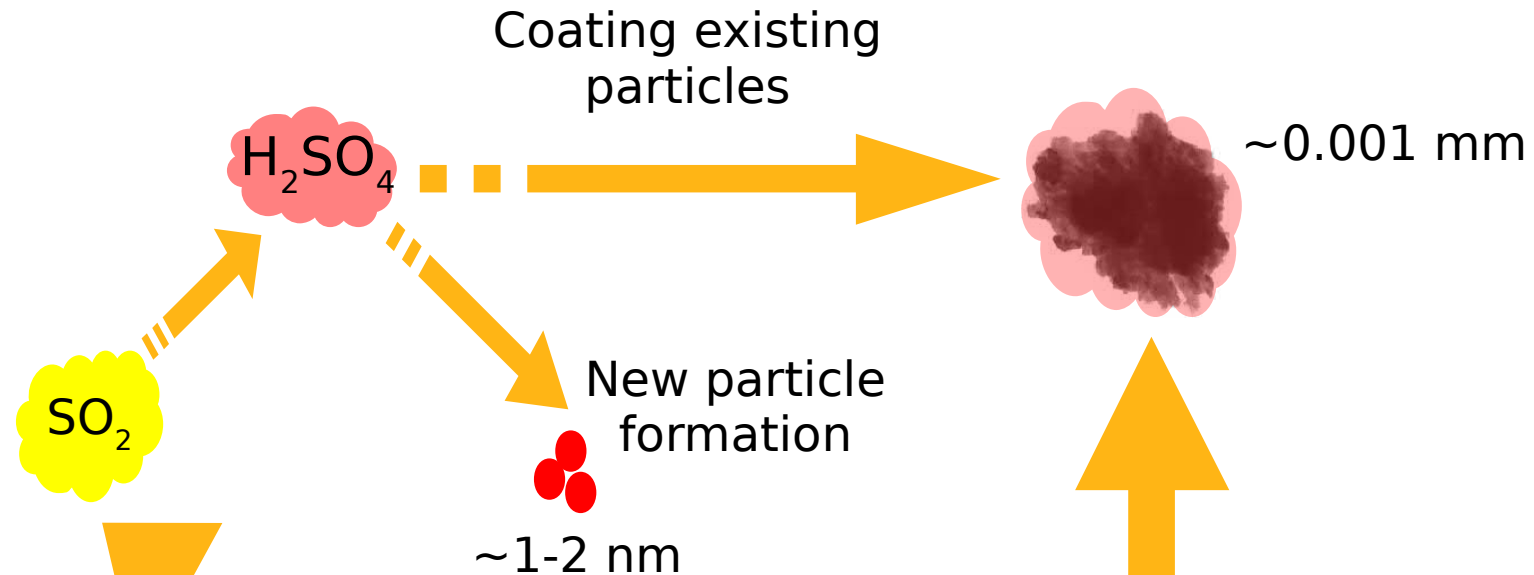


Secondary aerosol formation

Primary emission

# How do aerosols enter the atmosphere?

Example: wind-blown dust and secondary formation from sulfur dioxide



Secondary aerosol formation

Secondary aerosol

Primary emission

Primary aerosol

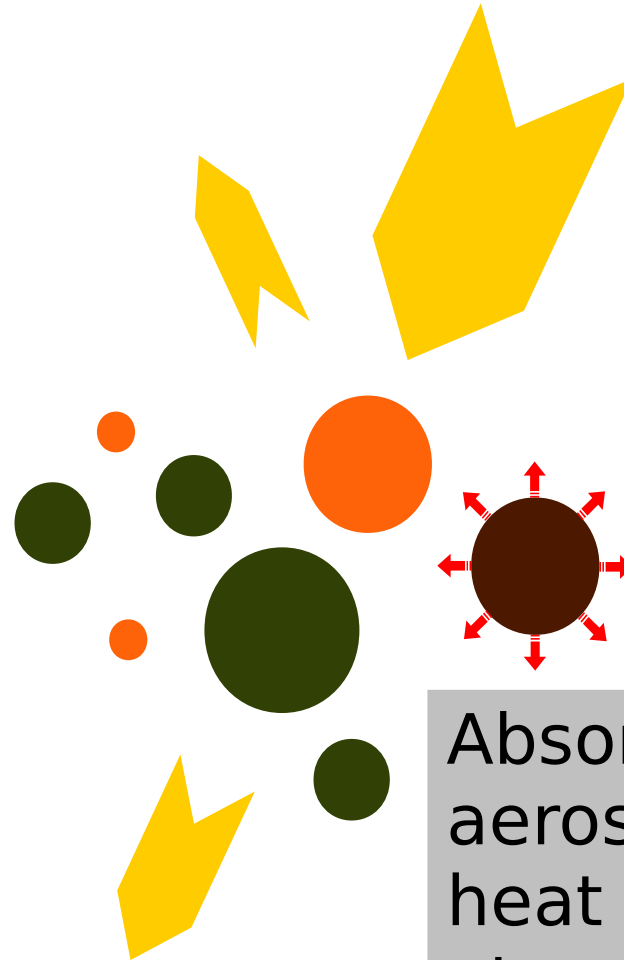
**Why would we want to include  
aerosols/chemistry in a climate model?**



# Aerosols reflect and absorb radiation



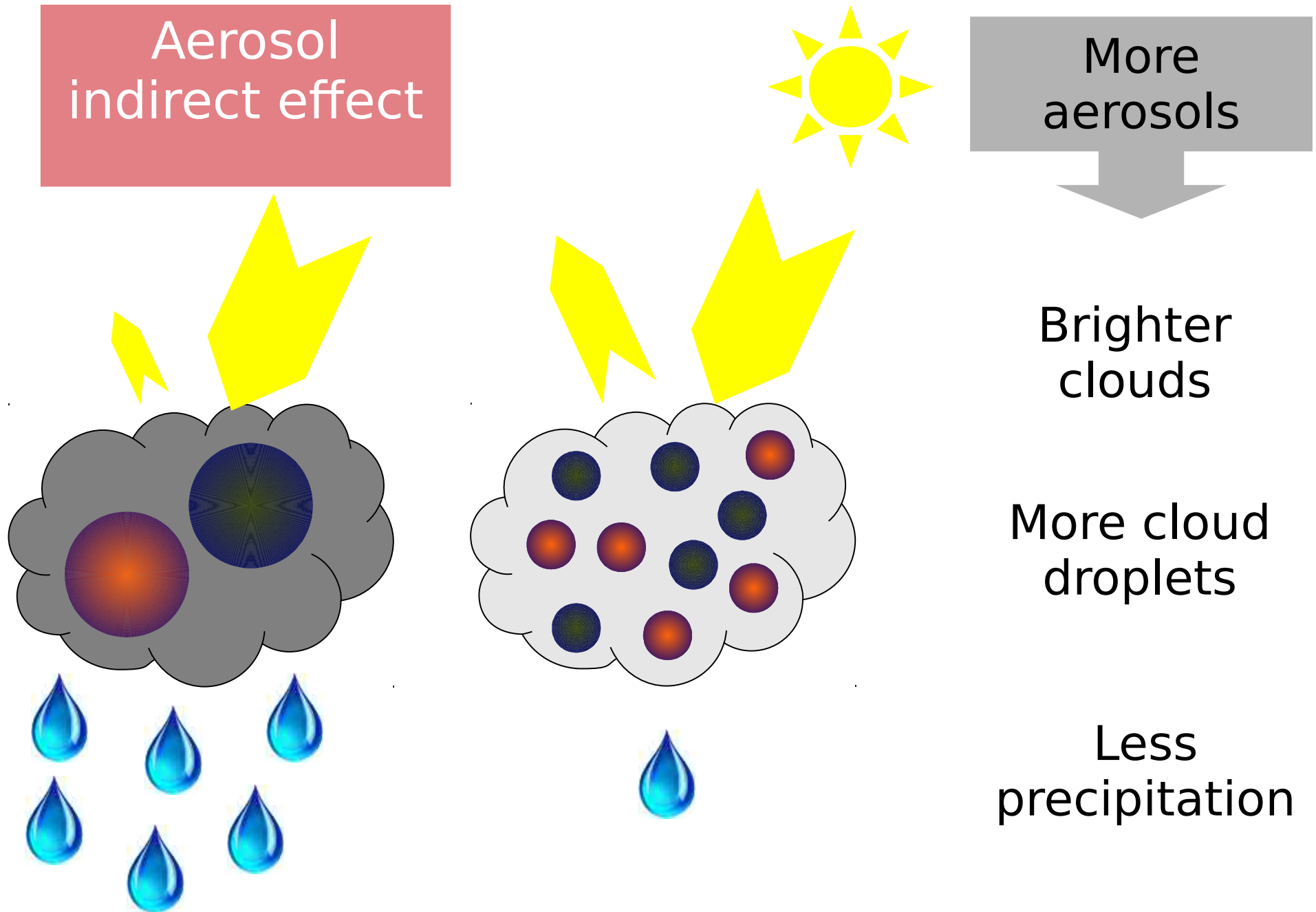
Aerosol direct  
effect



Absorbing  
aerosols  
heat the  
atmosphere

Aerosols reduce the  
radiation reaching the  
surface

# Aerosols act as cloud condensation nuclei



# Role of clouds in the atmosphere

**Radiation budget and climate:** Clouds reflect effectively incoming sunlight back to space. Similarly, clouds absorb and re-emit infrared radiation emitted by the Earth's surface

**Hydrological cycle:** Clouds turn water vapor into precipitating hydrometeors (rain drops, snow flakes, hail etc), thereby wetting land surfaces and filling rivers and lakes.

**Cleaning of the atmosphere:** Precipitating clouds scavenge both gaseous and particulate pollutants from the atmosphere

**Atmospheric chemistry:** Clouds serve as a medium for aqueous-phase chemical reactions. By this way, clouds influence the concentrations of many soluble trace gases and modify the chemical composition (and size) of atmospheric aerosol particles.

**Vertical transportation:** Vertical motion of air in the atmospheric is often associated with clouds. These include i) cycling of turbulent eddies in the boundary layer, ii) exchange of moisture, trace gases and aerosol particles between the boundary layer and free troposphere, iii) transportation material from the free troposphere to the stratosphere.

# Aerosols and clouds

In addition to making the existence of clouds possible, aerosol particle modify many cloud properties, including

**cloud albedo** (higher aerosol number concentrations make clouds more reflective)

**cloud lifetime** (many clouds live longer at higher aerosol concentrations)

**cloud precipitating efficiency** (aerosol particle may either suppress or accelerate precipitation)

**cloud formation probability** (large concentrations of absorbing aerosol may inhibit cloud formation altogether)



# Why add aerosols in Earth System / Climate models?

- Aerosol-radiation interactions
- Aerosol-cloud interactions
- Health effects
- Environmental effects
  - Deposition
  - Long-range nutrient dispersion
- Anthropogenic climate forcing
- Natural Earth System feedbacks via aerosols

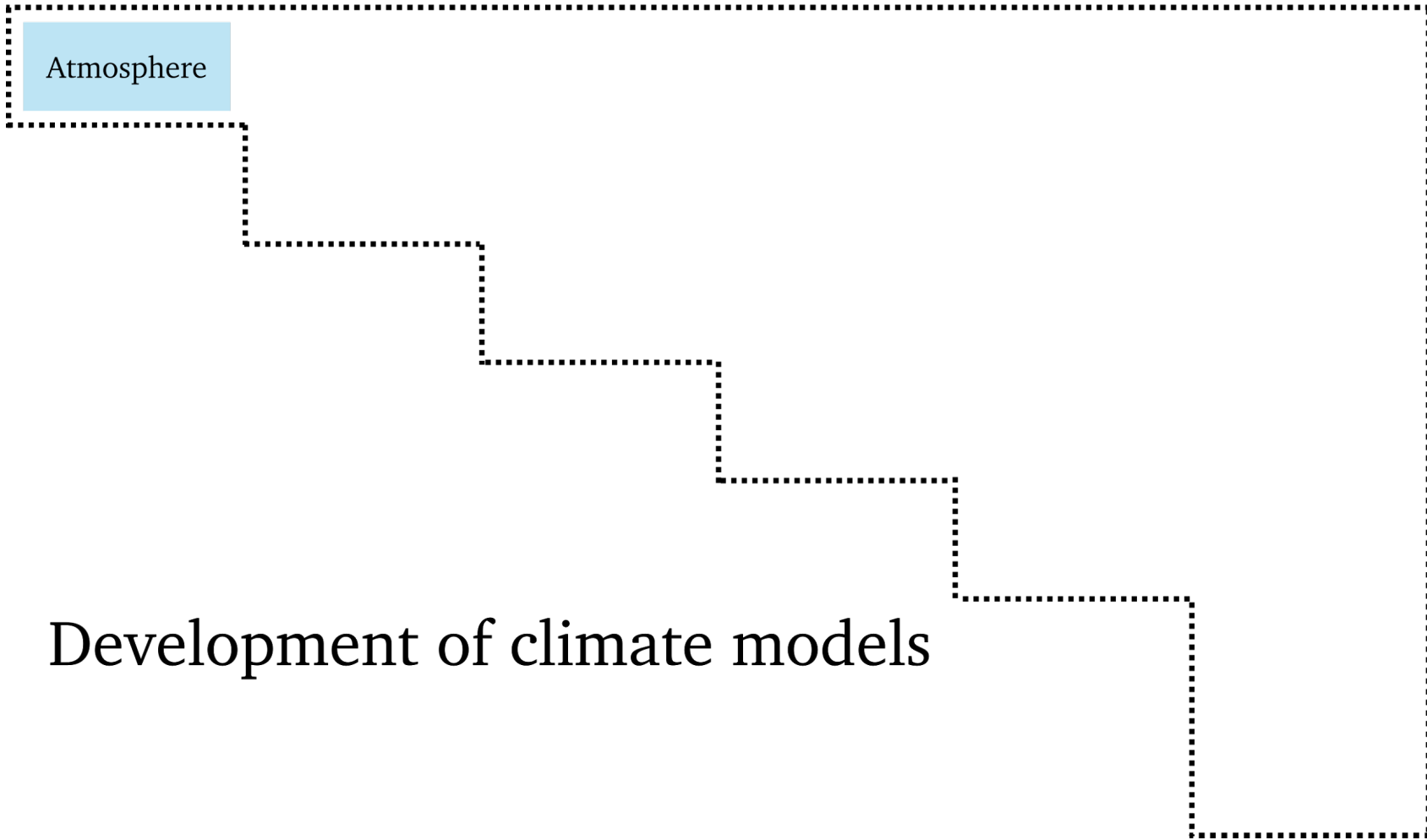


Development of climate models

1970s

Atmosphere

Development of climate models



1970s

1980s

Atmosphere

Atmosphere

Land surface

Sea and  
sea ice

Development of climate models





1970s

1980s

Early  
1990s

Atmosphere

Atmosphere

Atmosphere

Land surface

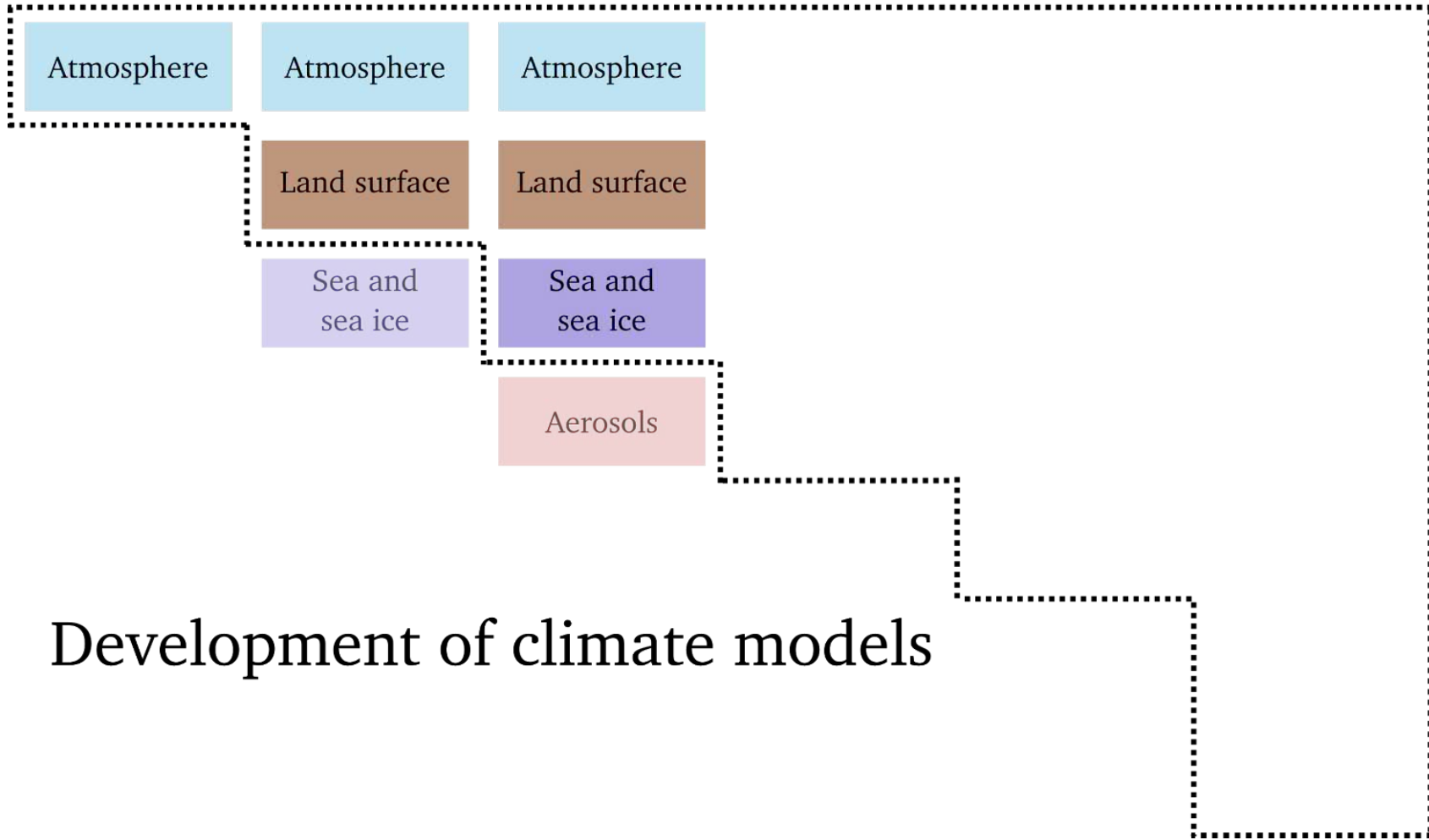
Land surface

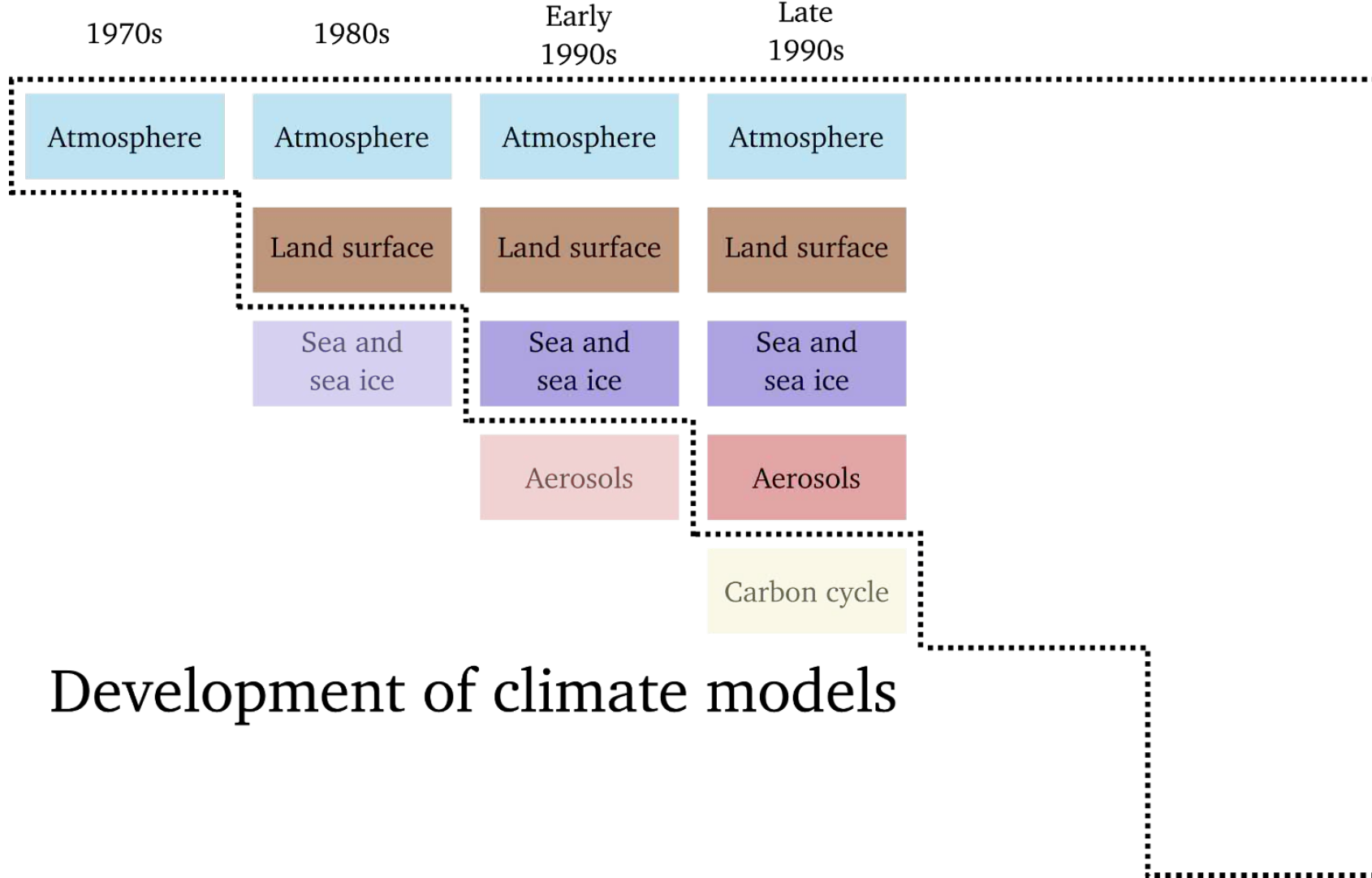
Sea and  
sea ice

Sea and  
sea ice

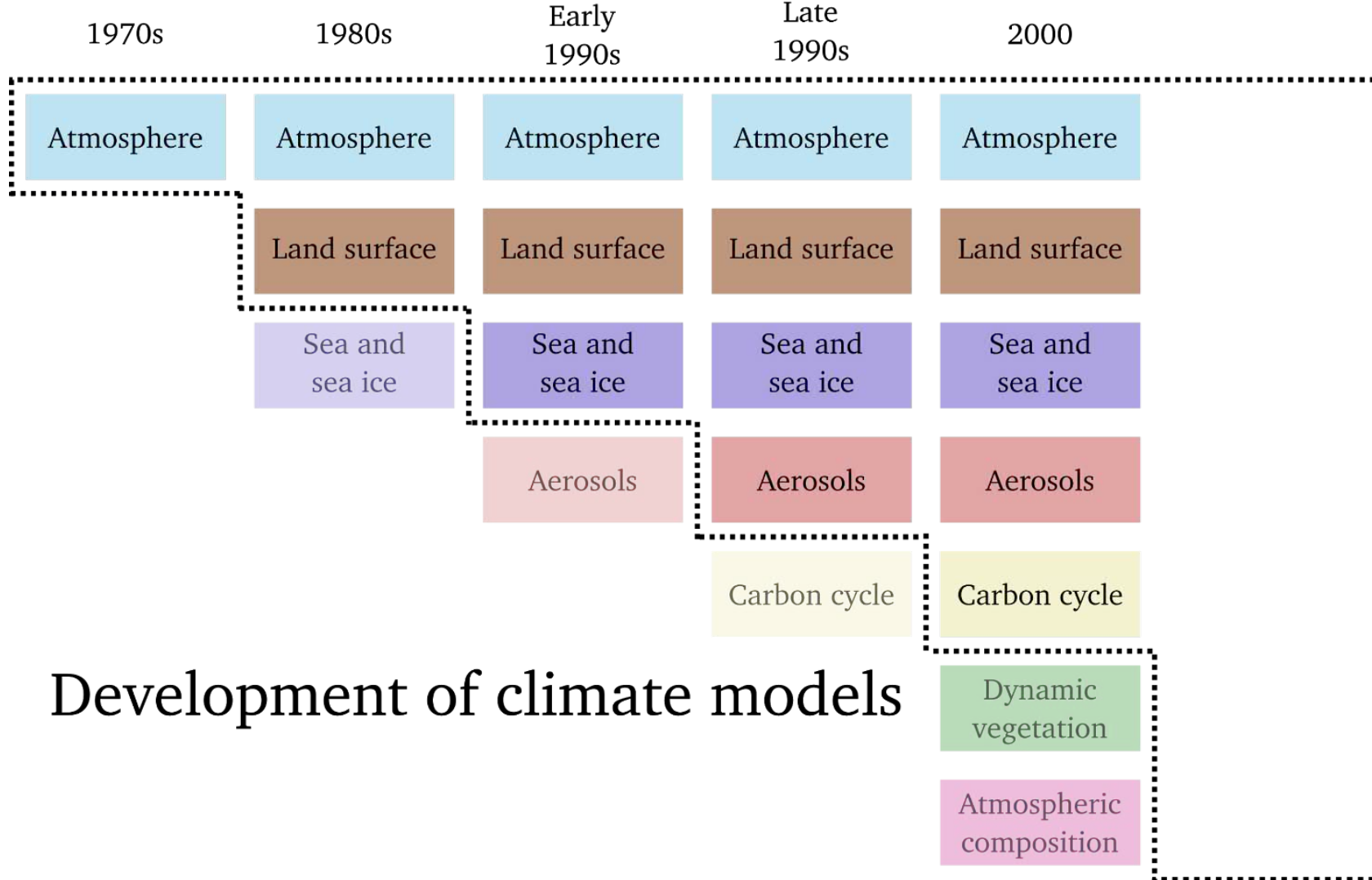
Aerosols

Development of climate models

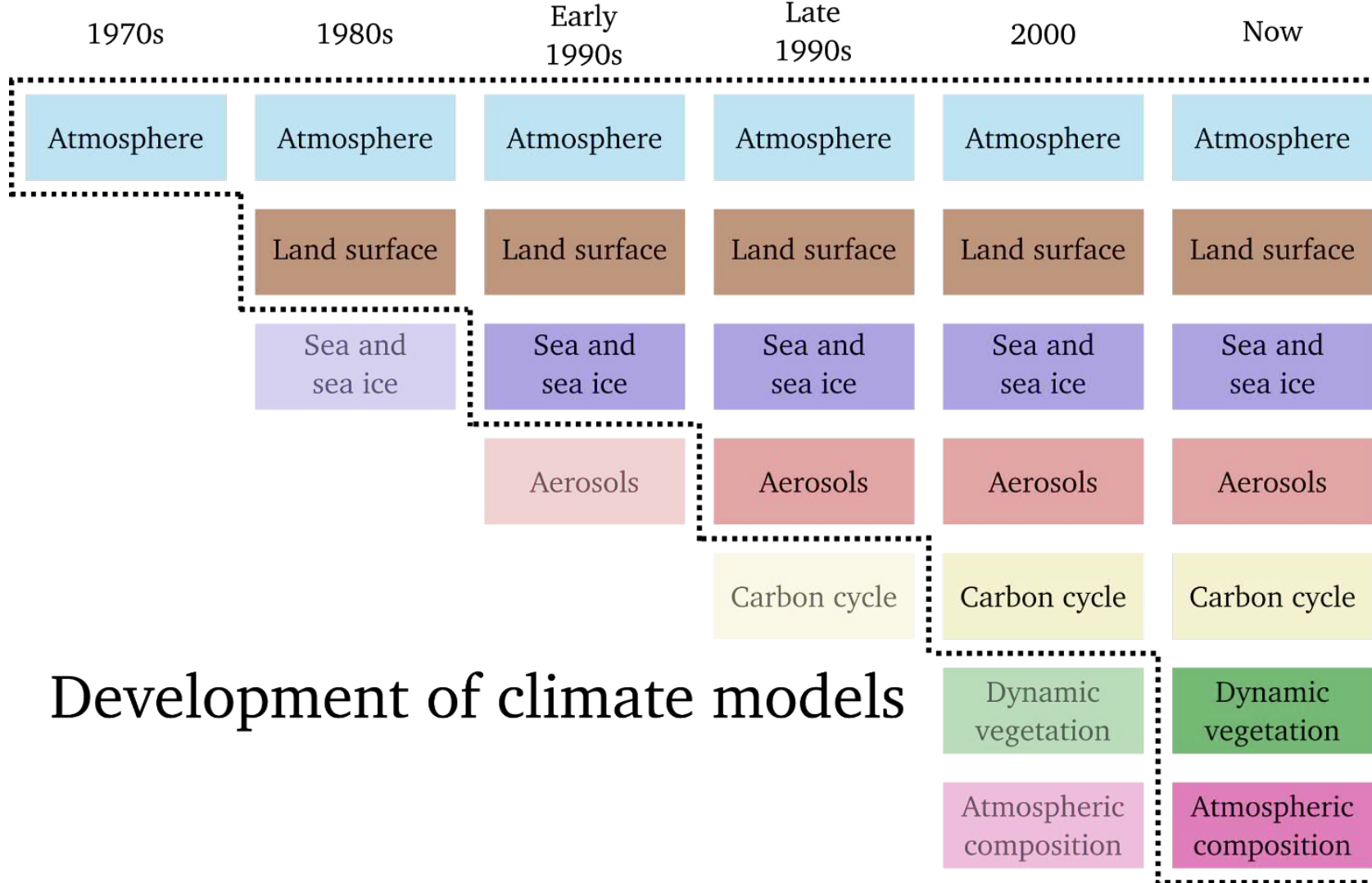




## Development of climate models

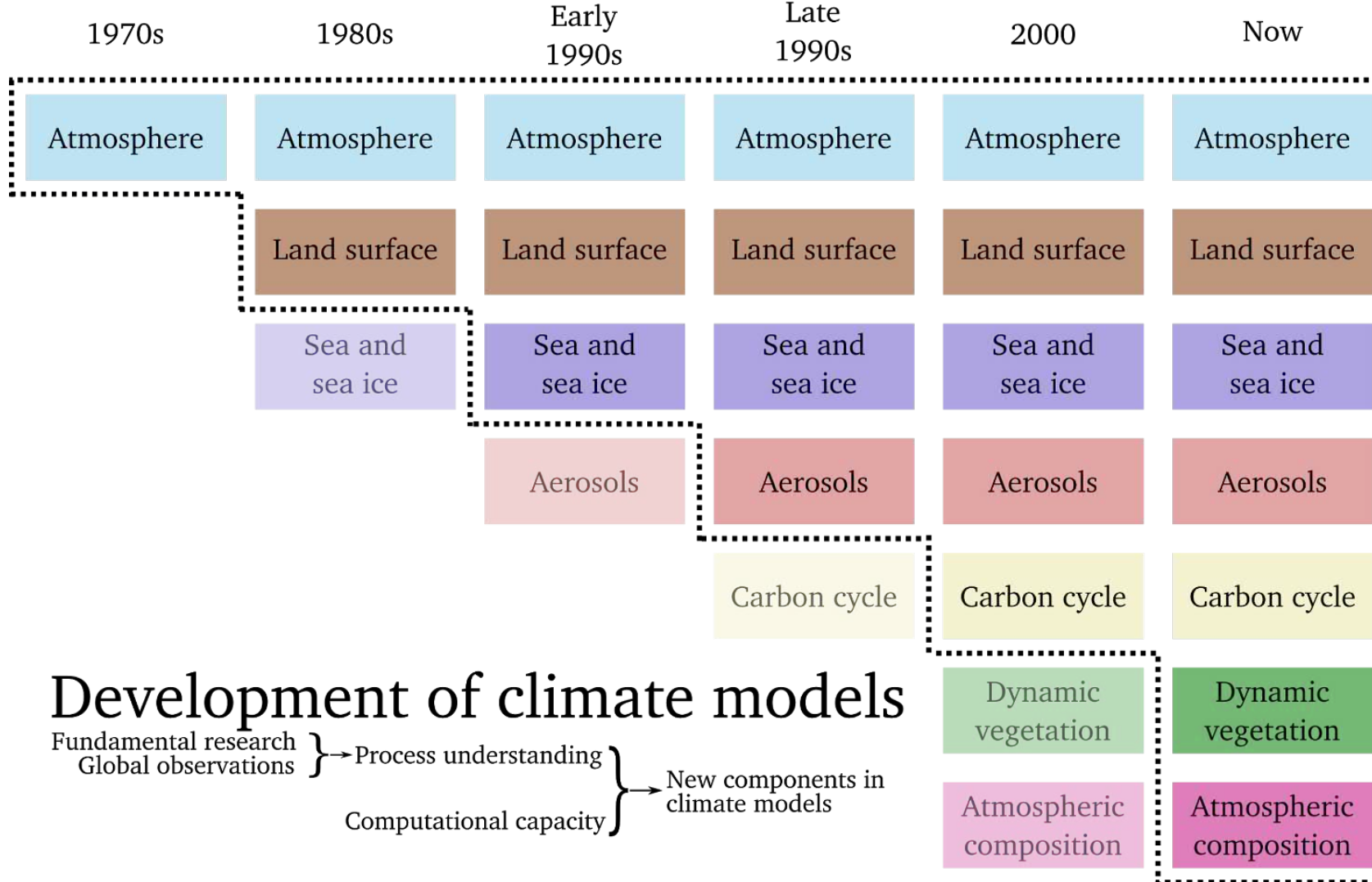


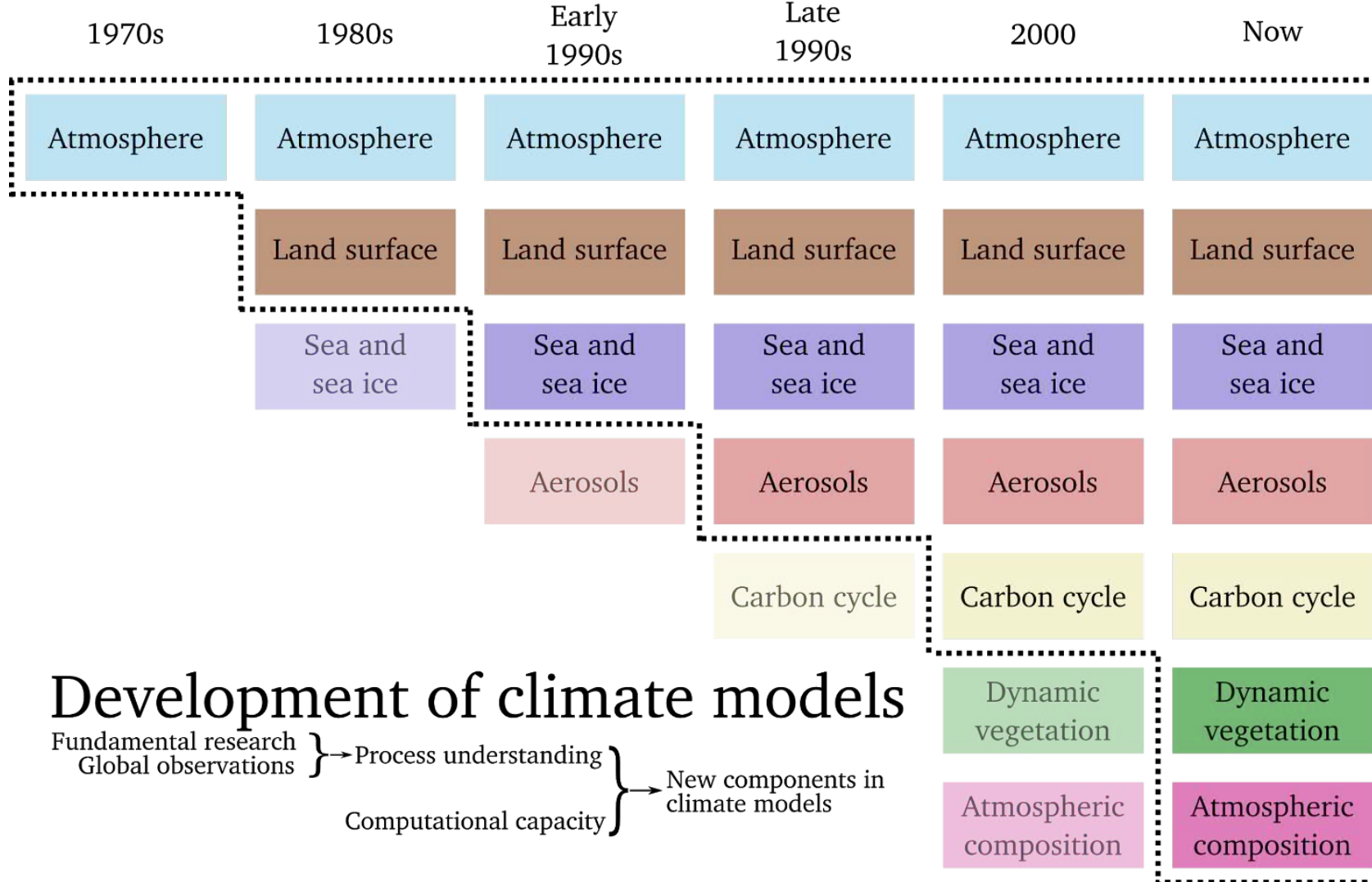
## Development of climate models



## Development of climate models

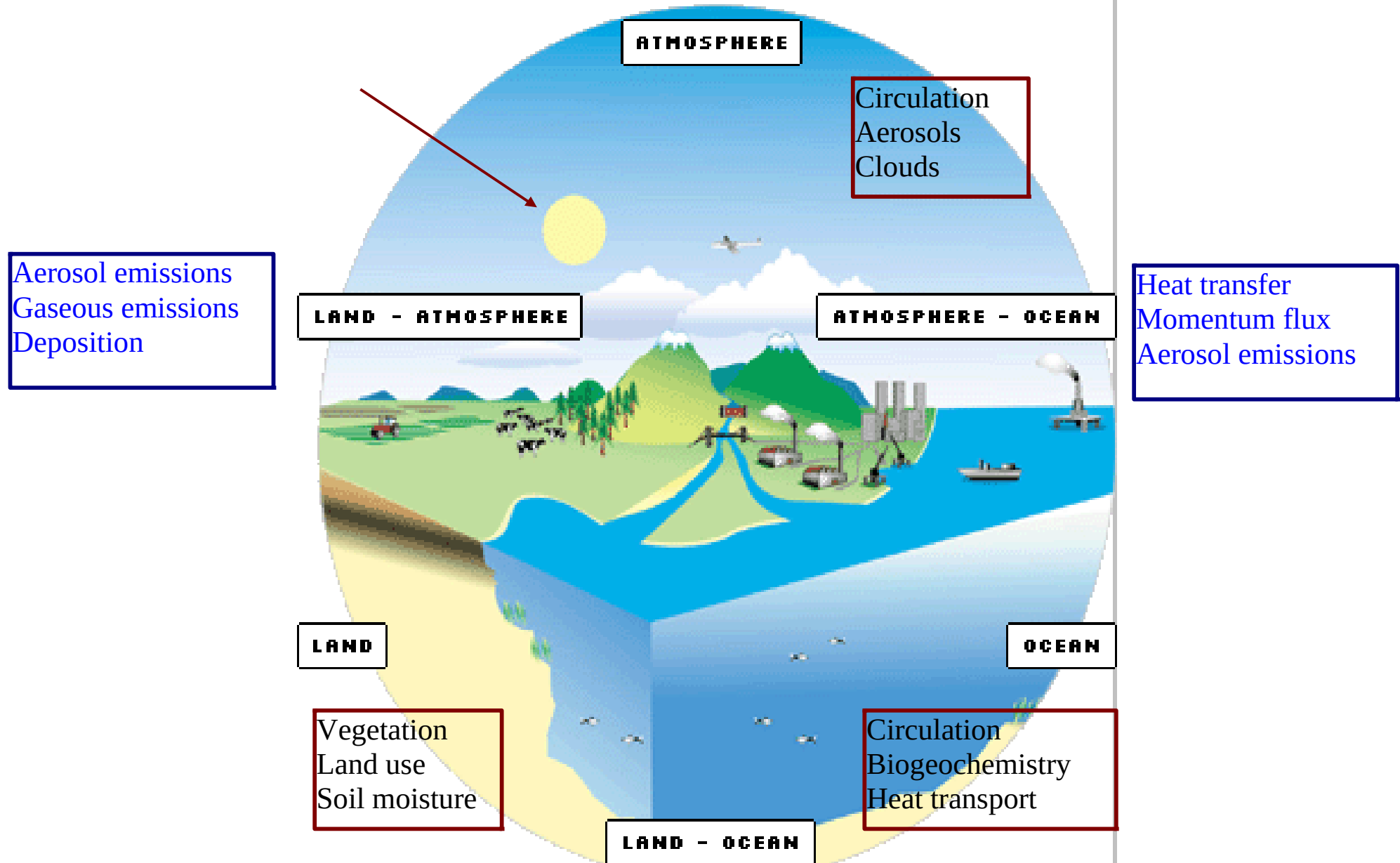






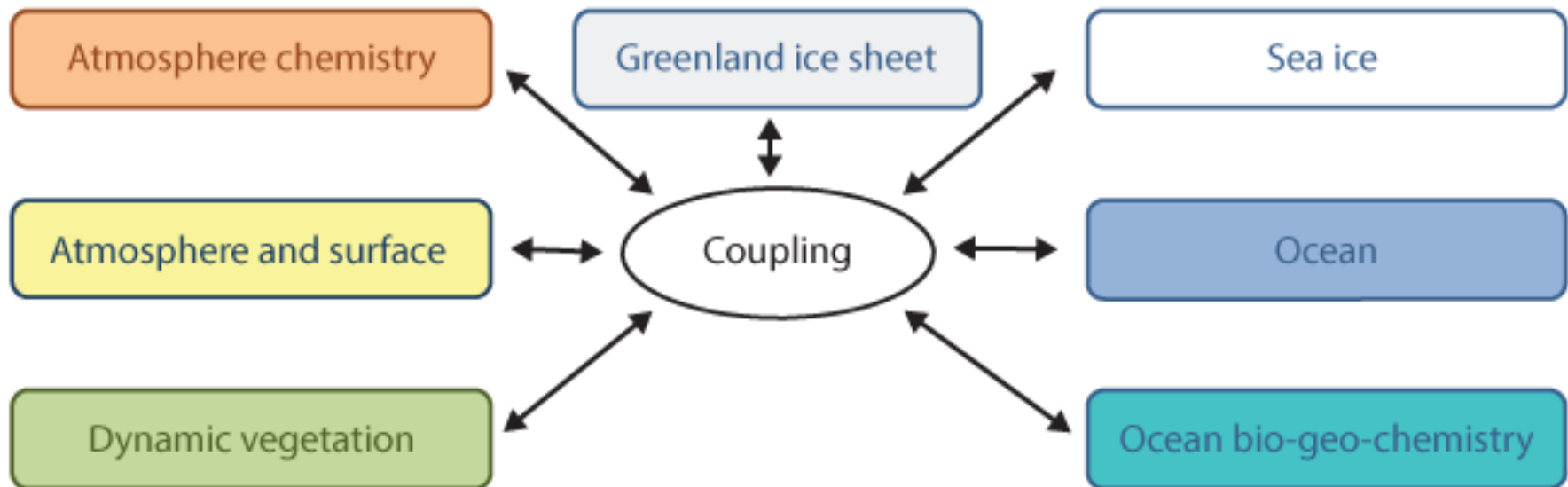
Climate models are already several millions  
lines of code, with scientific domains  
competing for computational resources

# Earth System (Model)



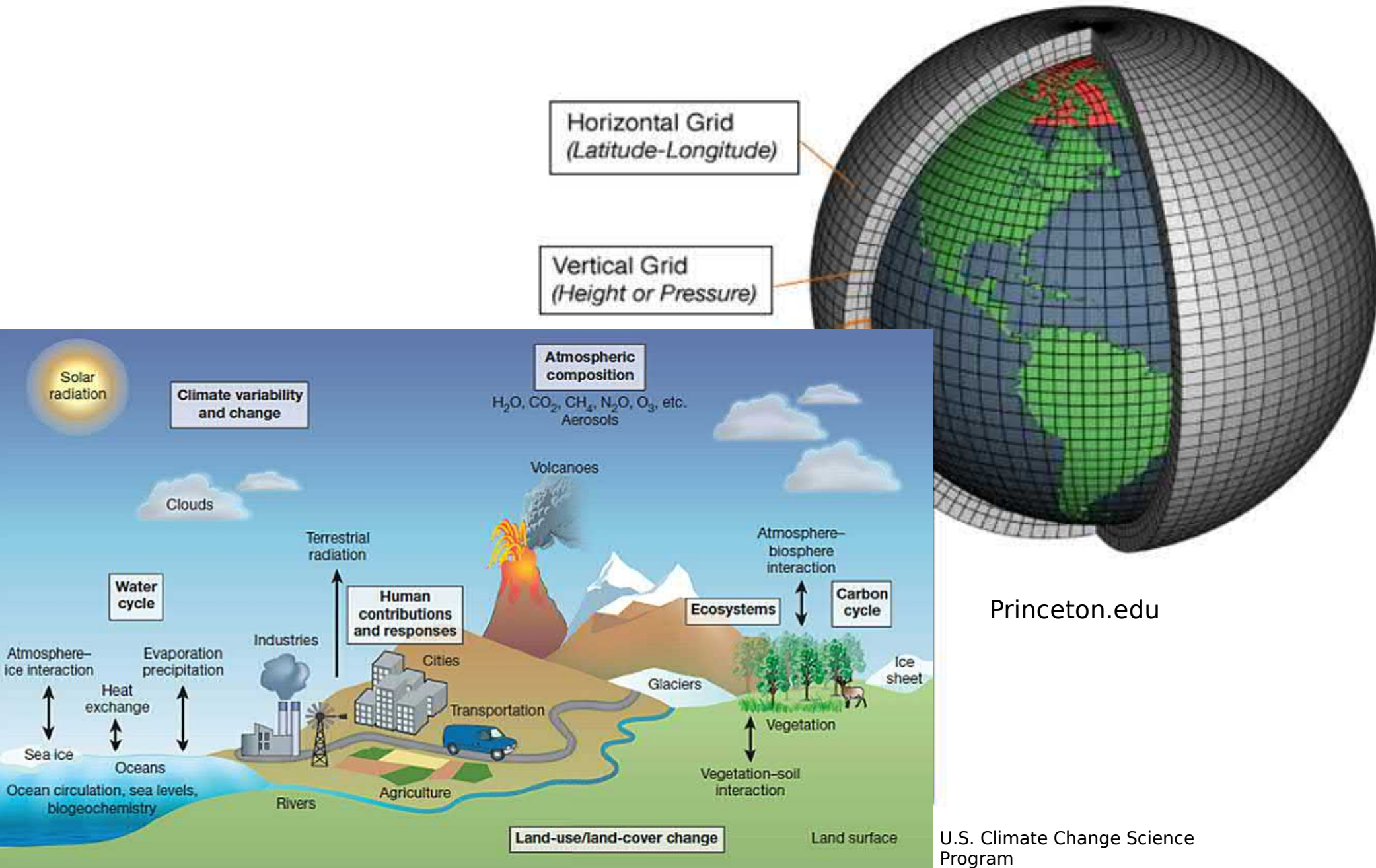
# Example: EC-Earth3

- **Atmosphere:** IFS
- **Atmospheric transport and chemistry:** TM5
  - Carbon bond (CB05) mechanism (51 species, 156 reactions)
- **Ocean:** NEMO, **sea-ice:** LIM, **biogeochemistry:** PISCES
- **Dynamic vegetation:** LPJ-GUESS
- **Ice sheets:** PISM



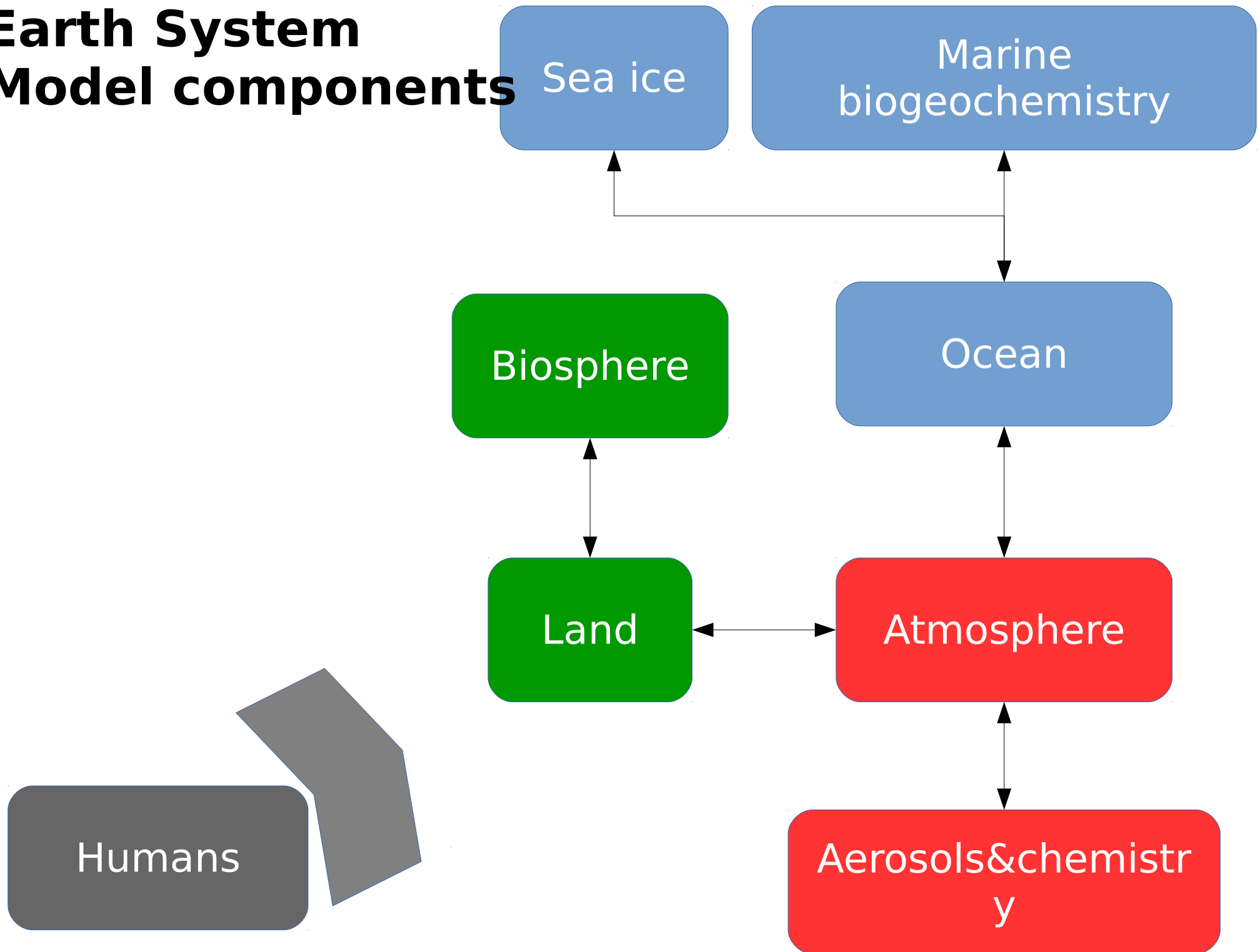
**How to describe aerosols/chemistry  
in a global climate model?**

# Earth System Models



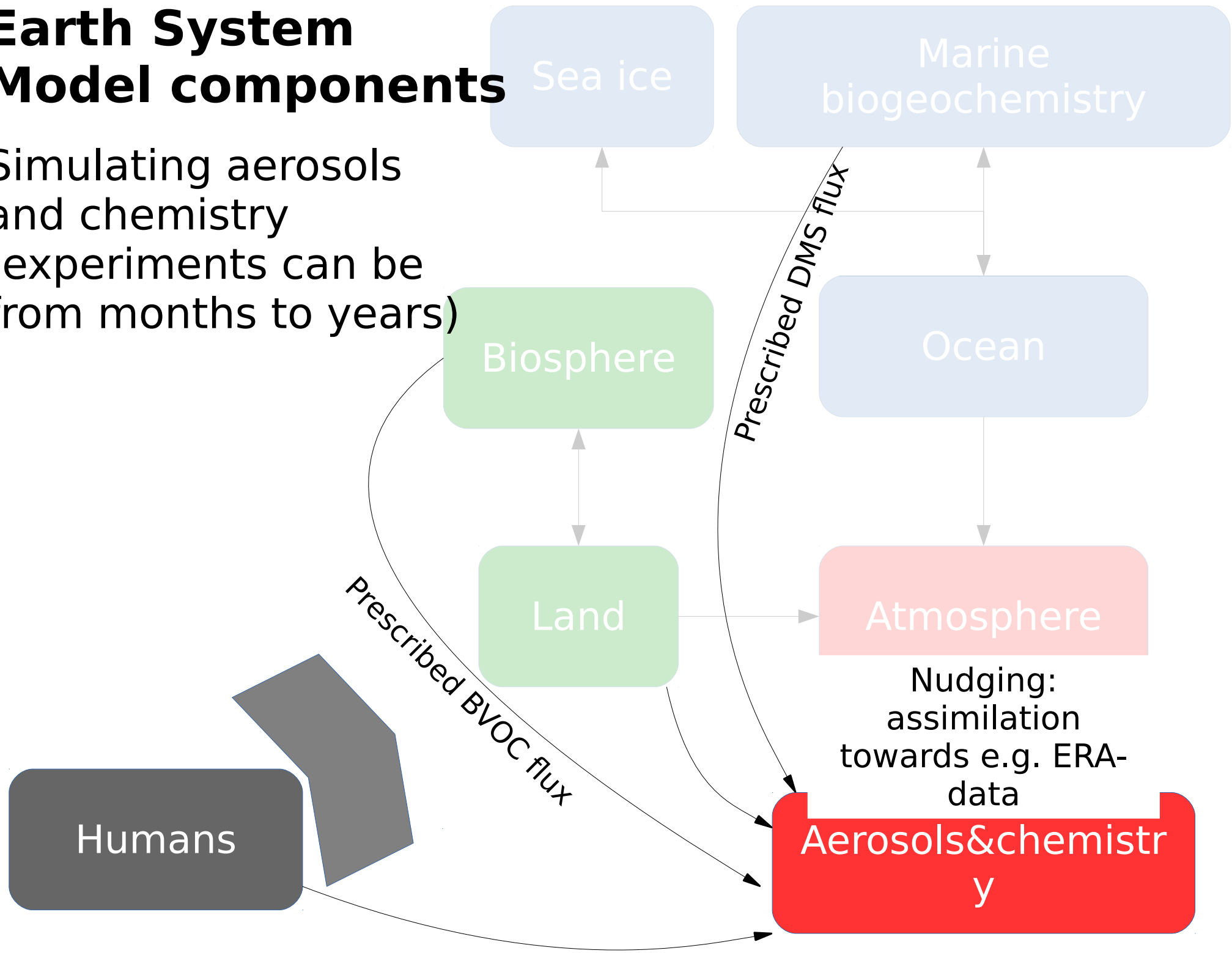


# Earth System Model components



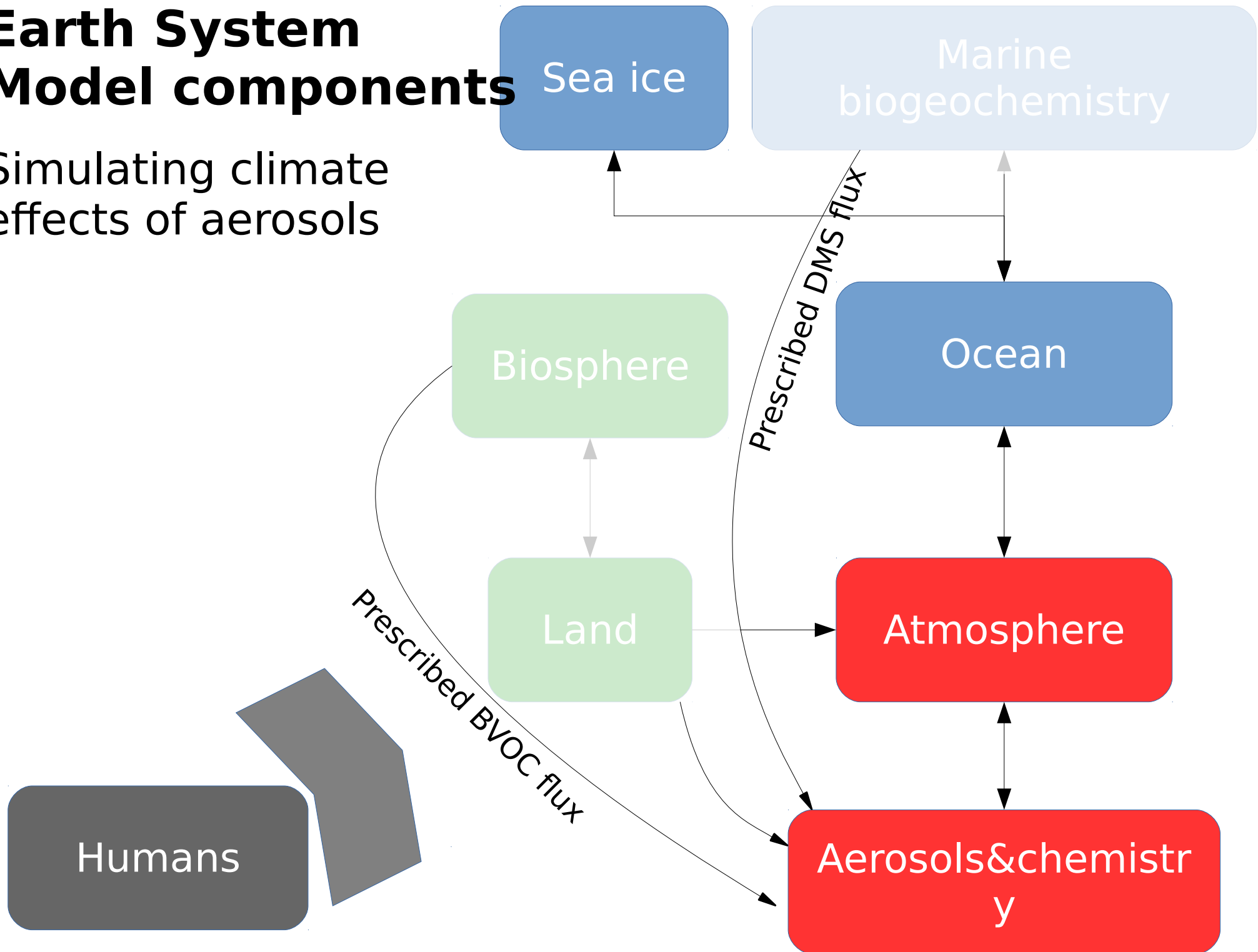
# Earth System Model components

Simulating aerosols  
and chemistry  
(experiments can be  
from months to years)



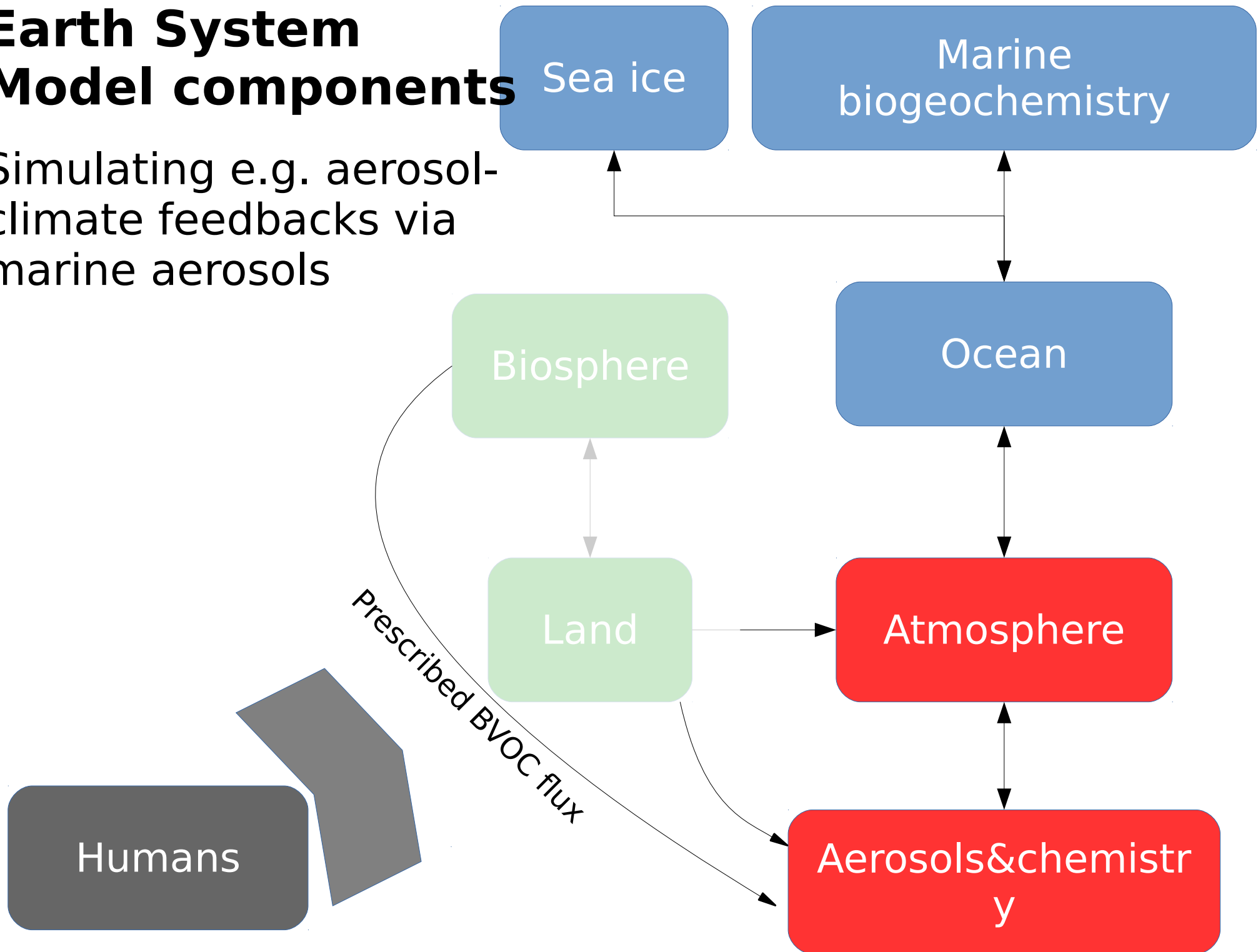
# Earth System Model components

Simulating climate  
effects of aerosols



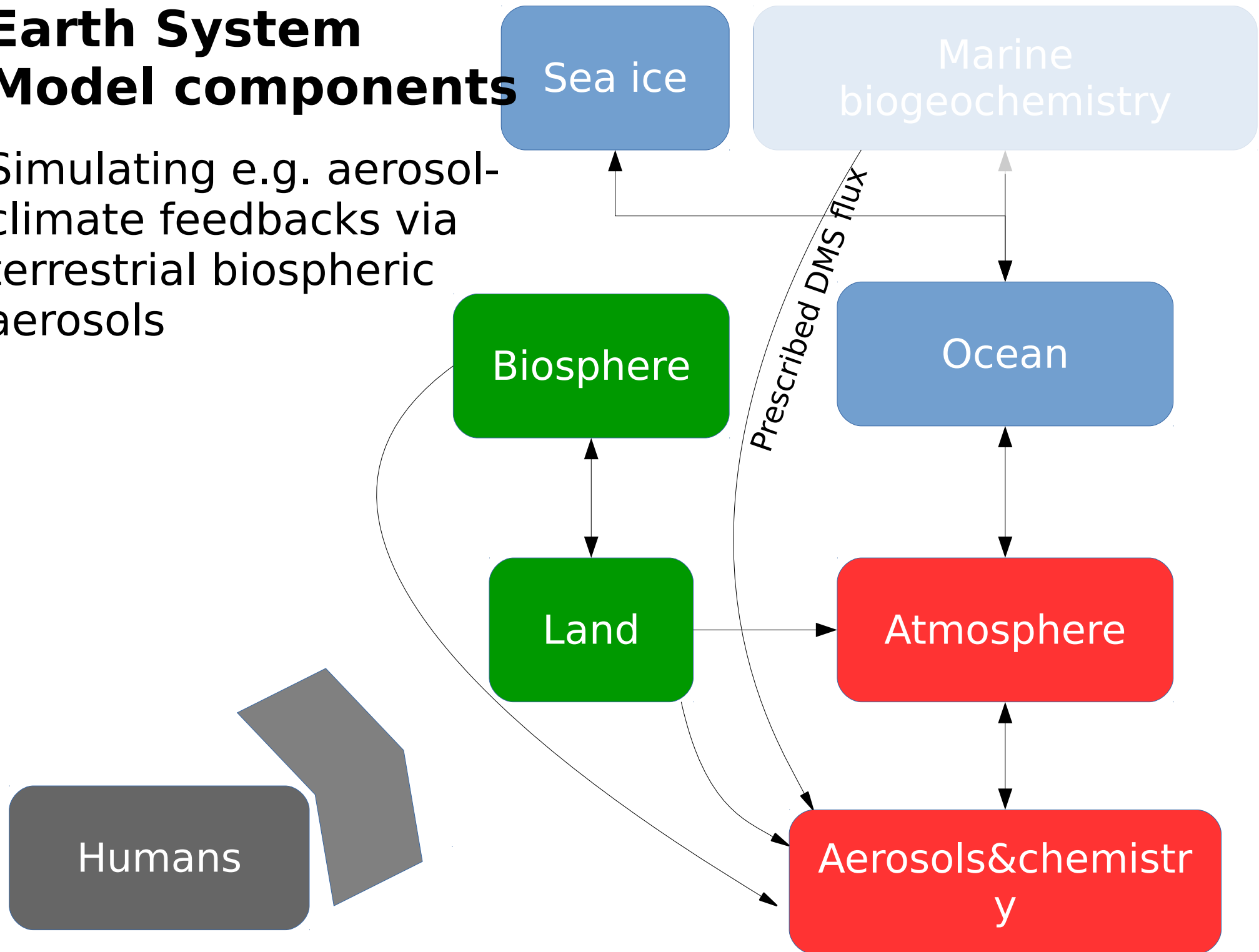
# Earth System Model components

Simulating e.g. aerosol-  
climate feedbacks via  
marine aerosols



# Earth System Model components

Simulating e.g. aerosol-  
climate feedbacks via  
terrestrial biospheric  
aerosols



# Earth System Model: choice of components

Choice of ESM components is based on

- timescale of the experiment: years, decades or millenia
- variables of interest: air quality, climate change, process study
- computational resources

Model of everything related to Earth

Population model

Dynamic vegetation model

Ocean circulation model

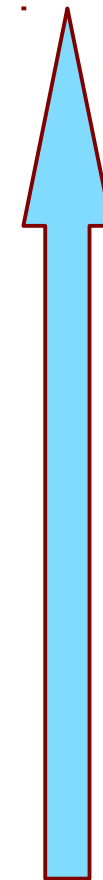
Prescribed vegetation (type, LAI)

Mixed layer ocean

Cloud microdynamics

Prescribed sea surface temperatures and sea ice

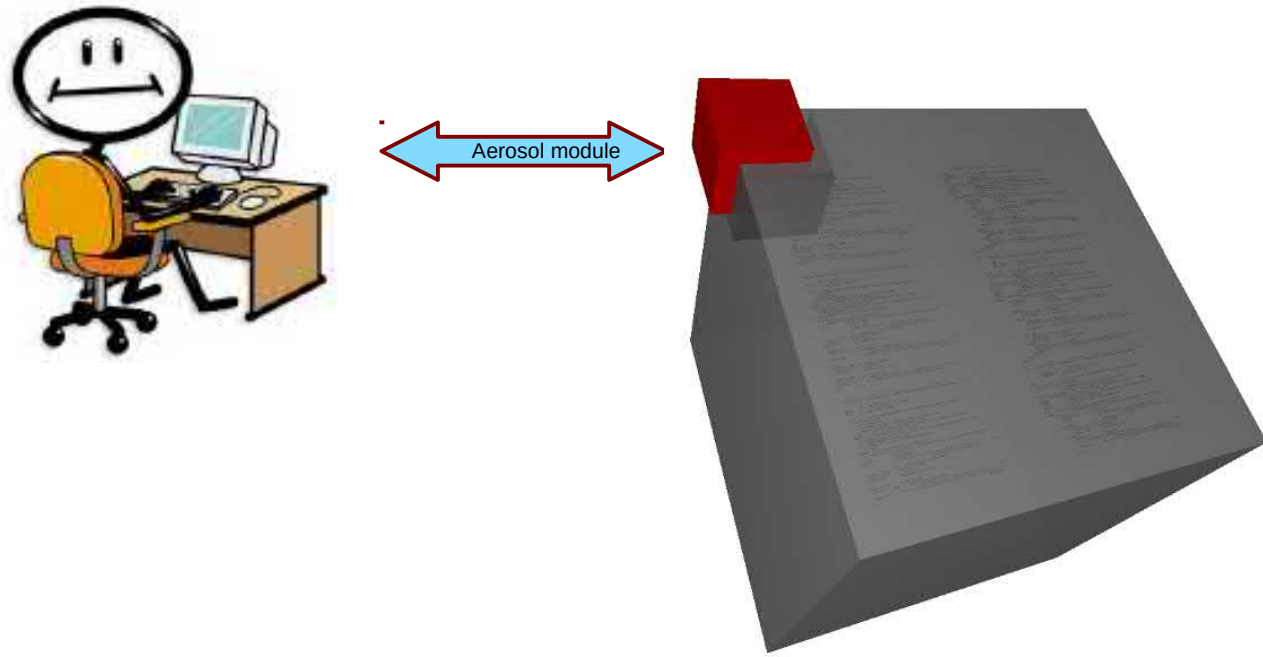
Prescribed meteorology



Complexity  
Computational  
expense  
Simulated noise

# Earth System Model: black box modeling

- ESM can easily have millions of lines of code
- A single researcher usually contributes only to a single module
  - Rest of the model is considered black box (“need to know” basis)

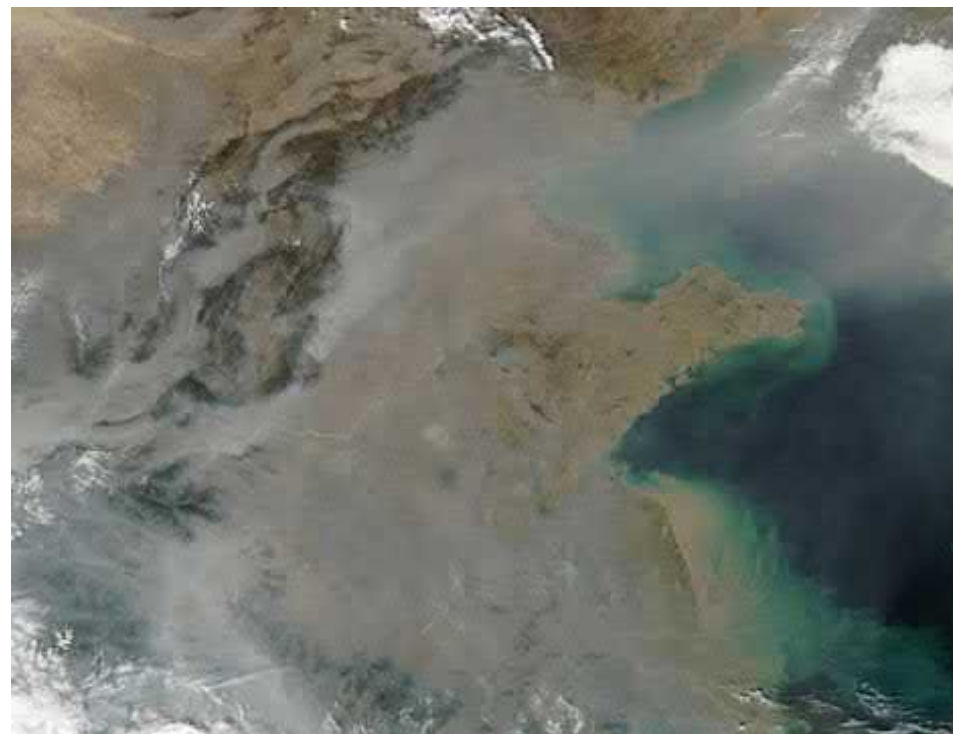


# What details do we need for global aerosol modeling?

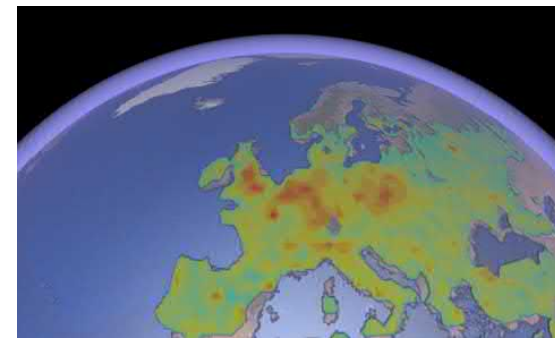
- Spatial distribution
  - unlike long-lived greenhouse gases, aerosols have a highly inhomogeneous spatial distribution
  - climate effect of an aerosol concentration (change) depends strongly on the location
    - **need to describe the spatial distribution**
- Composition
  - different aerosol types induce distinct climate effects (e.g. scattering, absorption)
    - **need to describe aerosols species composition**
- Size distribution
  - aerosol size determines e.g. potential to act as cloud condensation nuclei (CCN)
    - **need to describe aerosol size distribution**
- Processes
  - Aerosols enter atmosphere either by direct emission or atmospheric formation (chemistry)
  - Particle size distribution is changing rapidly via aerosol microphysics
    - **need to describe atmospheric chemistry and aerosol microphysics**



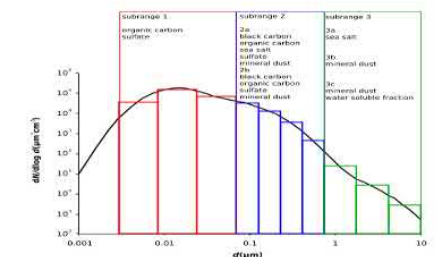
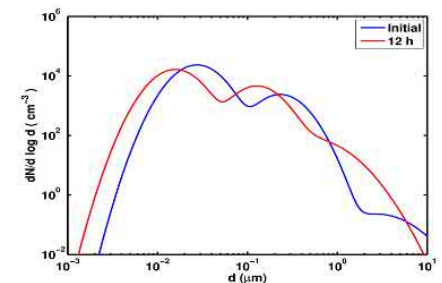
What aerosol (and gas-phase)  
components need to be  
considered in a climate model?



# Global aerosol models

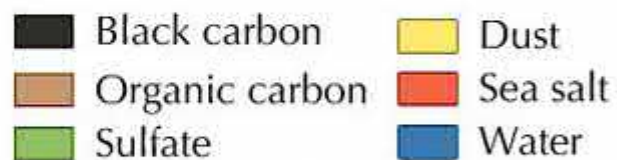


- First approximations use fixed aerosol climatologies
  - Monthly/yearly average radiative properties of aerosol
  - Based on previous simulations and satellite observations
- Aerosol mass-only models (Bulk-models)
  - No (or very limited) aerosol microphysical processes
- Modal size-resolved aerosol microphysics models
  - Aerosol distribution is represented with superposition of several log-normal modes
- Sectional size-resolved aerosol microphysics models
  - Better representation of aerosol processes, especially for growth and cloud processes





Example of global aerosol microphysics: M7 (used in e.g. ECHAM and EC-Earth)

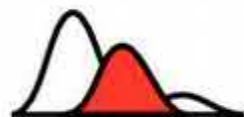


**Nucleation**

**Aitken**



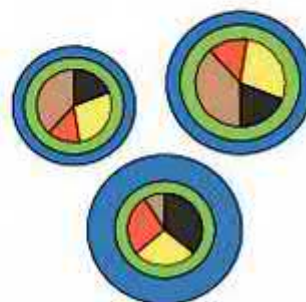
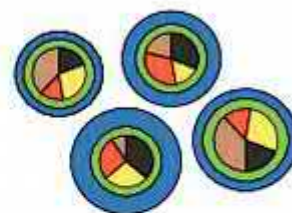
**Accumulation**



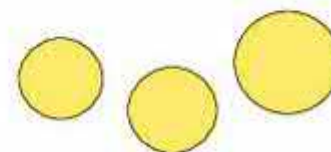
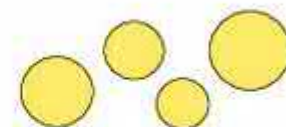
**Coarse**



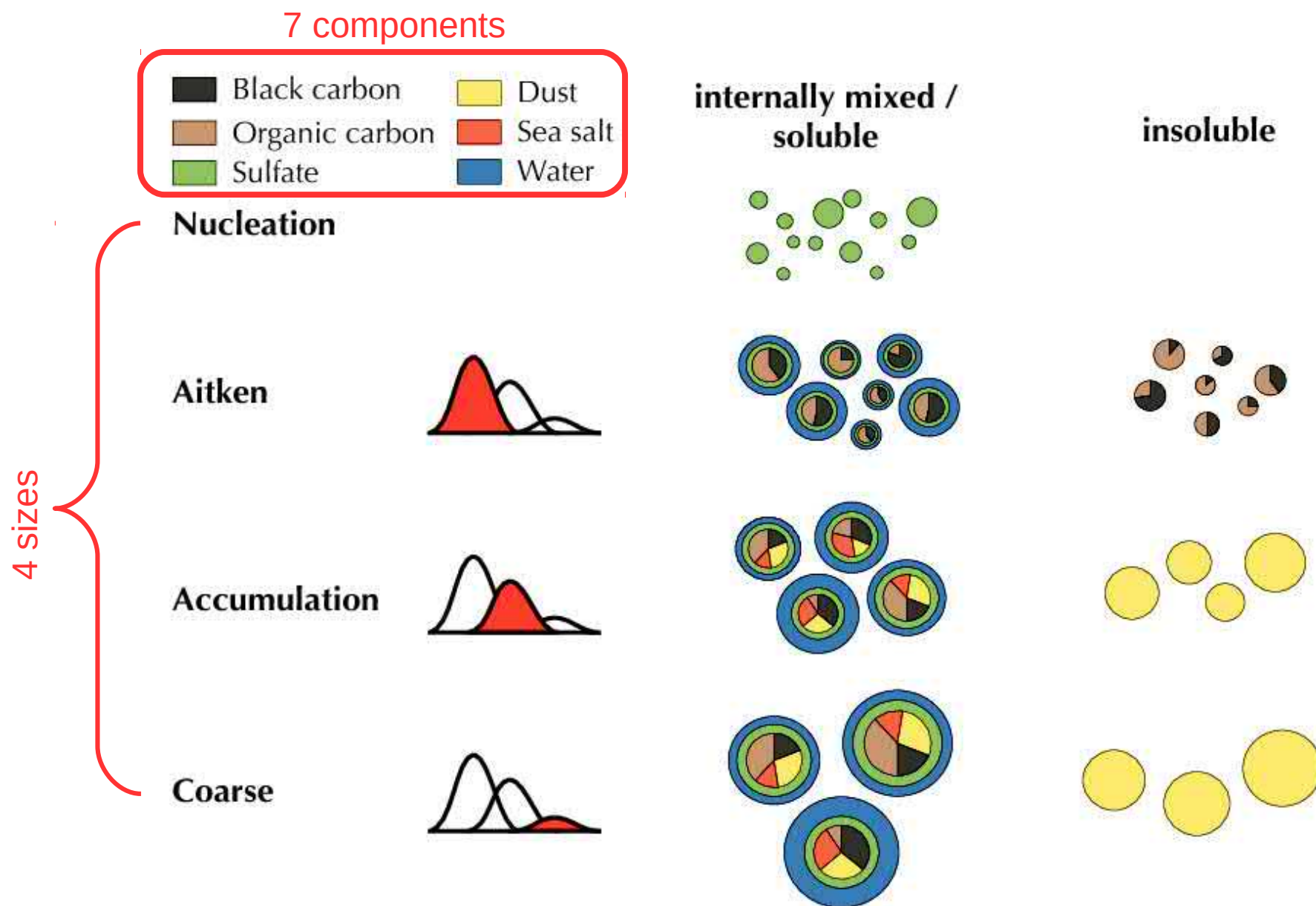
**internally mixed /  
soluble**



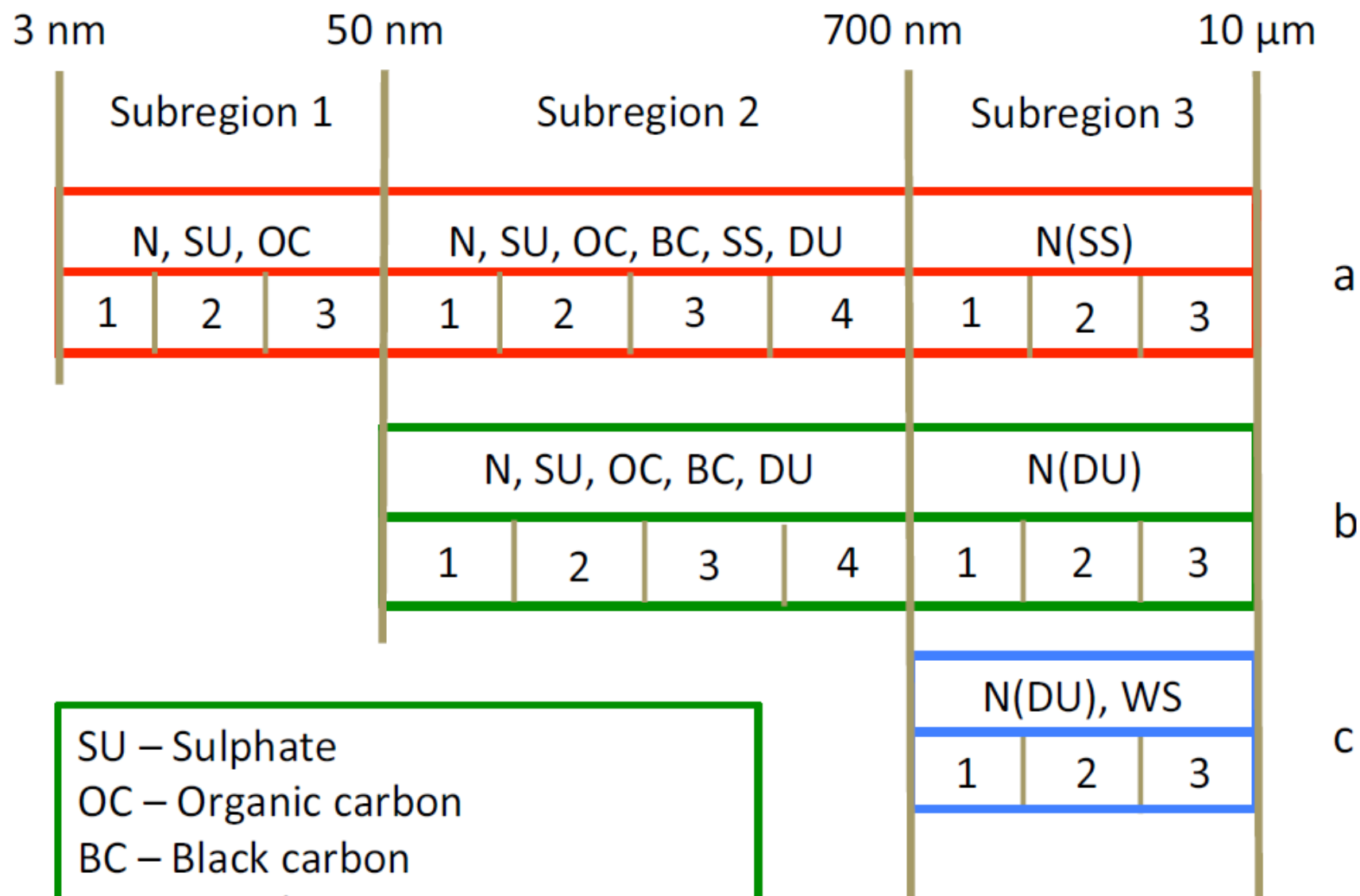
**insoluble**



Example of global aerosol microphysics: M7 (used in e.g. ECHAM and EC-Earth)

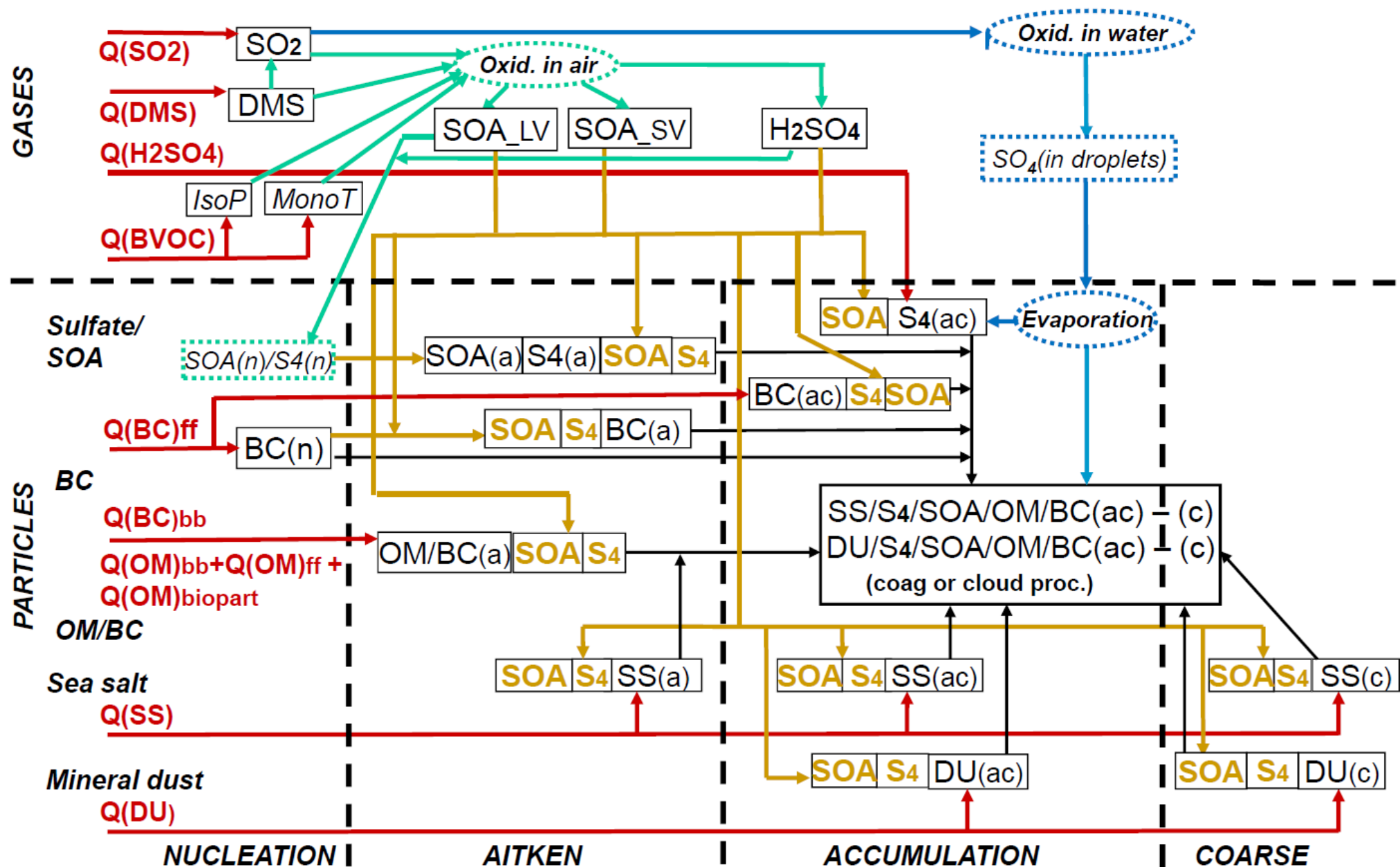


# Example of global aerosol microphysics: SALSA (used in ECHAM)



SU – Sulphate  
OC – Organic carbon  
BC – Black carbon  
SS – Sea salt  
DU – Dust  
WS – Water soluble fraction  
N() – Number concentration only

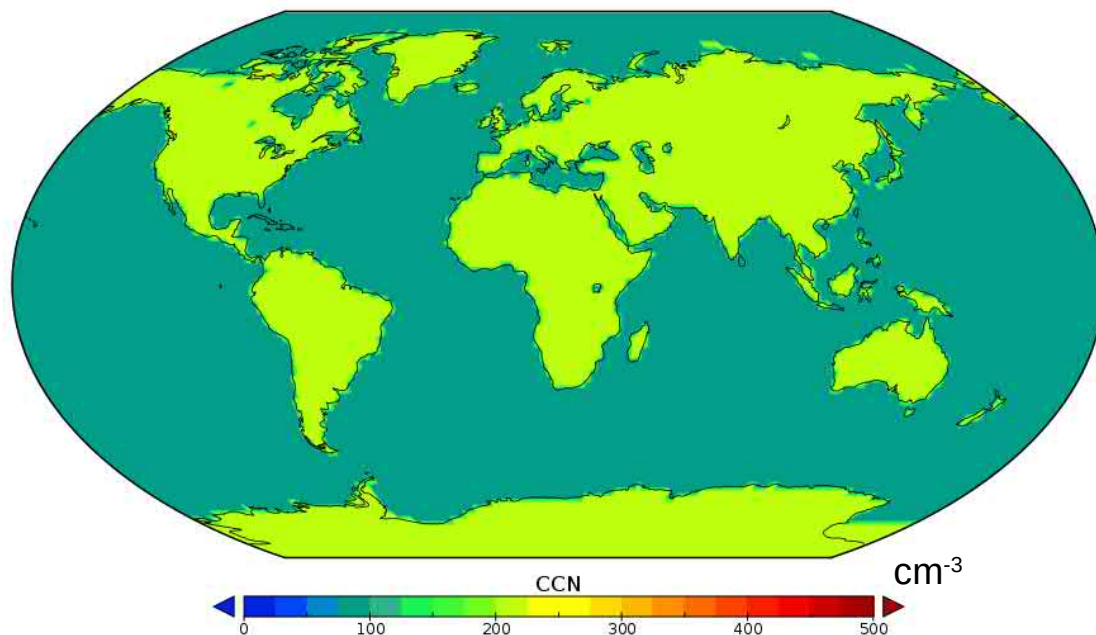
# Example of global aerosol microphysics: NorESM



## No aerosol information

If aerosols are not simulated, model needs to assume a prescribed monthly/annual distribution which can vary in vertical and horizontal

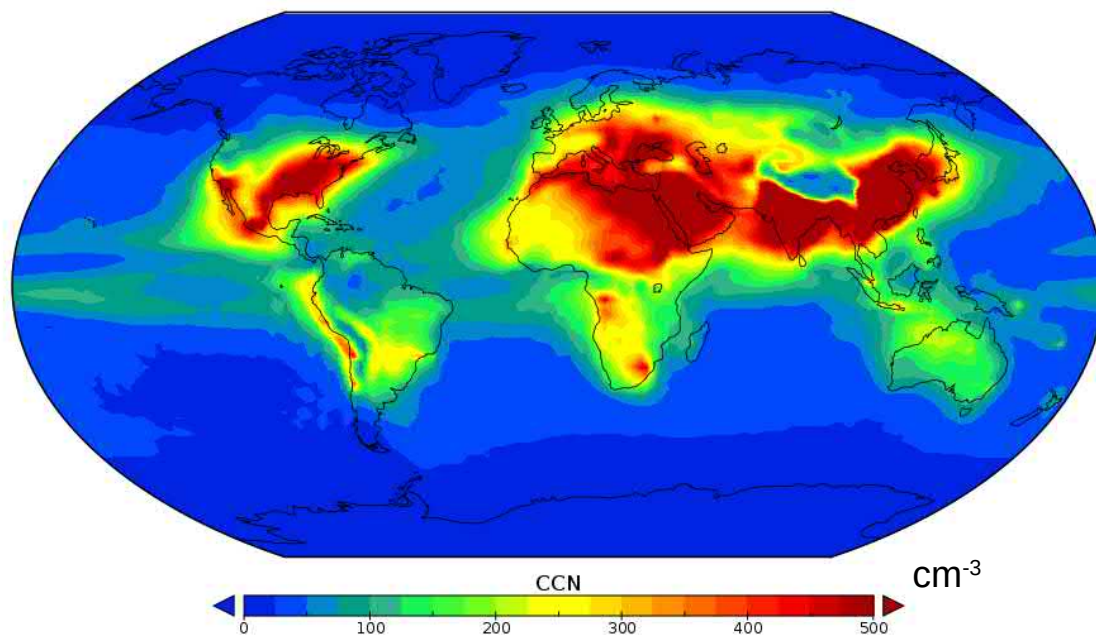
*Example: ECHAM5 assumes aerosol concentrations of 80  $\text{cm}^{-3}$  over ocean and 220  $\text{cm}^{-3}$  over land (for cloud activation)*



## Interactive aerosol model

If aerosol size distribution and chemical composition is prognosticated by the model, cloud condensation nuclei (CCN) can be diagnosed as  $N(d_p > d_{\text{limit}})$  or at different supersaturations with (kappa-)Köhler.

*Example: ECHAM5-HAM CCN(0.2%) annual average supersaturation*





# **Atmospheric chemistry**

# Atmospheric chemistry in climate models

- Complete atmospheric chemistry is impossible to model
  - E.g. Master Chemical Mechanism (near-explicit chemical mechanism for VOC degradation): 142 primary compounds, >6000 resulting species, over 13500 reactions
- Tracers are expensive
- Typically 2+ options for chemistry
  - 1) Fixed oxidant fields, basic sulfur chemistry, limited organic chemistry – FAST
  - 2) Extended (“full”) chemistry, 30-80 chemical species, 100-200 reactions – EXPLICIT  
(Examples: MOZART, CB05 chemical mechanisms)

# Atmospheric chemistry in climate models

- Tracers are expensive
- Typically 2+ options for chemistry
  - 1) Fixed oxidant fields, basic sulfur chemistry, limited organic chemistry - FAST
  - 2) Extended ("full") chemistry, 30-80 chemical species, 100-200 reactions - EXPLICIT

For example, chemistry mechanism in EC-Earth:

27 transported species  
15 non-transported species

Chemical trace species	(continued)	(continued)
O <sub>3</sub>	ORGNTR <sup>[5]</sup>	OH
NO <sub>x</sub>	ISOP	NO <sub>2</sub>
H <sub>2</sub> O <sub>2</sub>	SO <sub>2</sub>	NO <sub>3</sub>
CH <sub>4</sub>	DMS	N <sub>2</sub> O <sub>5</sub>
CO	NH <sub>3</sub>	HNO <sub>4</sub>
HNO <sub>3</sub>	NH <sub>4</sub> <sup>+</sup> <sup>[8]</sup>	CH <sub>3</sub> COCHO
CH <sub>3</sub> OOH	MSA	C <sub>2</sub> O <sub>3</sub>
CH <sub>2</sub> O	SO <sub>4</sub> <sup>2-</sup> <sup>[6]</sup>	ROR <sup>[9]</sup>
PAR <sup>[1]</sup>	NO <sub>3</sub> <sup>-</sup> <sup>[7]</sup>	RXPAR <sup>[10]</sup>
C <sub>2</sub> H <sub>4</sub>	<sup>222</sup> Rn	XO <sub>2</sub> <sup>[11]</sup>
OLE <sup>[2]</sup>	<sup>210</sup> Pb	XO <sub>2</sub> N <sup>[12]</sup>
ALD2 <sup>[3]</sup>	NO	NH <sub>2</sub>
PAN	HO <sub>2</sub>	
ROOH <sup>[4]</sup>	CH <sub>3</sub> O <sub>2</sub>	

# Atmospheric chemistry in climate models

Reactants	Products	Rate expression	Reference
NO + O <sub>3</sub>	NO <sub>2</sub>	$3.0\text{E-}12 \cdot \exp(-1500/T)$	[1]
NO + HO <sub>2</sub>	NO <sub>2</sub> + OH	$3.5\text{E-}12 \cdot \exp(250/T)$	[1]
NO + CH <sub>3</sub> O <sub>2</sub>	CH <sub>2</sub> O + HO <sub>2</sub> + NO <sub>2</sub>	$2.8\text{E-}12 \cdot \exp(300/T)$	[1]
NO <sub>2</sub> + OH (+ M)	HNO <sub>3</sub>	$K_0 = 1.8\text{E-}30 \cdot (300/T)^{3.0}$ $K_\infty = 2.8\text{E-}11$	[1]
OH + HNO <sub>3</sub>	NO <sub>3</sub>	$K_0 = 2.41\text{E-}14 \cdot (460/T)$ $K_2 = 6.51\text{E-}34 \cdot (1335/T)$ $K_3 = 2.69\text{E-}17 \cdot (2199/T)$	[1]
NO <sub>2</sub> + O <sub>3</sub>	NO <sub>3</sub>	$1.2\text{E-}13 \cdot \exp(-2540/T)$	[1]
NO + NO <sub>3</sub>	NO <sub>2</sub> + NO <sub>2</sub>	$1.5\text{E-}11 \cdot \exp(170/T)$	[1]
NO <sub>2</sub> + NO <sub>3</sub>	N <sub>2</sub> O <sub>5</sub>	$K_0 = 2.0\text{E-}30 \cdot (300/T)^{4.4}$ $K_\infty = 1.4\text{E-}12 \cdot (300/T)^{0.7}$	[1]
N <sub>2</sub> O <sub>5</sub>	NO <sub>2</sub> + NO <sub>3</sub>	$2.7\text{E-}27 \cdot \exp(11\,000/T)$	[1]
OH + HNO <sub>4</sub>	NO <sub>2</sub>	$1.3\text{E-}12 \cdot \exp(380/T)$	[1]
NO <sub>2</sub> + HO <sub>2</sub>	HNO <sub>4</sub>	$K_0 = 2.0\text{E-}31 \cdot (300/T)^{3.4}$ $K_\infty = 2.9\text{E-}12 \cdot (300/T)^{1.1}$	[1]
HNO <sub>4</sub> (+ M)	NO <sub>2</sub> + HO <sub>2</sub>	$2.1\text{E-}27 \cdot \exp(10900/T)$	[1]
O( <sup>1</sup> D) (+ M)		$3.3\text{E-}11 \cdot \exp(55/T) \cdot [\text{O}_2]$ $+ 2.15\text{E}11 \cdot \exp(110/T) \cdot [\text{N}_2]$	[1]
O( <sup>1</sup> D) + H <sub>2</sub> O	OH + OH	$1.63\text{E-}10 \cdot \exp(60/T)$	[1]
O <sub>3</sub> + HO <sub>2</sub>	OH	$1.0\text{E-}14 \cdot \exp(-490/T)$	[1]

Example, chemistry  
mechanism in EC-Earth

Reactants	Products	Rate expression	Reference
CO + OH	HO <sub>2</sub>	$K_0 = 5.9E-33*(300/T)^{1.4}$ $K_\infty = 1.1E-12*(300/T)^{-1.3}$ $K_0 = 1.5E-13*(300/T)^{-0.6}$ $K_\infty = 2.1E9*(300/T)^{-6.1}$	[1]
O <sub>3</sub> + OH	HO <sub>2</sub>	$1.7E-12*\exp(-940/T)$	[1]
OH + H <sub>2</sub> O <sub>2</sub>	HO <sub>2</sub>	$1.8E-12$	[1]
OH + CH <sub>2</sub> O	CO + HO <sub>2</sub>	$5.5E-12*\exp(125/T)$	[1]
OH + CH <sub>4</sub>	CH <sub>3</sub> O <sub>2</sub>	$2.45E-12*\exp(-1775/T)$	[1]
OH + CH <sub>3</sub> OOH	0.7 CH <sub>3</sub> O <sub>2</sub> + 0.3 CH <sub>2</sub> O + 0.3 OH	$3.8E-12*\exp(200/T)$	[1]
OH + ROOH	0.7 XO <sub>2</sub> + 0.3 OH	$3.01E-12*\exp(190/T)$	[2]
CH <sub>3</sub> O <sub>2</sub> + HO <sub>2</sub>	CH <sub>3</sub> OOH	$4.1E-13*\exp(750/T)$	[1]
CH <sub>3</sub> O <sub>2</sub> + CH <sub>3</sub> O <sub>2</sub>	1.33 CH <sub>2</sub> O + 0.67 HO <sub>2</sub>	$9.5E-14*\exp(390/T)$	[1]
OH + HO <sub>2</sub>		$4.8E-11*\exp(250/T)$	[1]
HO <sub>2</sub> + HO <sub>2</sub>	H <sub>2</sub> O <sub>2</sub>	$3.5E-13*\exp(430/T)$ $1.77E-33*\exp(1000/T)$ $1.4E-21*\exp(2200/T)$	[1]
OH + H <sub>2</sub>	HO <sub>2</sub>	$2.8E-12*\exp(-1800/T)$	[1]
NO <sub>3</sub> + CH <sub>2</sub> O	HNO <sub>3</sub> + CO + HO <sub>2</sub>	$5.8E-16$	[1]
ALD2 + OH	C <sub>2</sub> O <sub>3</sub>	Average of : $4.4E-12*\exp(365/T)$ $5.1E-12*\exp(405/T)$	[3]
ALD2 + NO <sub>3</sub>	C <sub>2</sub> O <sub>3</sub> + HNO <sub>3</sub>	Average of : $1.4E-12*\exp(-1860/T)$ $6.5E-15$	[3]
NO + C <sub>2</sub> O <sub>3</sub>	CH <sub>2</sub> O + XO <sub>2</sub> + HO <sub>2</sub> + NO <sub>2</sub>	$8.1E-12*\exp(270/T)$	[1]
NO <sub>2</sub> + C <sub>2</sub> O <sub>3</sub>	PAN	$K_0 = 2.7E-28*(300/T)^{7.1}$ $K_\infty = 1.2E-11*(300/T)^{0.9}$	[3]

Example, chemistry  
mechanism in EC-Earth



Reactants	Products	Rate expression	Reference
PAN	$\text{NO}_2 + \text{C}_2\text{O}_3$	$K_0 = 4.9\text{E}-3 \cdot \exp(-12100/T)$ $K_\infty = 5.4\text{E}16 \cdot \exp(-13\,830/T)$	[3]
$\text{C}_2\text{O}_3 + \text{C}_2\text{O}_3$	$2 \text{CH}_2\text{O} + 2 \text{XO}_2 + 2 \text{HO}_2$	$2.9\text{E}-12 \cdot \exp(500/T)$	[1]
$\text{C}_2\text{O}_3 + \text{HO}_2$	$\text{CH}_2\text{O} + \text{XO}_2 + \text{HO}_2 +$ $0.79 \text{OH} + 0.21 \text{ROOH}$	$4.3\text{E}-13 \cdot \exp(1040/T)$	[1]
$\text{OH} + \text{PAR}$	$0.87 \text{XO}_2 + 0.76 \text{ROR} + 0.11 \text{HO}_2 +$ $0.11 \text{ALD2} + 0.11 \text{RXPAR} + 0.13 \text{XO}_2\text{N}$	$8.1\text{E}-13$	[4]
ROR	$1.1 \text{ALD2} + 0.96 \text{XO}_2 + 0.04 \text{XO}_2\text{N} +$ $0.02 \text{ROR} + 2.1 \text{RXPAR} + 0.94 \text{HO}_2$	$1\text{E}15 \cdot \exp(-8000/T)$	[4]
ROR	$\text{HO}_2$	$1600.0^{(*)}$	[4]
$\text{OH} + \text{OLE}$	$\text{CH}_2\text{O} + \text{ALD2} + \text{XO}_2 + \text{HO}_2 + \text{RXPAR}$	Average of : $1.86\text{E}-11 \cdot \exp(175/T)$ $8.12\text{E}-12 \cdot \exp(610/T)$ $2.6\text{E}-12 \cdot \exp(610/T)$	[3] [3] [3]
$\text{O}_3 + \text{OLE}$	$0.44 \text{ALD2} + 0.64 \text{CH}_2\text{O} + 0.25 \text{HO}_2 + 0.29 \text{XO}_2 +$ $0.37 \text{CO} + 0.9 \text{RXPAR} +$ $0.4 \text{OH}$	Average of : $8.5\text{E}-16 \cdot \exp(-1520/T)$ $1.4\text{E}-15 \cdot \exp(-2100/T)$ $1.0\text{E}-17$	[3] [3] [3]
$\text{NO}_3 + \text{OLE}$	$0.91 \text{XO}_2 + \text{CH}_2\text{O} + 0.09 \text{XO}_2\text{N} + \text{NO}_2 + \text{ALD2}$ $+ \text{RXPAR}$	Average of : $4.0\text{E}-14 \cdot \exp(-400/T)$ $6.0\text{E}-16$ $3.5\text{E}-15$	[3] [3] [3]
$\text{OH} + \text{C}_2\text{H}_4 (+\text{M})$	$\text{HO}_2 + 1.56 \text{CH}_2\text{O} + 0.22 \text{ALD2} + \text{XO}_2$	$K_0 = 1.0\text{E}-28 \cdot (300/T)^{4.5}$ $K_\infty = 8.8\text{E}-12 \cdot (300/T)^{0.85}$	
$\text{O}_3 + \text{C}_2\text{H}_4$	$\text{CH}_2\text{O} + 0.26 \text{HO}_2 + 0.12 \text{OH} + 0.43 \text{CO}$	$1.2\text{E}-14 \cdot \exp(-2630/T)$	[1]
$\text{OH} + \text{CH}_3\text{COCHO}$	$\text{XO}_2 + \text{C}_2\text{O}_3$	$1.5\text{E}-11$	[3]

Example, chemistry  
mechanism in EC-Earth

Reactants	Products	Rate expression	Reference
OH + ISOP	0.85 XO <sub>2</sub> + 0.61 CH <sub>2</sub> O + 0.58 OLE + 0.85 HO <sub>2</sub> + 0.15 XO <sub>2</sub> N + 0.03 CH <sub>3</sub> COCHO + 0.63 PAR	2.7E-11*exp(390/T)	[3]
O <sub>3</sub> + ISOP	0.9 CH <sub>2</sub> O + 0.55 OLE + 0.36 CO + 0.15 C <sub>2</sub> O <sub>3</sub> + 0.63 PAR + 0.3 HO <sub>2</sub> + 0.18 XO <sub>2</sub> + 0.03 CH <sub>3</sub> COCHO + 0.28 OH	1.04E-14*exp(-1995/T)	[3]
NO <sub>3</sub> + ISOP	0.9 HO <sub>2</sub> + 0.9 ORGNTR + 0.45 OLE + 0.12 ALD2 + 0.08 CH <sub>3</sub> COCHO + 0.1 NO <sub>2</sub> + 0.03 CH <sub>2</sub> O	3.15E-12*exp(-450/T)	[3]
NO + XO <sub>2</sub>	NO <sub>2</sub>	2.6E-12*exp(365/T)	[2]
XO <sub>2</sub> + XO <sub>2</sub>		6.8E-14 <sup>[KC81]</sup>	[2]
			[3]
NO + XO <sub>2</sub> N	ORGNTR	2.6E-12*exp(365/T) <sup>[KC79]</sup>	[2]
HO <sub>2</sub> + XO <sub>2</sub>	ROOH	7.5E-13*exp(700/T) <sup>[KC82]</sup>	[2]
PAR + RXPAR		8E-11	[4]
OH + ORGNTR	NO <sub>2</sub> + XO <sub>2</sub>	5.9E-13*exp(-360/T)	[2]
HO <sub>2</sub> + XO <sub>2</sub> N	ROOH	(KC81*KC82)/KC79	[5]
DMS + OH	SO <sub>2</sub>	1.1E-11*exp(-240/T)	[1]
DMS + OH	0.75 SO <sub>2</sub> + 0.25 MSA	1.0E-39*exp(5820/T)	[1]
		5.0E-30*exp(6280/T)	
DMS + NO <sub>3</sub>	SO <sub>2</sub>	1.9E-13*exp(520/T)	[6]
OH + SO <sub>2</sub>	SO <sub>4</sub> <sup>2-</sup>	K <sub>0</sub> = 3.3E-31*(300/T) <sup>4.3</sup> K <sub>∞</sub> = 1.6E-12*(300/T)	[1]
OH + NH <sub>3</sub>	NH <sub>2</sub>	1.7E-12*exp(-710/T)	[1]
NO + NH <sub>2</sub>		4.0E-12*exp(450/T)	[1]
NO <sub>2</sub> + NH <sub>2</sub>		2.1E-12*exp(650/T)	[1]
HO <sub>2</sub> + NH <sub>2</sub>		3.4E-11	[1]
O <sub>2</sub> + NH <sub>2</sub>		6.0E-21	[1]
O <sub>3</sub> + NH <sub>2</sub>		4.3E-12*exp(-930/T)	[1]

Example, chemistry  
mechanism in EC-Earth

# Atmospheric chemistry in climate models

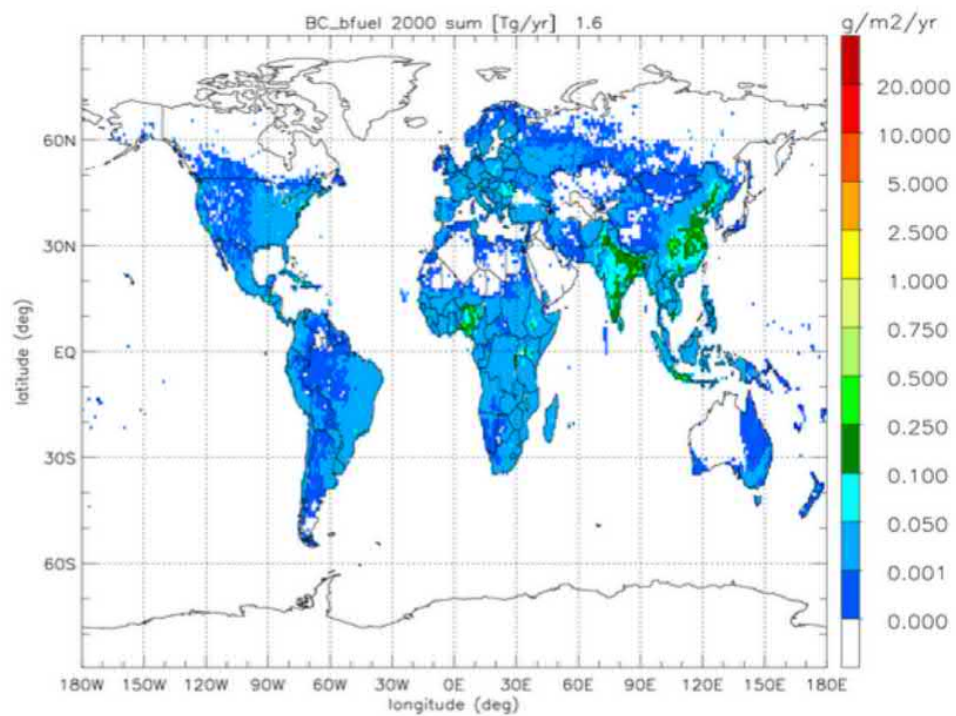
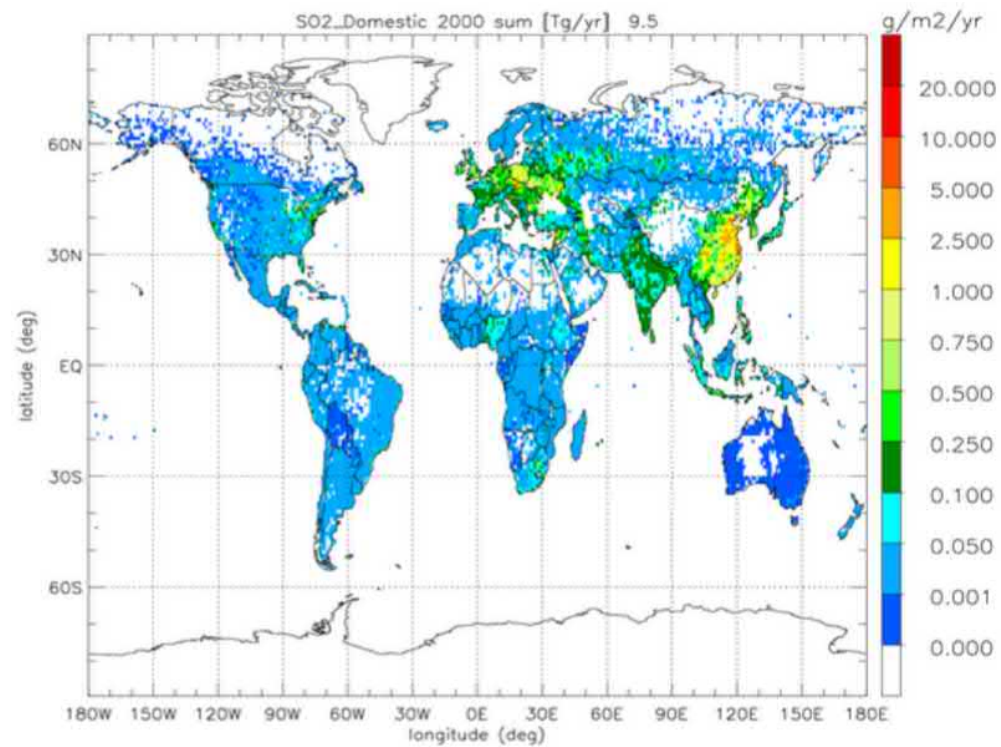
- In addition to gas-phase reactions, there is heterogeneous and aqueous-phase chemistry
  - e.g. oxidation of  $\text{SO}_2$  by  $\text{H}_2\text{O}_2$  and  $\text{O}_3$  in cloud-phase and aerosol-phase (aqueous)
  - Conversion of  $\text{N}_2\text{O}_5$  to  $\text{HNO}_3$  on cloud droplets
  - Organic reactions and formation of secondary organic aerosol in aqueous-phase



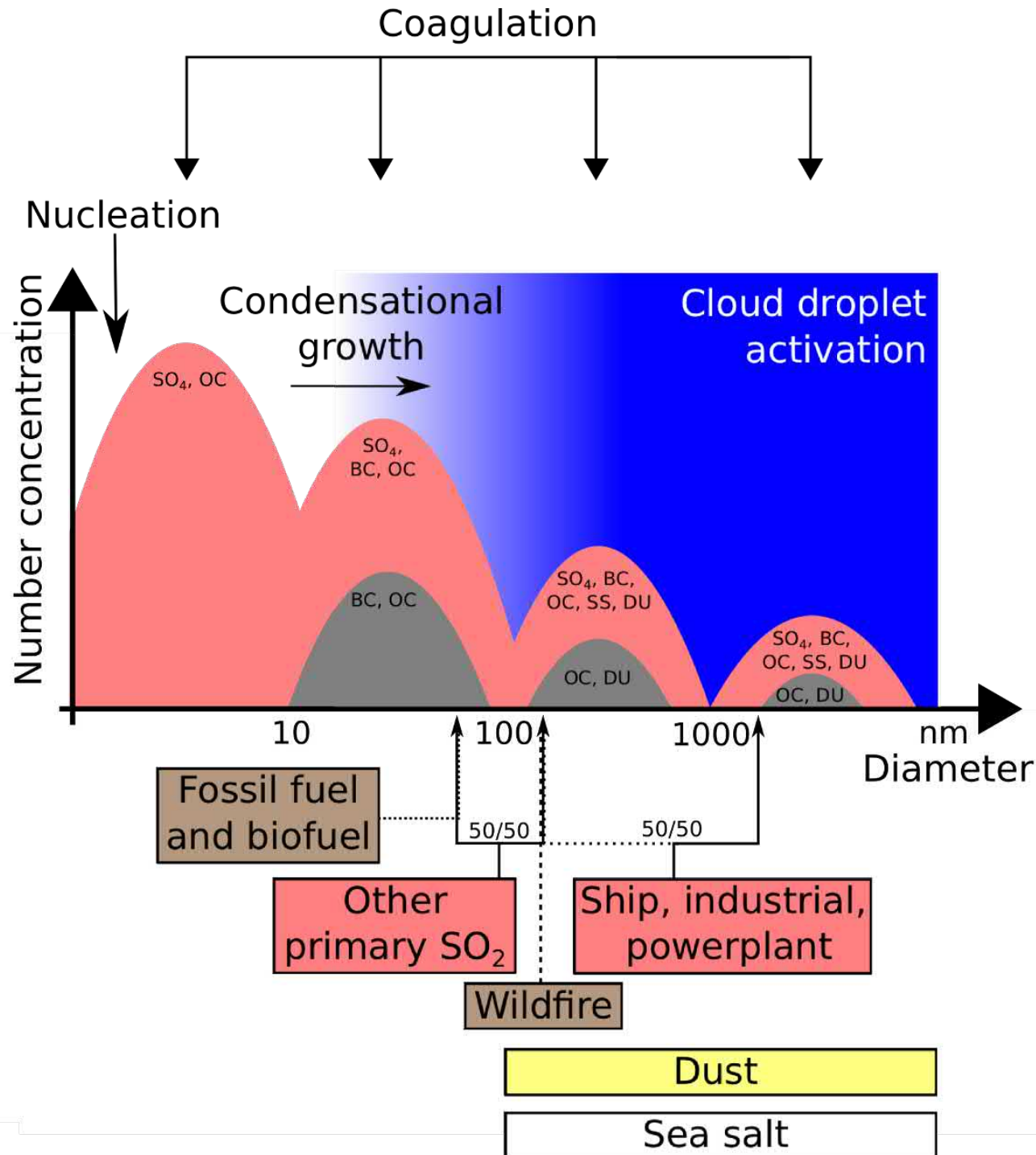
**How to include sources of aerosols?**

# Anthropogenic aerosol and precursor sources

- Typically, anthropogenic emissions are
  - Prescribed annual or monthly maps
  - Primary aerosols: black carbon, organic carbon
  - Precursors:  $\text{SO}_2$ ,  $\text{NH}_3$ , aromatics, ...
  - Sectoral information (industry, power generation, traffic, ...)
  - Limited vertical profiles: typically low (surface) and high (e.g. stack) emissions
  - No size information: model-specific assumptions for emission size-distribution, typically log-normal distribution



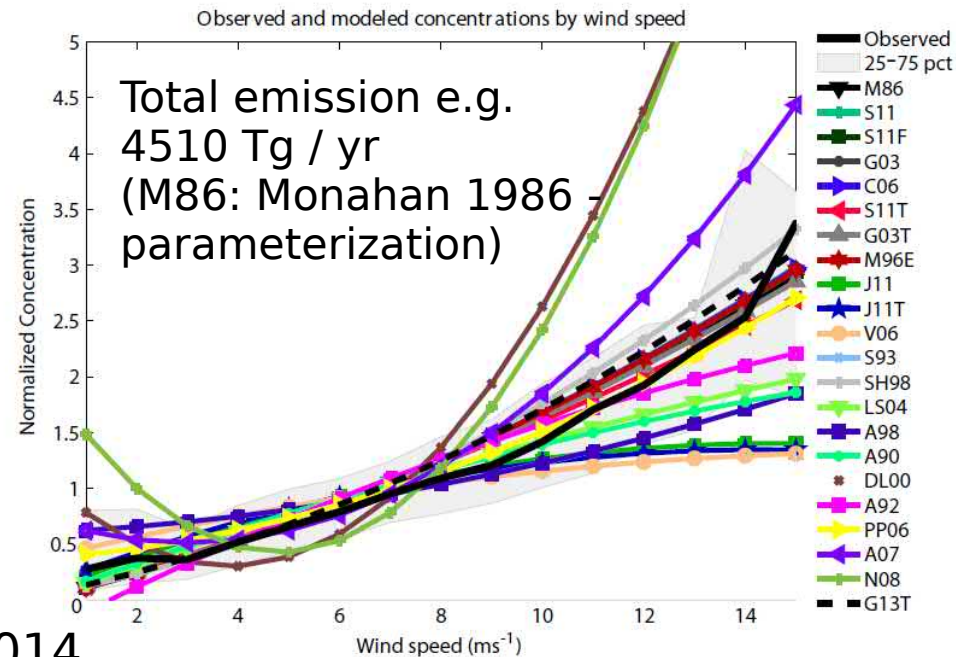
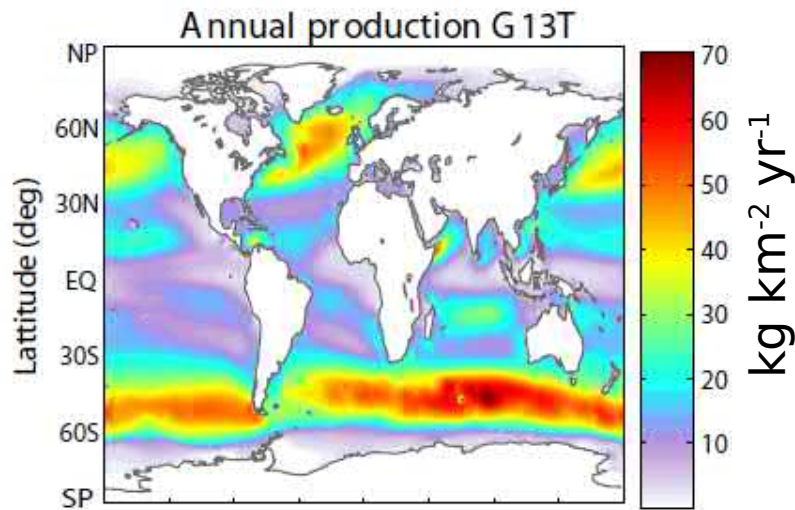
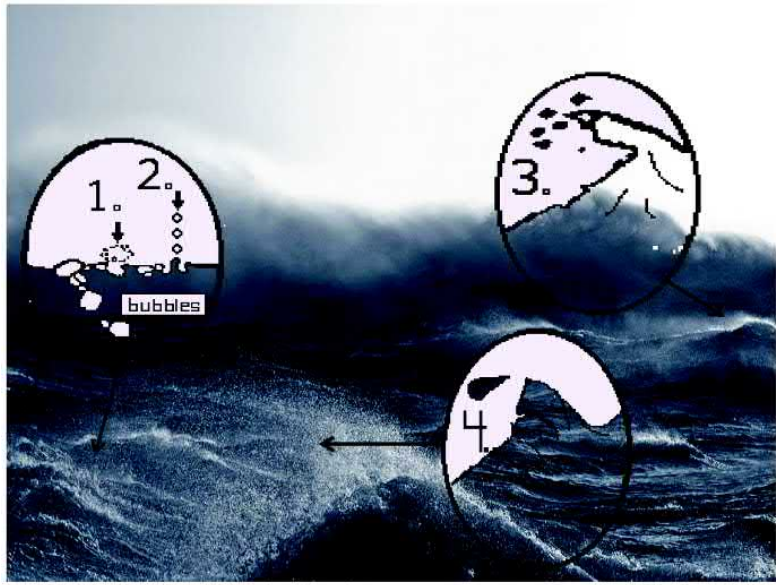
What size is assumed for aerosol emissions: M7 (used in e.g. ECHAM and EC-Earth)



# Sea spray sources

$$\frac{dF(D_p, U_{10}, T, S, O)}{dD_p} = W(U_{10}, D_p) \cdot \frac{dF_N D_p}{dD_p} \cdot T_W(T, D_p) \cdot S_W(S, D_p) \cdot O_W(O, D_p).$$

$D_p$  = dry diameter  
 $W$  = white-cap fraction  
 $U_{10}$  = 10m wind speed  
 $F_N$  = shape function  
 $T$  = ocean temperature  
 $S$  = ocean salinity  
 $O$  = sea state

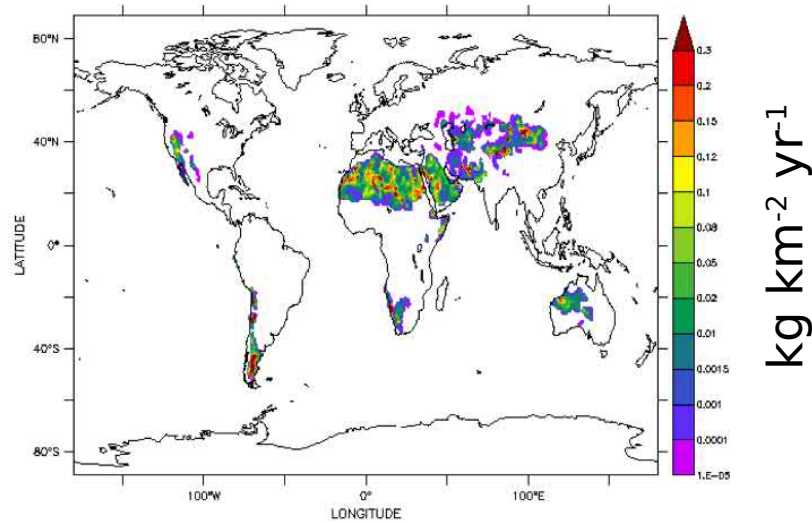


Grythe et al., 2014

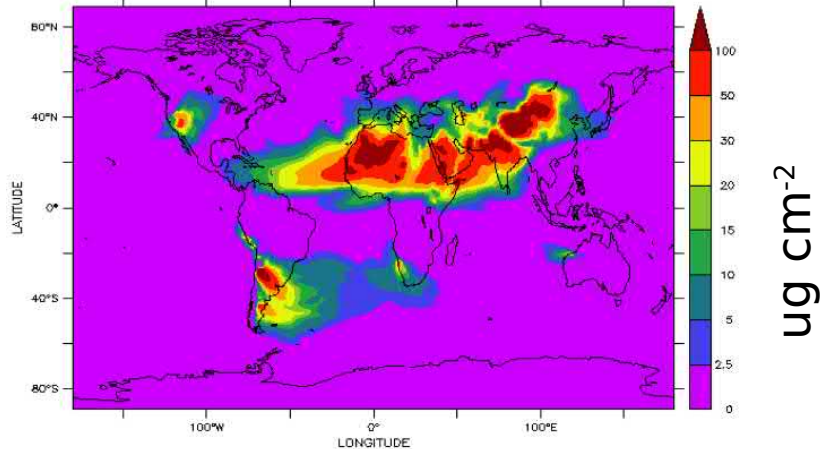


# Dust sources

Dust emission



Dust loading



**Dust emission flux F:**  
friction velocity  
threshold friction velocity  
clay content in the soil  
bare soil fraction  
source erodibility

Model	Emission [ $\text{Tg yr}^{-1}$ ]
CAM	4313
GISS	1507
GOCART	3157
SPRINTARS	3995
MATCH	981
MOZGN	2371
UMI	1688
ECMWF	514
LOA	1276
UIO_CTM	1572
LSCE	1158
ECHAM5-HAM	664
MIRAGE	2066
TM5	1683
AEROCOM-MEDIAN	1123

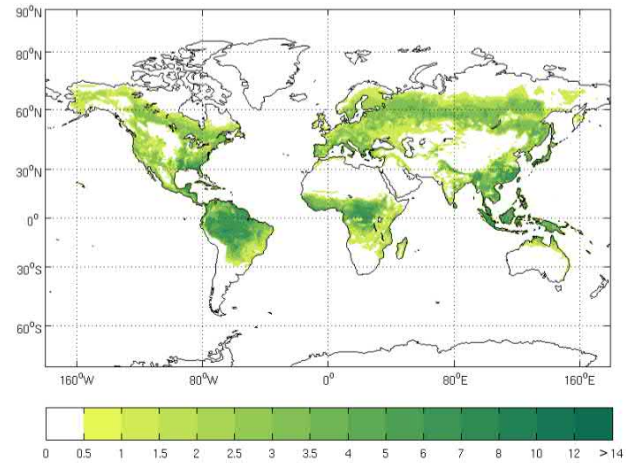
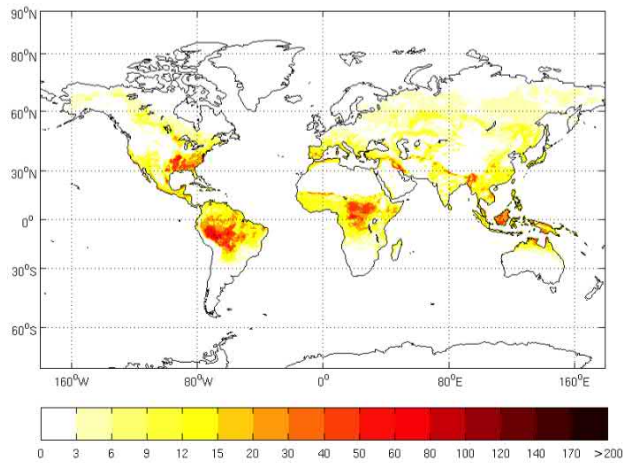
Huneus et al., 2011

# Biogenic sources

## Biogenic Volatile Organic Compounds (BVOCs)

Sindelarova et al.,  
2014

mg m<sup>-2</sup> day<sup>-1</sup>



Emission activity  
factor:

$$\gamma = C_{ce} \cdot LAI \cdot \gamma_P \cdot \gamma_T \cdot \gamma_A \cdot \gamma_{SM} \cdot \gamma_{CO_2}$$

normalization

Leaf Area Index

Light

Temperature

Leaf age

Soil moisture

CO<sub>2</sub> inhibition

# Other aerosol and precursor sources

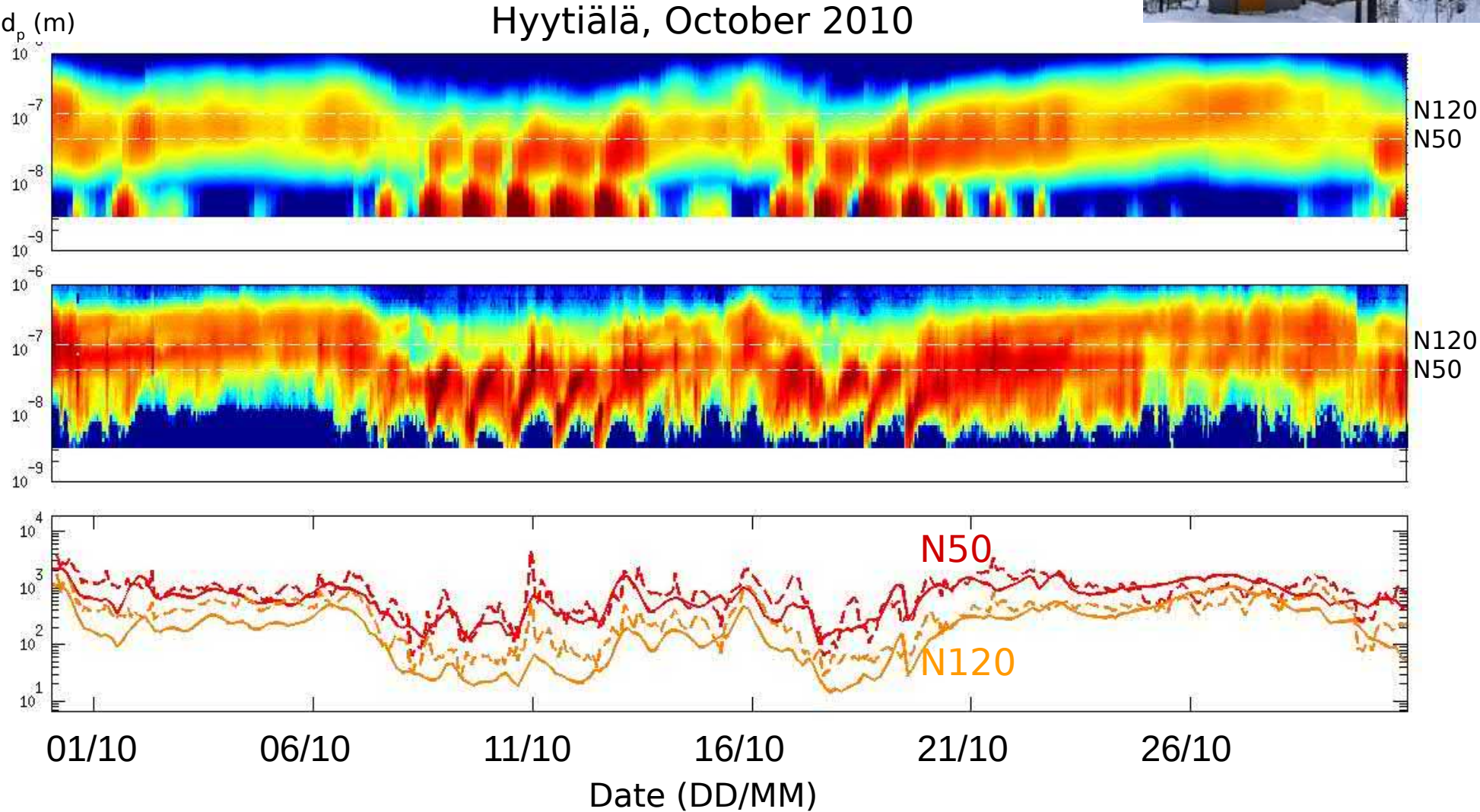
- Volcanic sources:  $\text{SO}_2$ , typically annual-mean for each source, with simplified vertical profile
- Wildfires
- Marine organics
- Primary biological aerosol particles (PBAPs)



Evaluation of model against  
in-situ DMPS observations



OBSERVATION MODEL



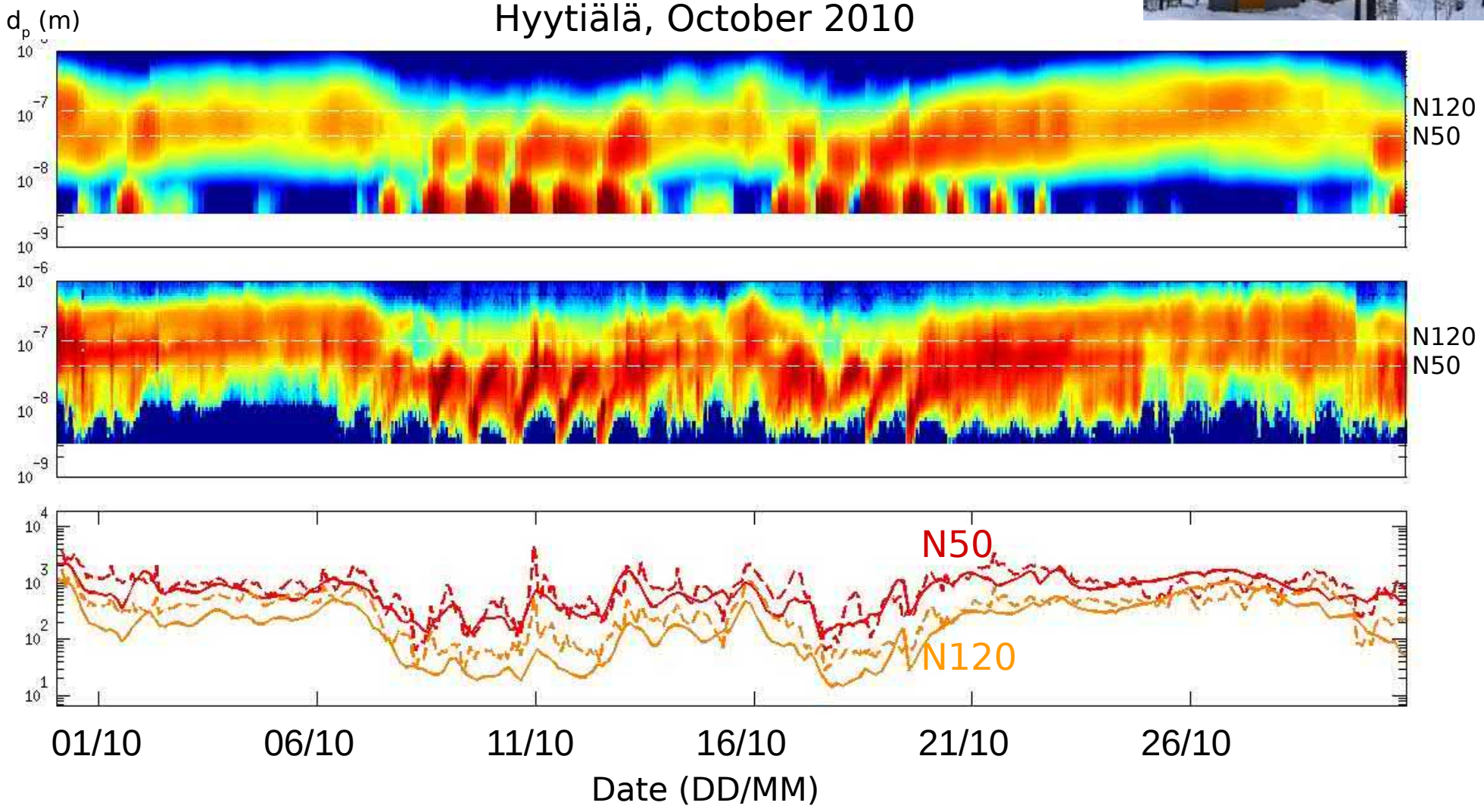
Evaluation of model against  
in-situ DMPS observations

Even a global model with 200  
km grid-size can predict  
events in Hyytiälä!



Hyytiälä, October 2010

OBSERVATION MODEL

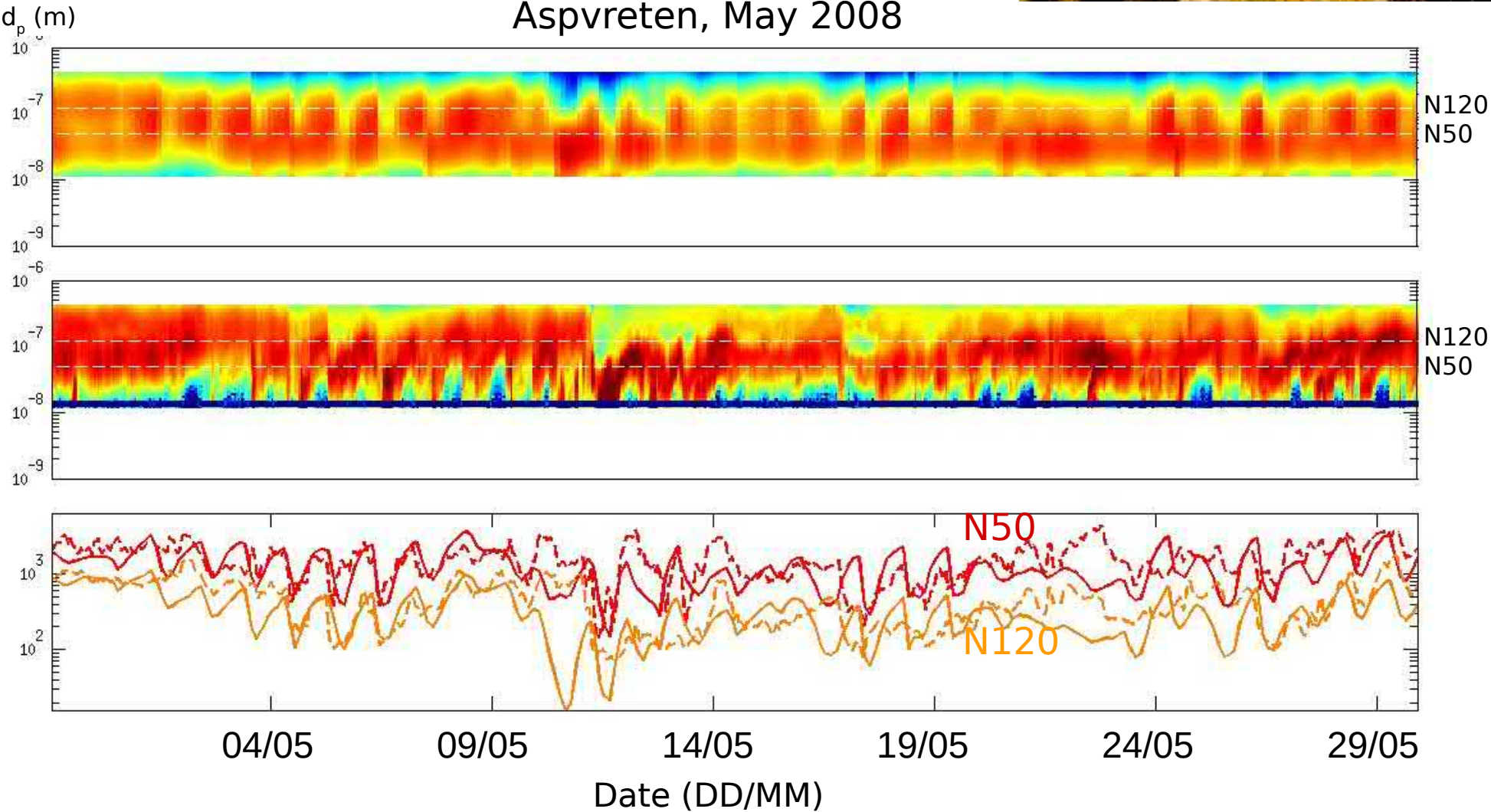




Evaluation of model against  
in-situ DMPS observations



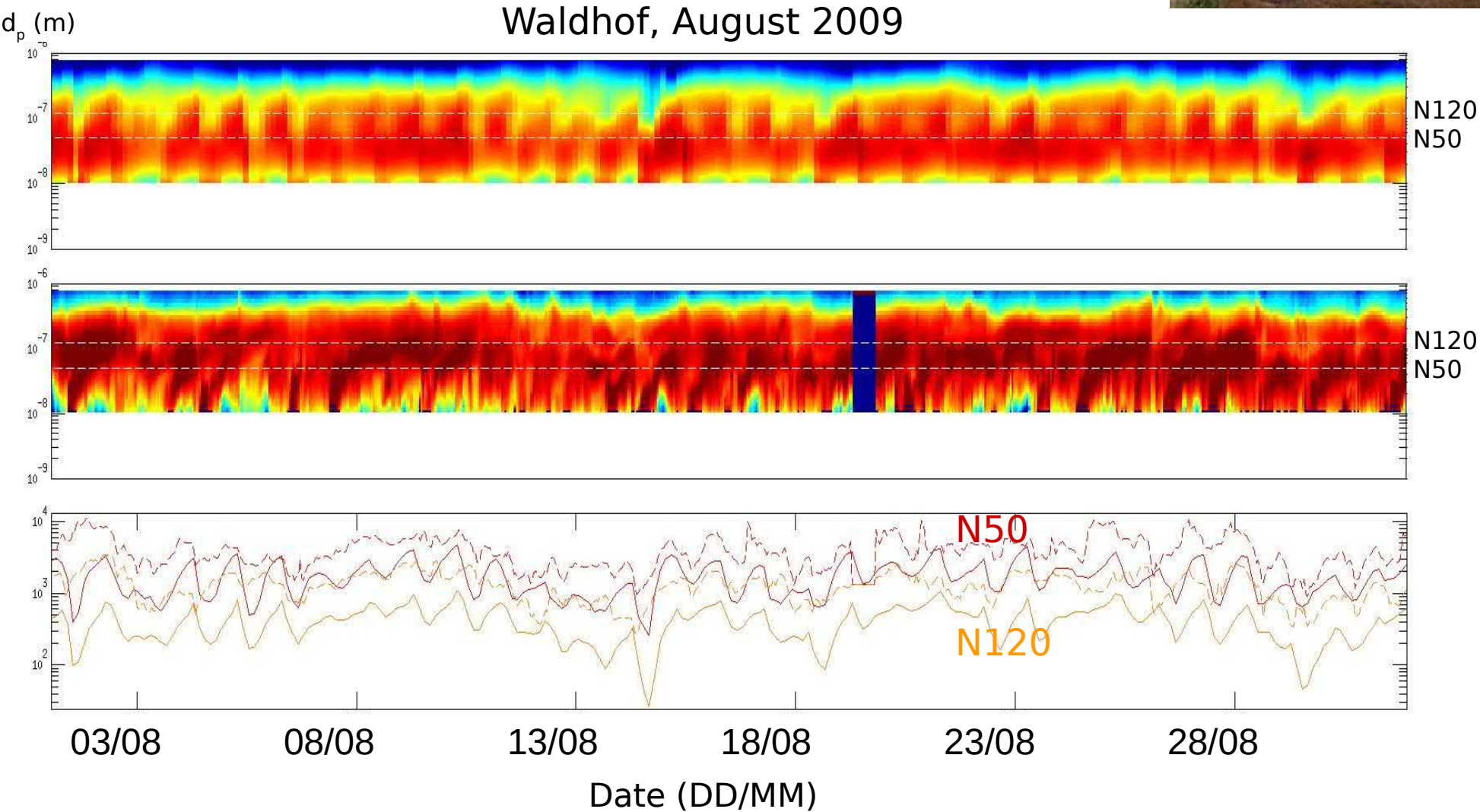
OBSERVATION MODEL



# Evaluation of model against in-situ DMPS observations



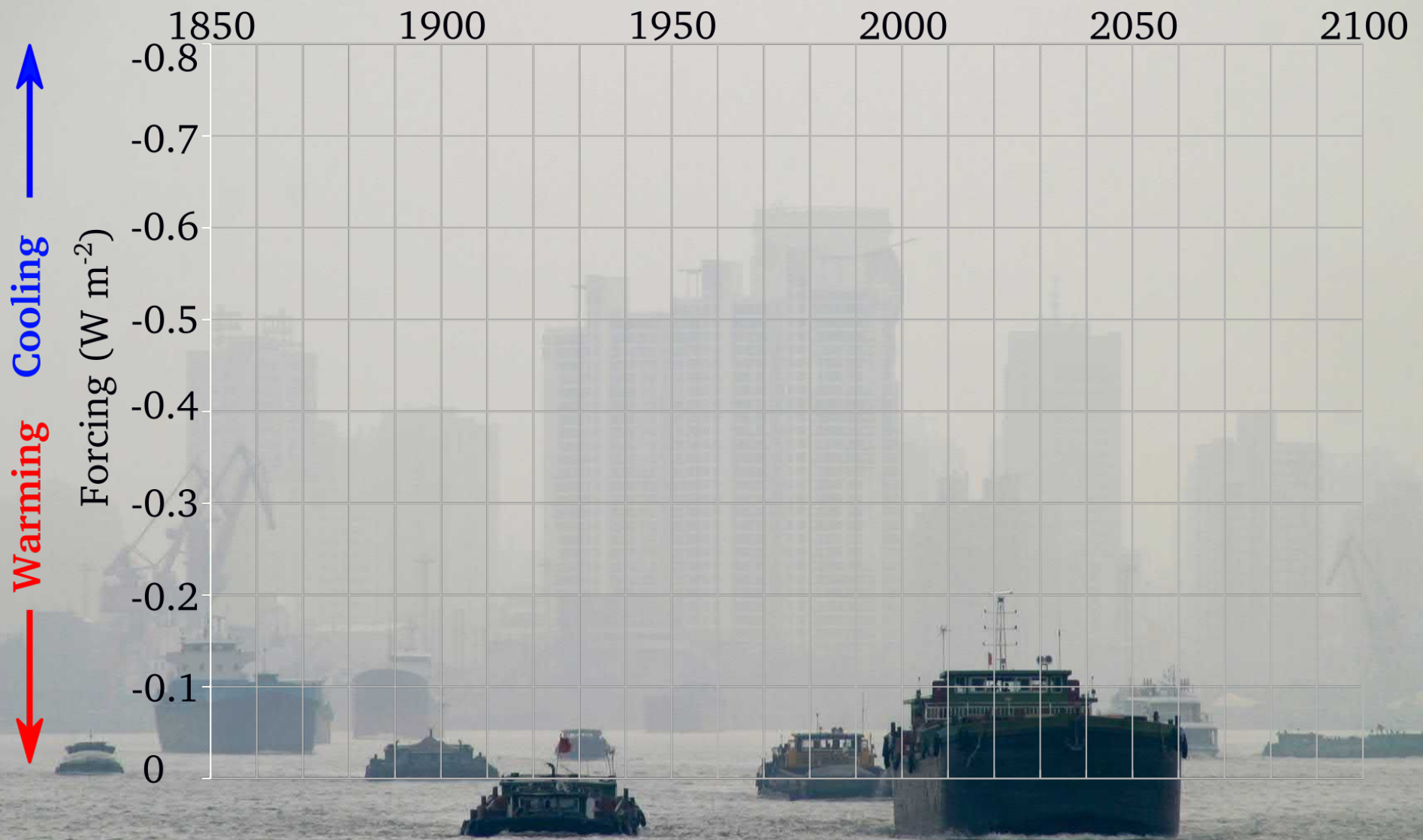
MODEL  
OBSERVATION



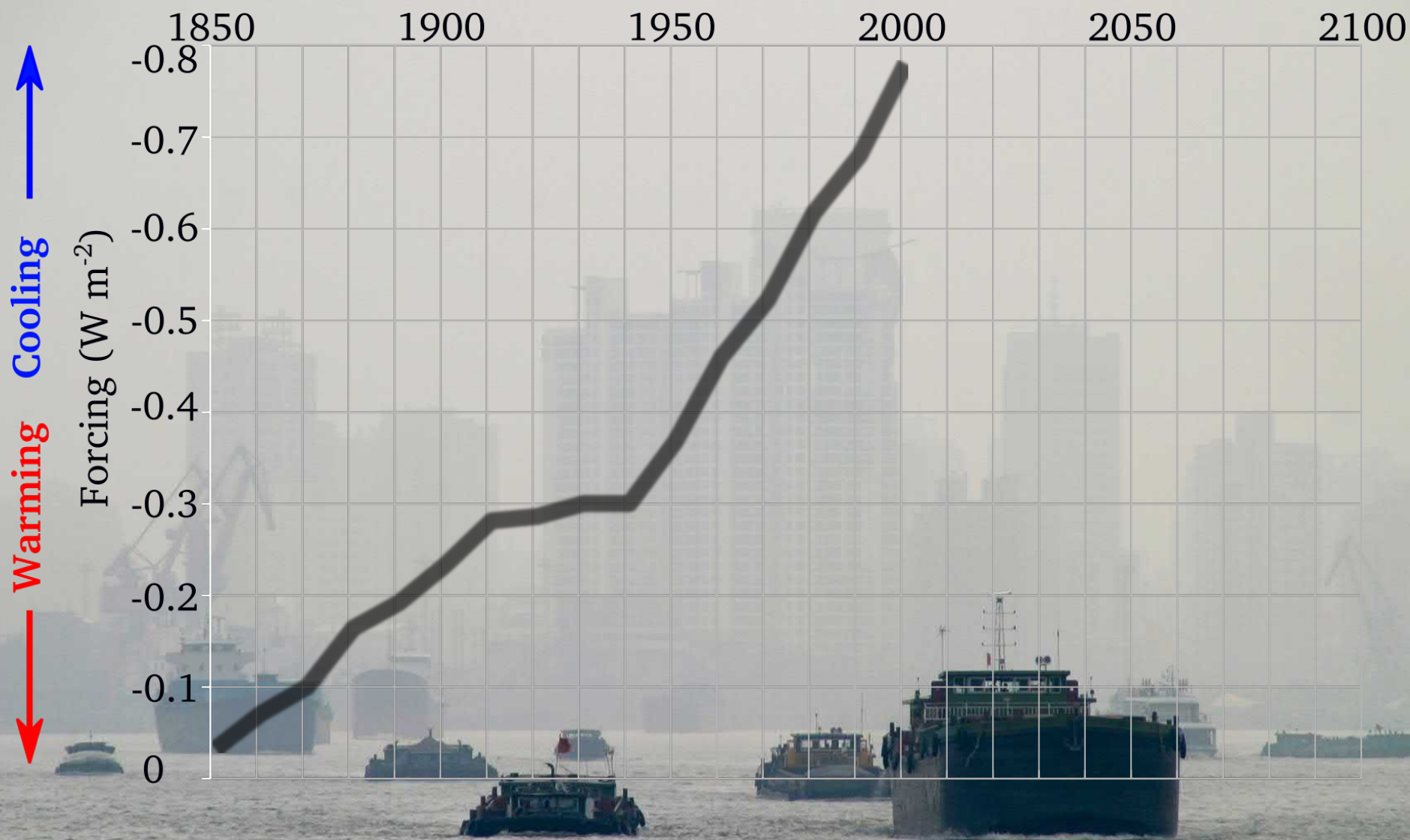
## **Aerosol forcing**

How are anthropogenic aerosols influencing climate?



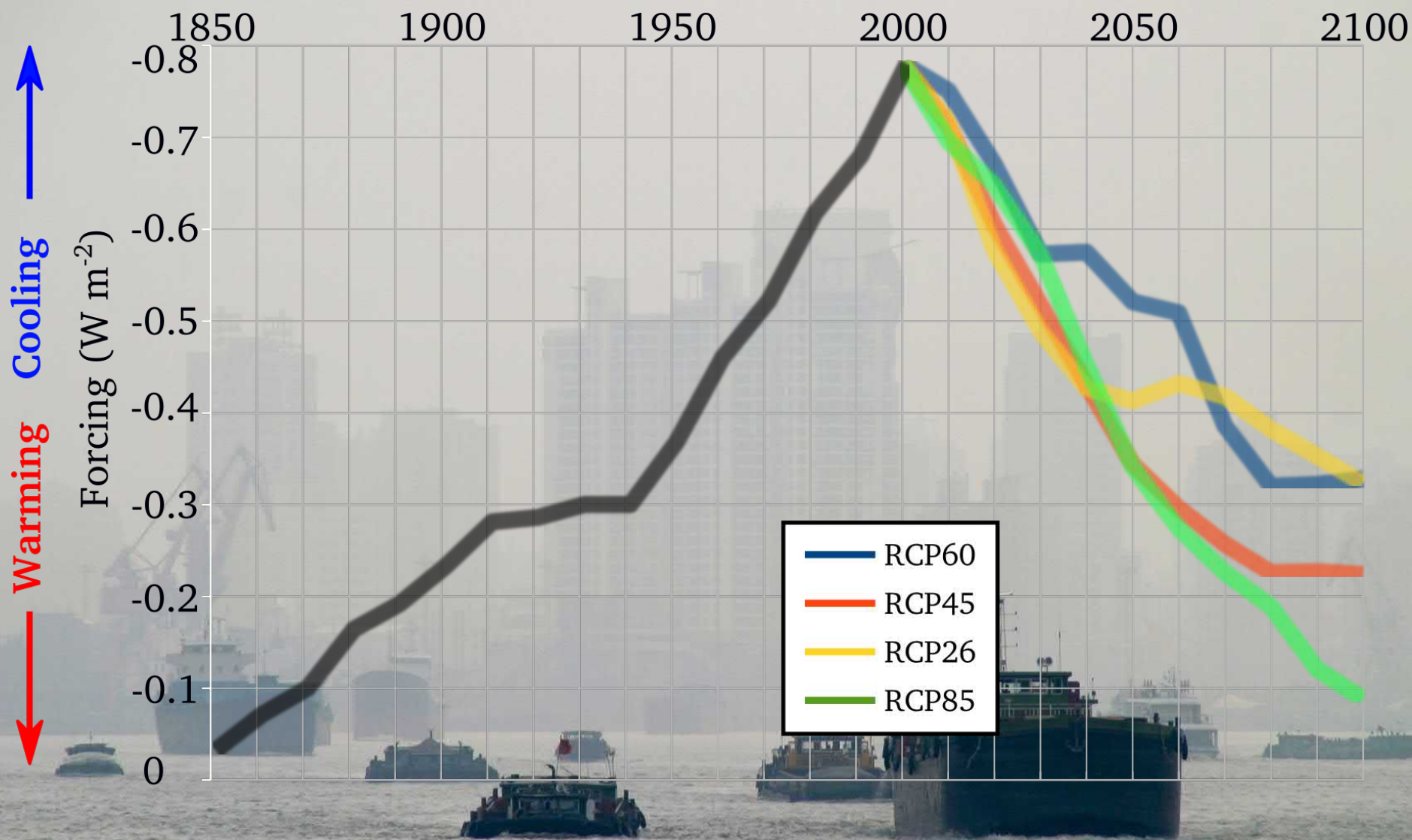


Aerosol forcing: more negative → more cooling effect  
from anthropogenic aerosols



Aerosol forcing: more negative  $\rightarrow$  more cooling effect  
from anthropogenic aerosols





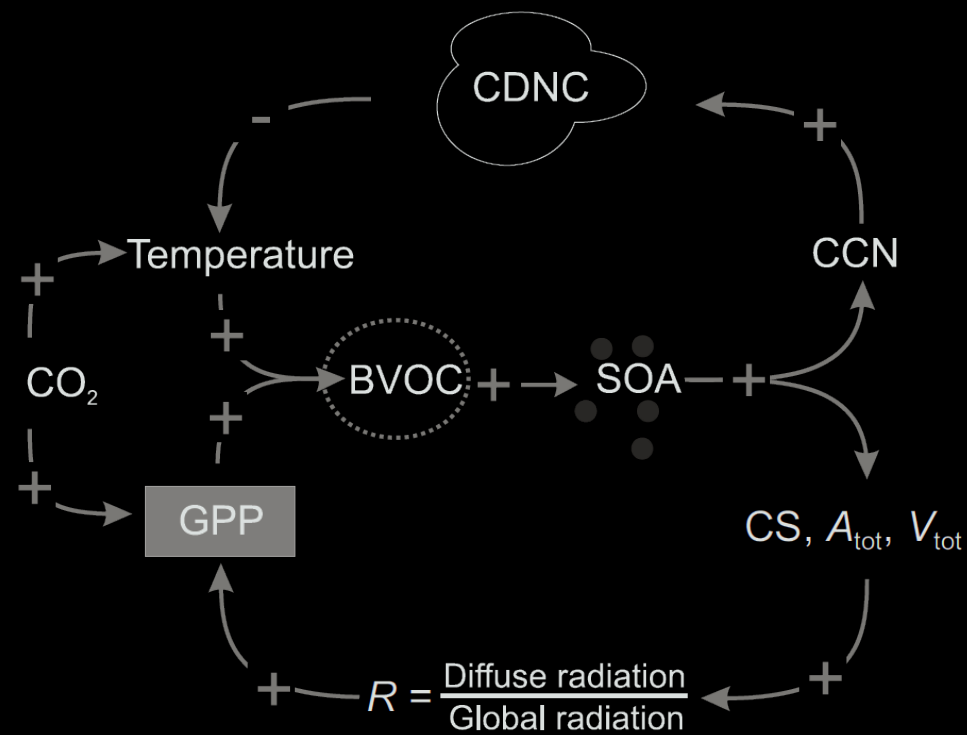
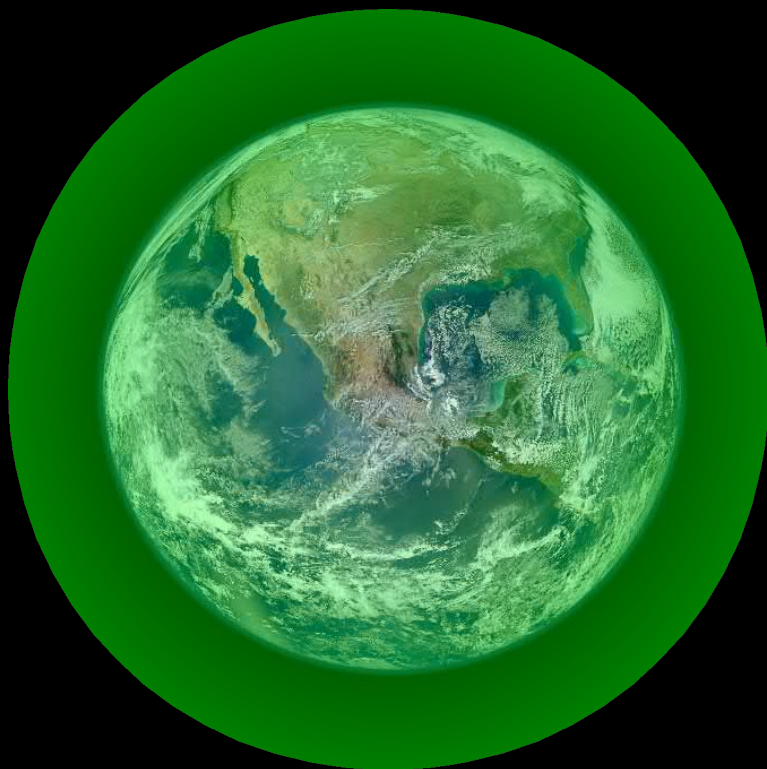
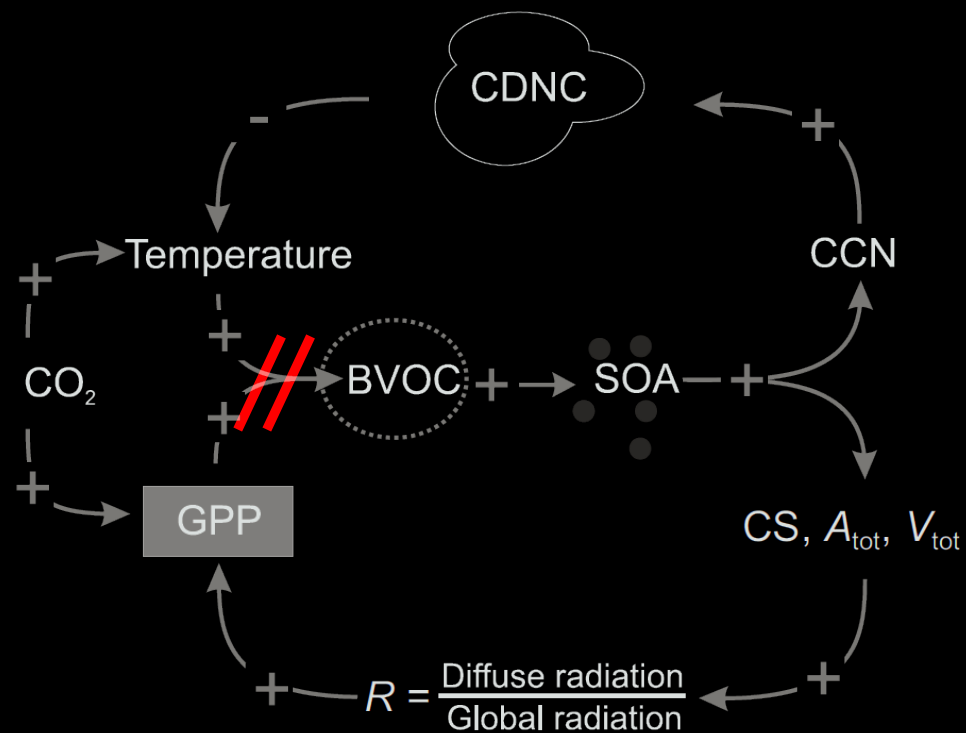
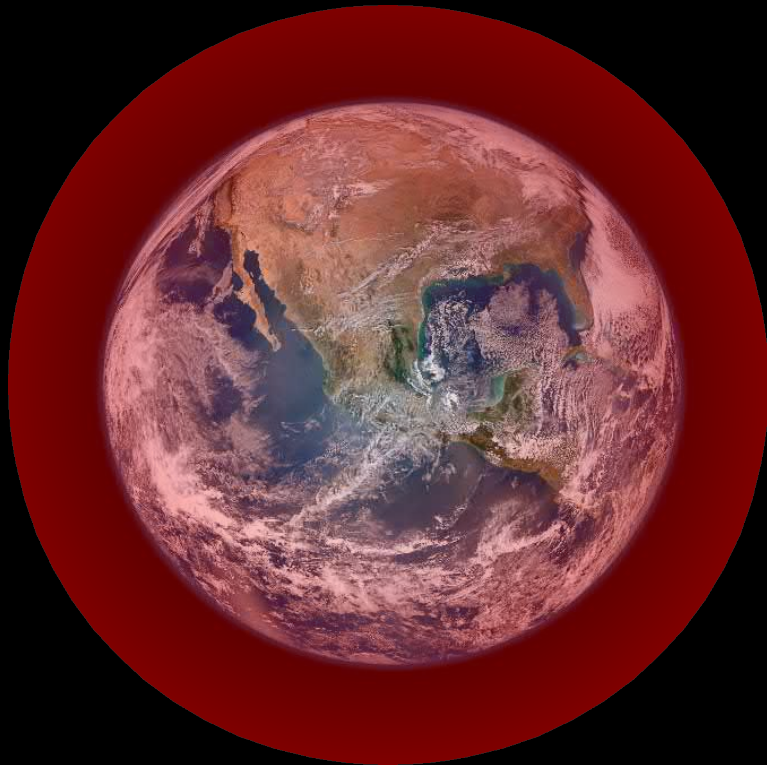
Aerosol forcing: more negative  $\rightarrow$  more cooling effect from anthropogenic aerosols

## **Aerosol-climate feedbacks**

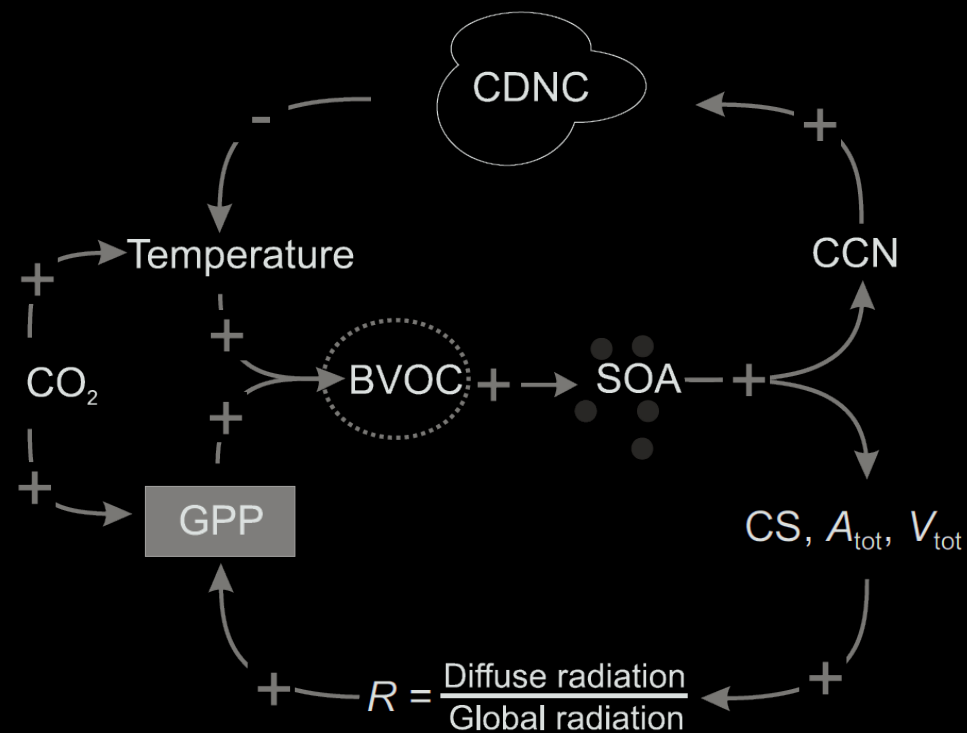
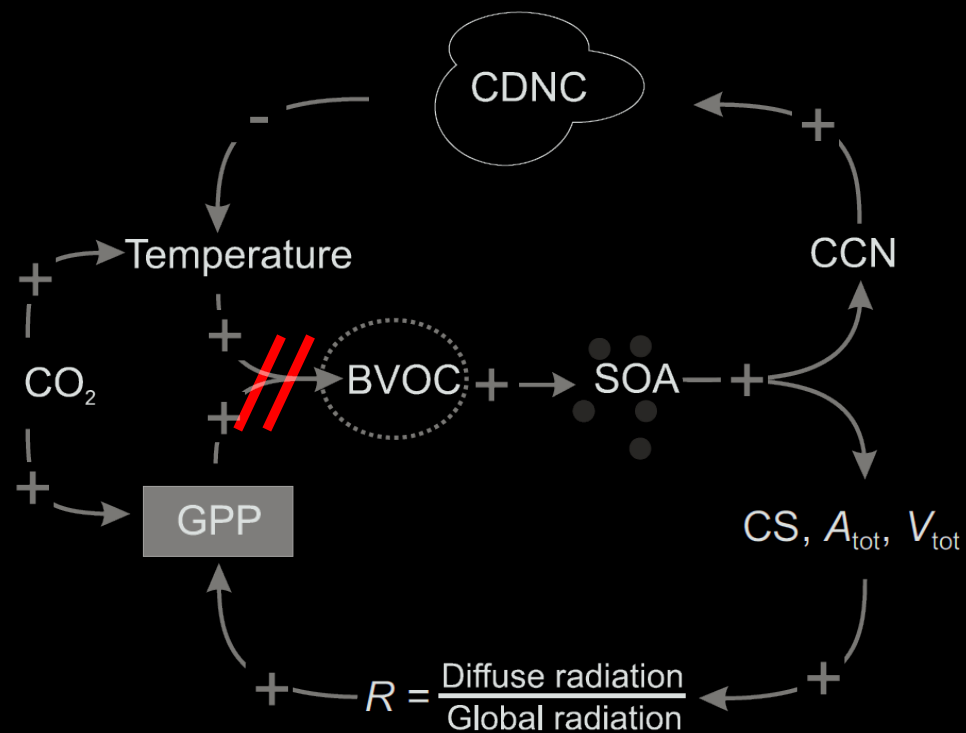
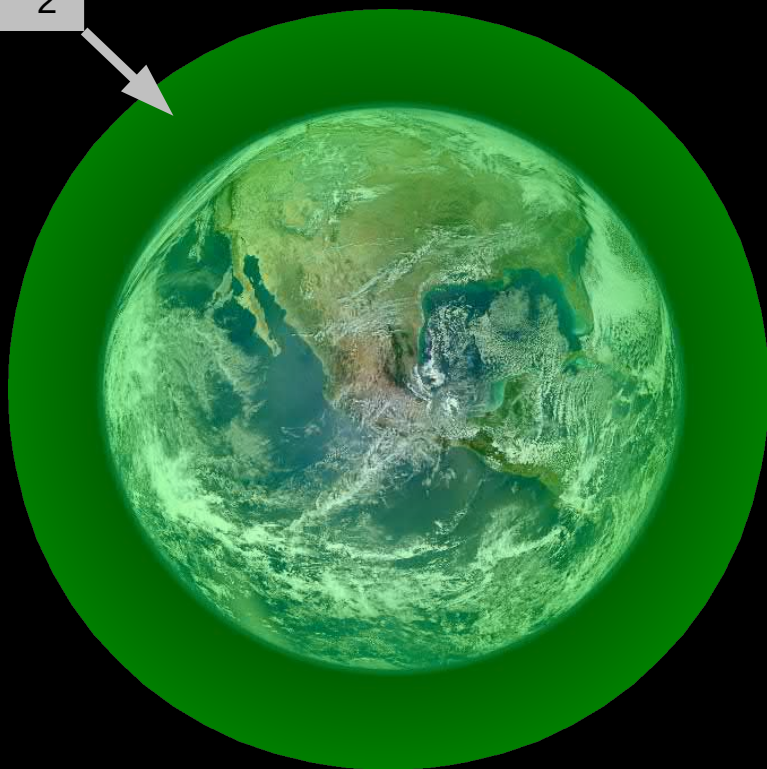
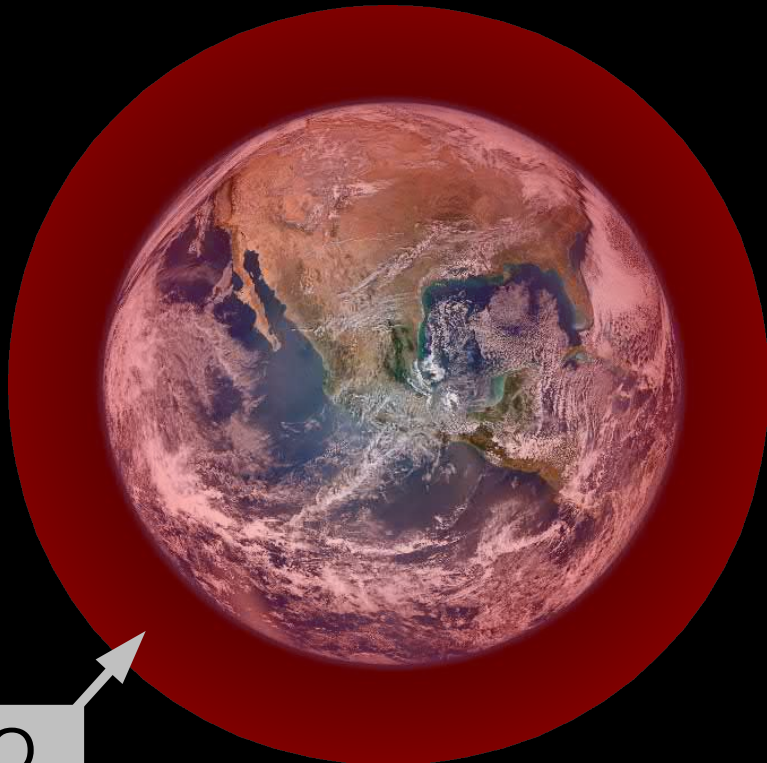
How does climate change modify aerosol sources or aerosol-climate effects?



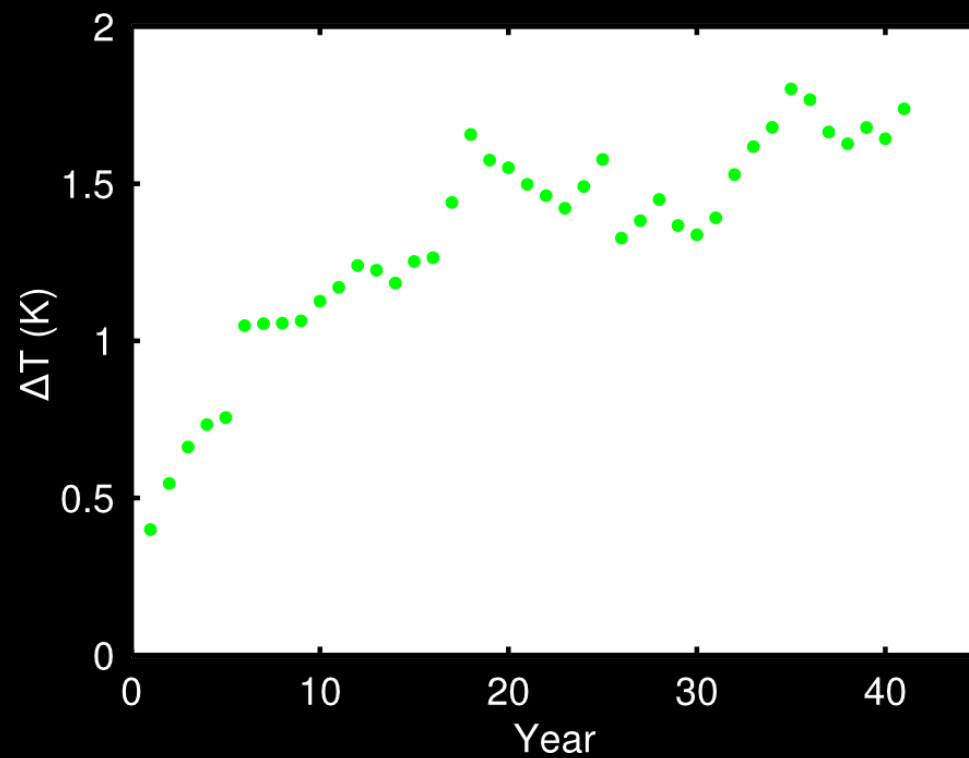
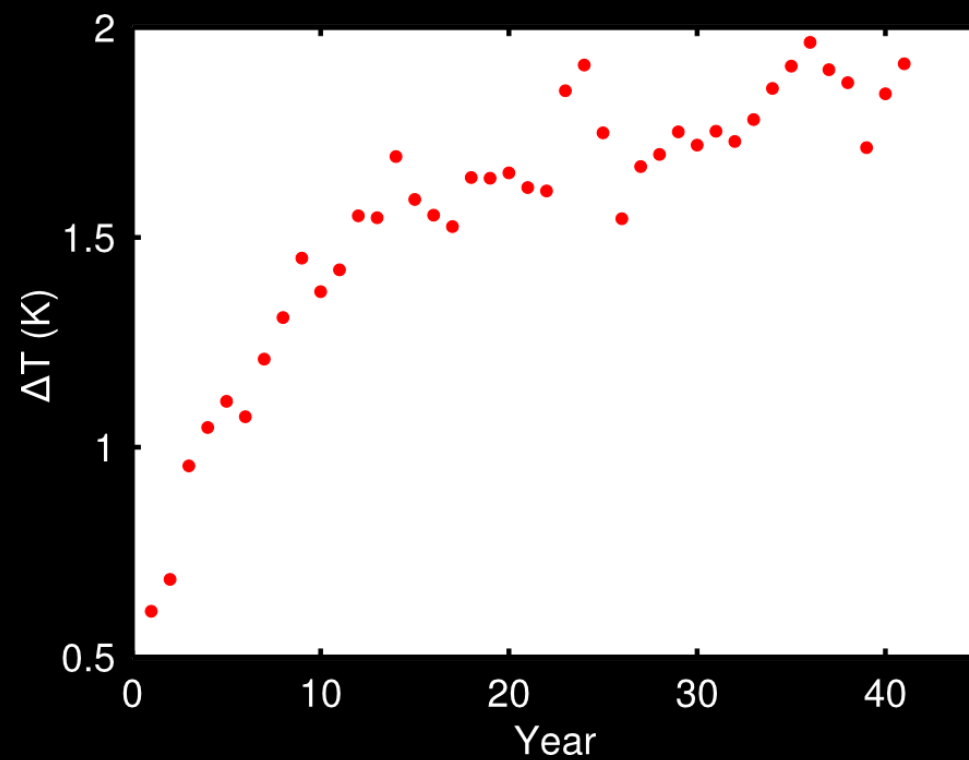
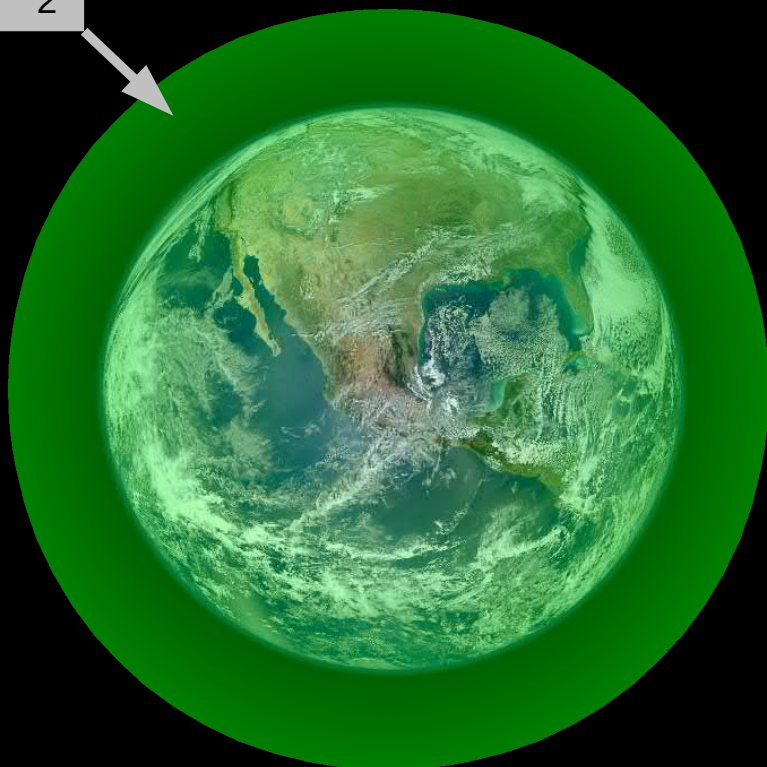
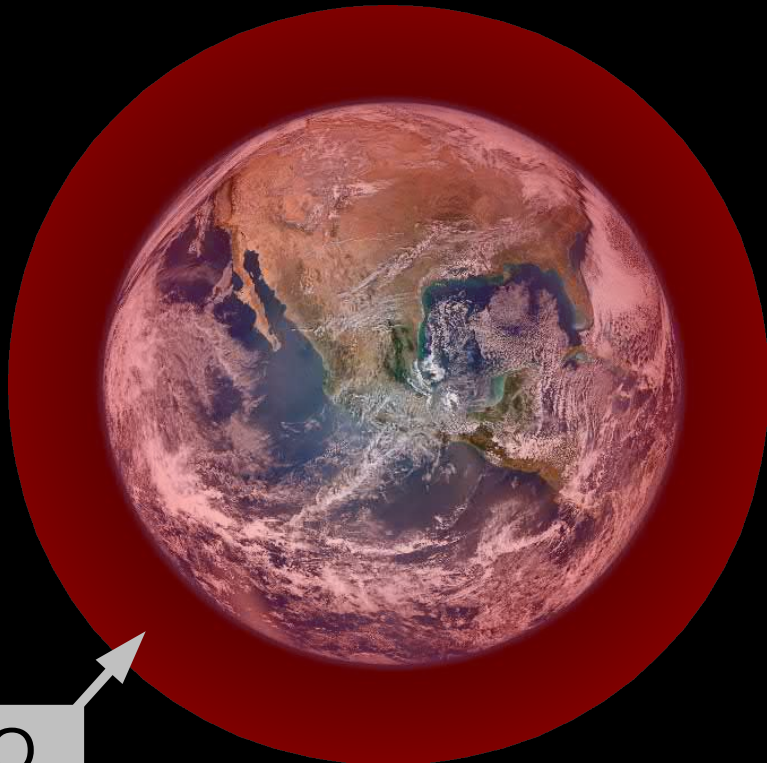




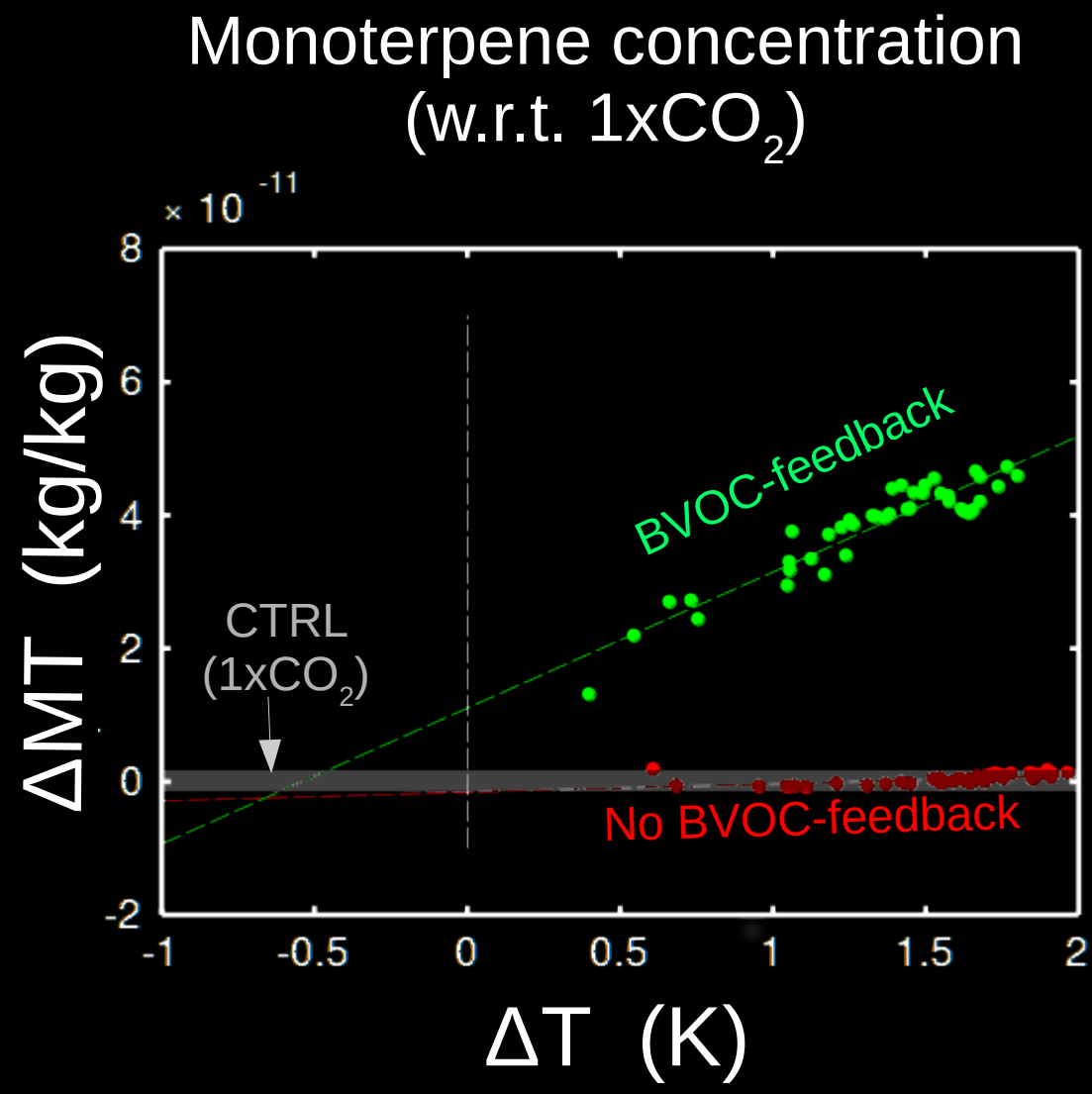
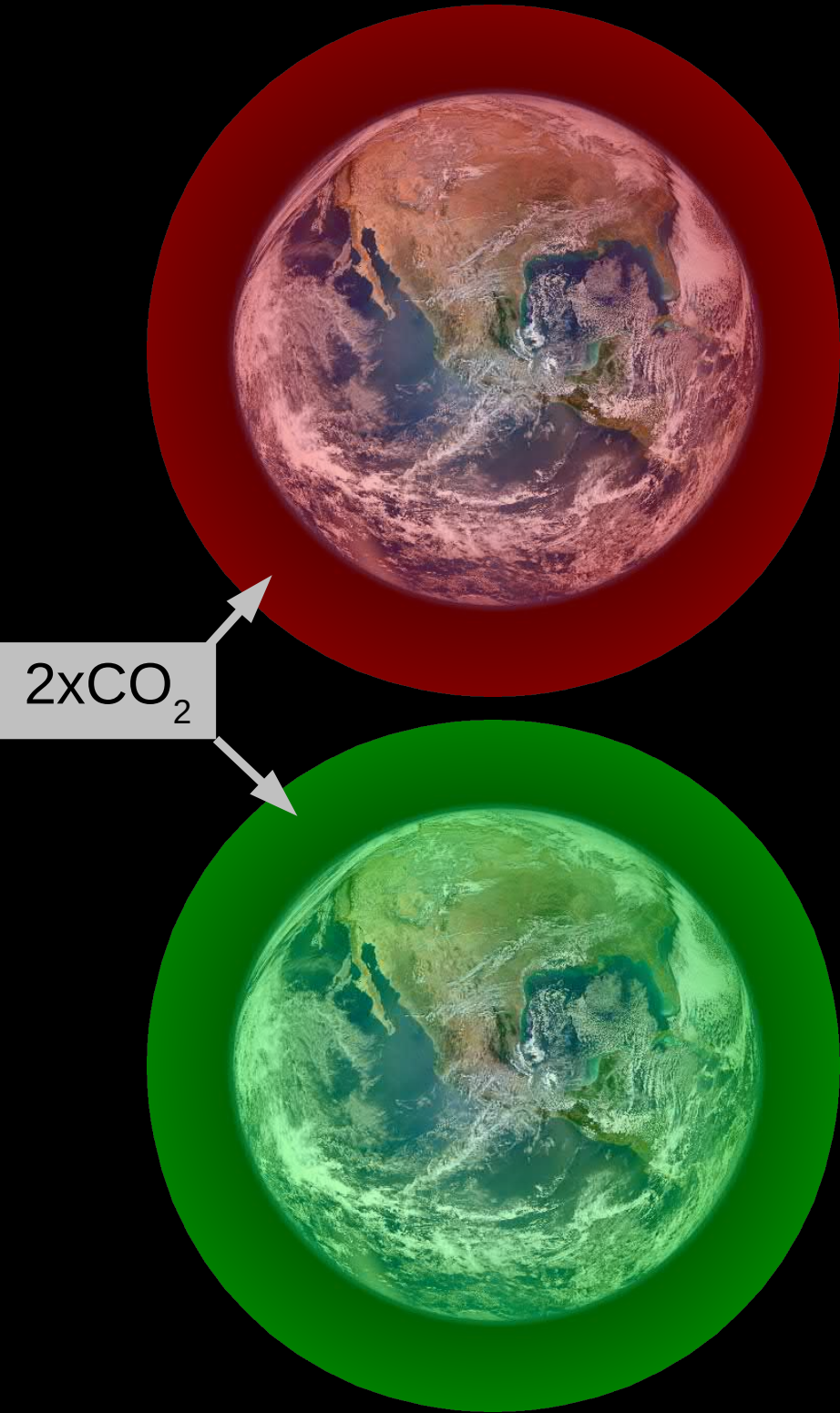
2xCO<sub>2</sub>



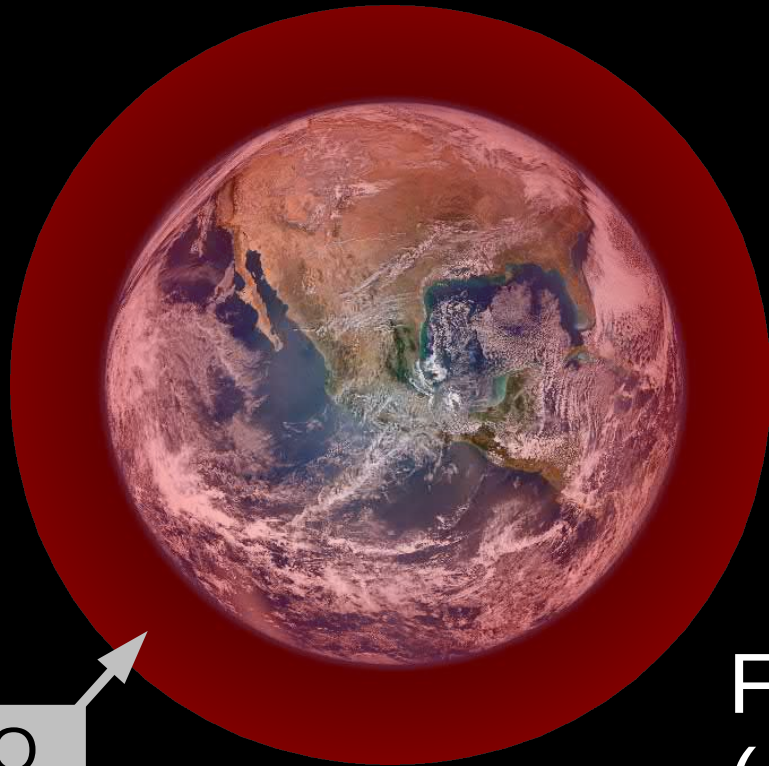
2xCO<sub>2</sub>





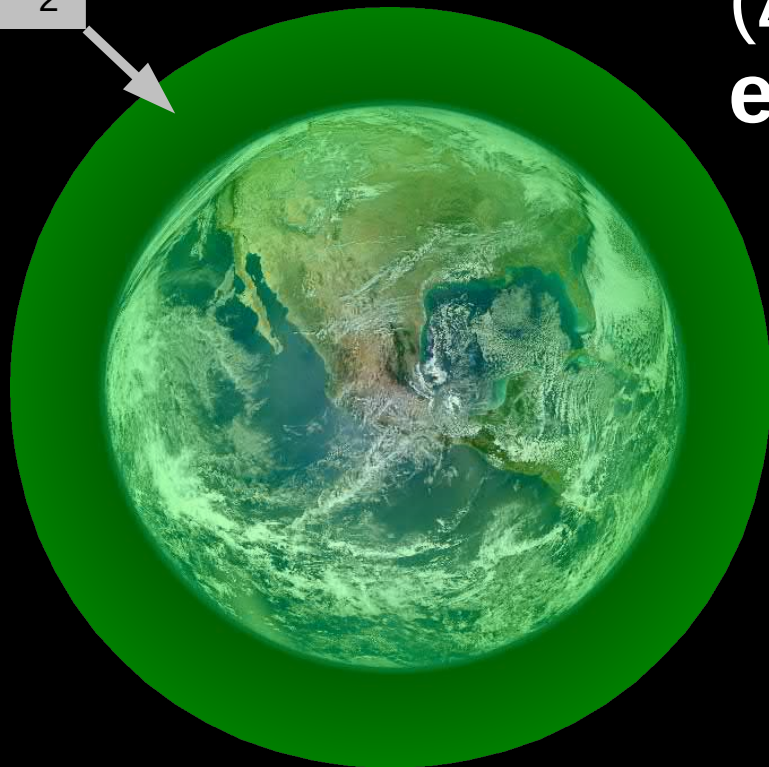






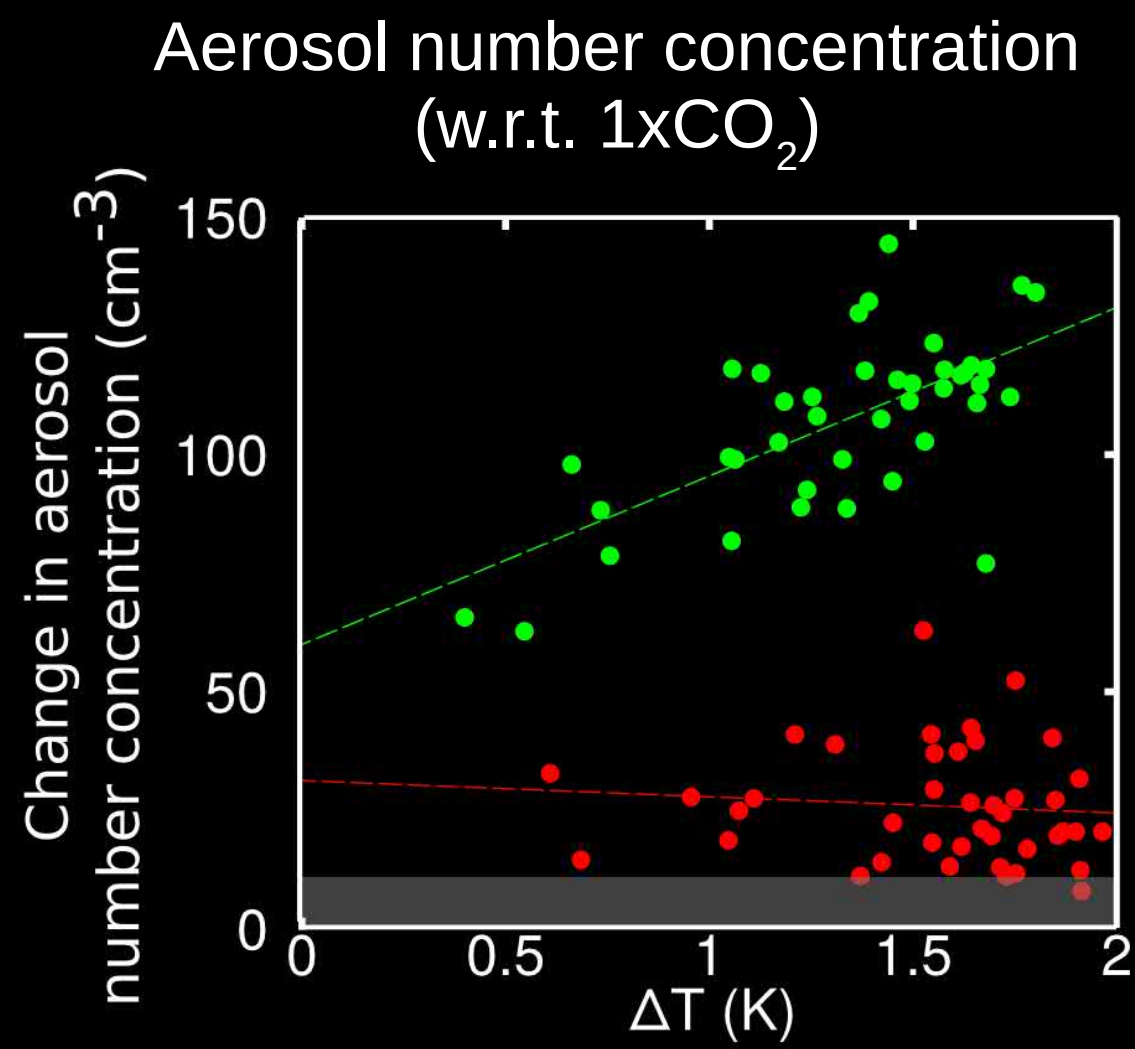
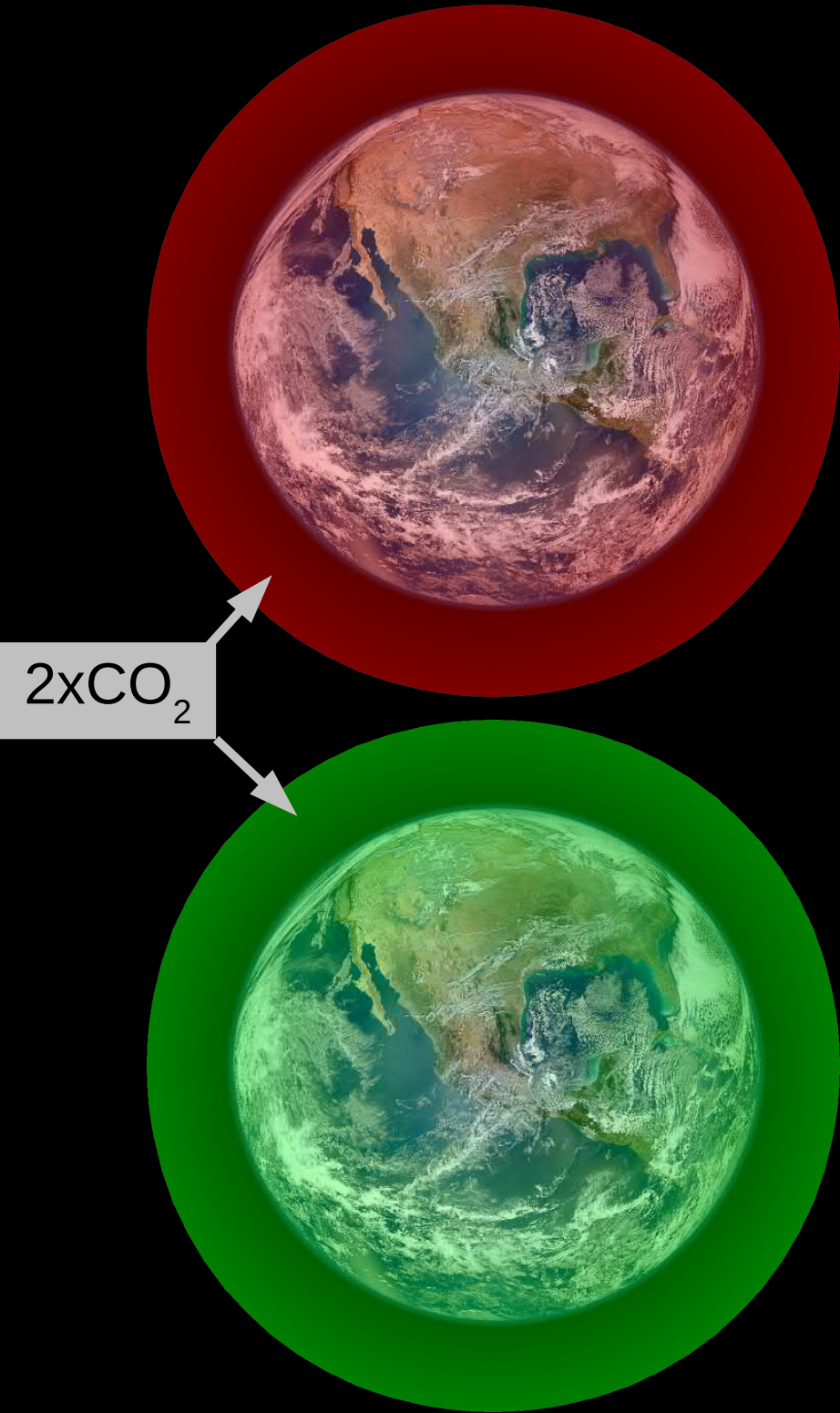
76 Tg yr<sup>-1</sup>

For equilibrium climate change  
( $\Delta T \approx 3.2$  K) **monoterpene  
emission** increases by 32%

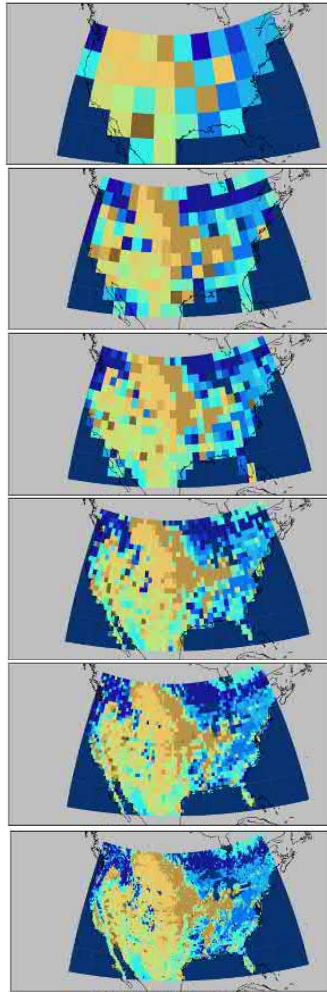


100 Tg yr<sup>-1</sup>

Heald et al. (2008): +19% (1.8K)  
Liao et al. (2006): +58% (4.8K)



**Climate model  
resolution** has  
improved  
significantly in last  
decades



## IPCC Assessment report (year)

FAR (1990)  
Resolution ~500 km

SAR (1995)  
Resolution ~250 km

TAR (2001)  
Resolution ~180 km

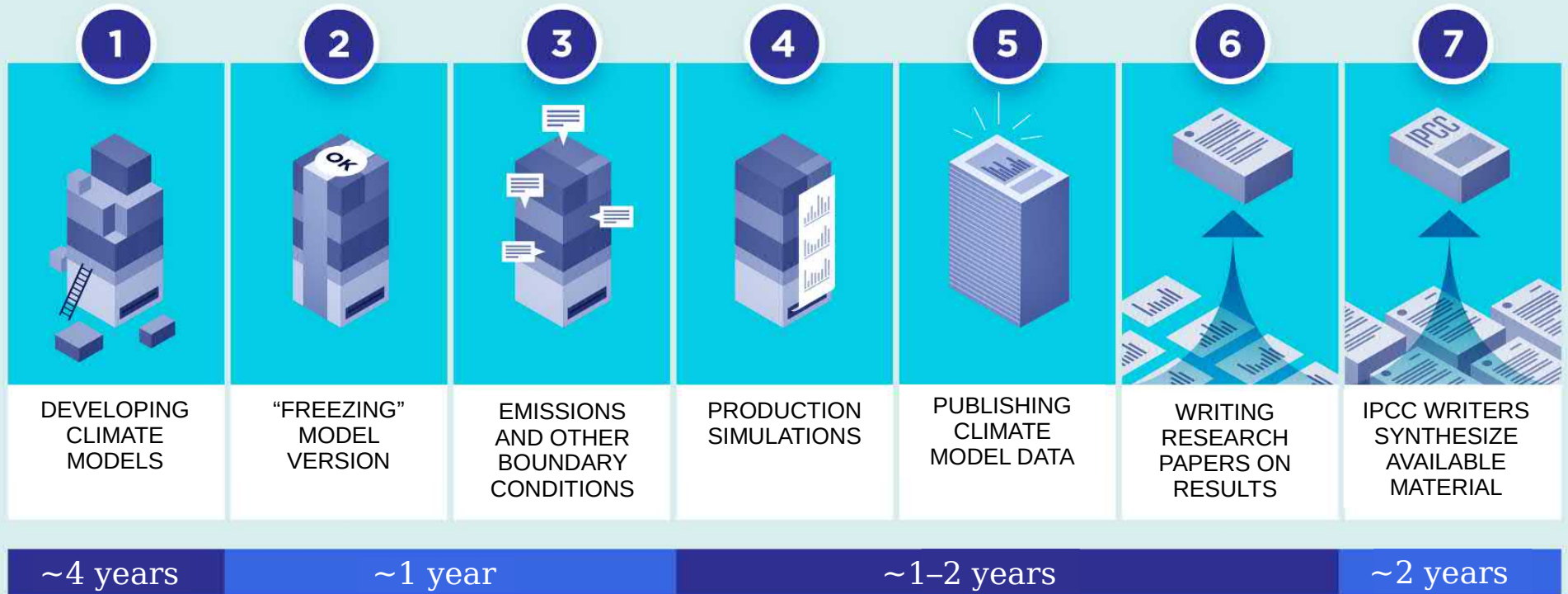
AR4 (2007)  
Resolution ~150 km

AR5 (2013)  
Resolution ~80 km

AR6 (2021)  
Resolution ?

# From climate simulations to IPCC reports

## Coupled Model Intercomparison Project (CMIP)



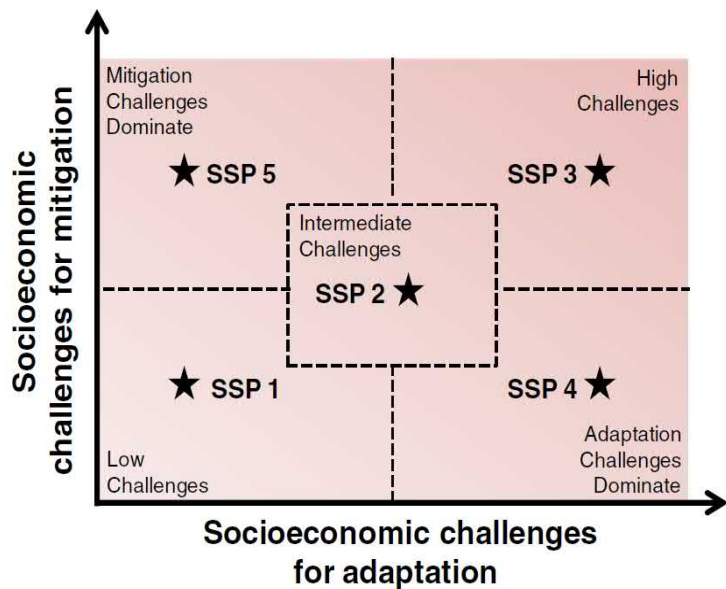


# Coupled Model Intercomparison Project Phase 6

From socio-economic pathways to climate projections

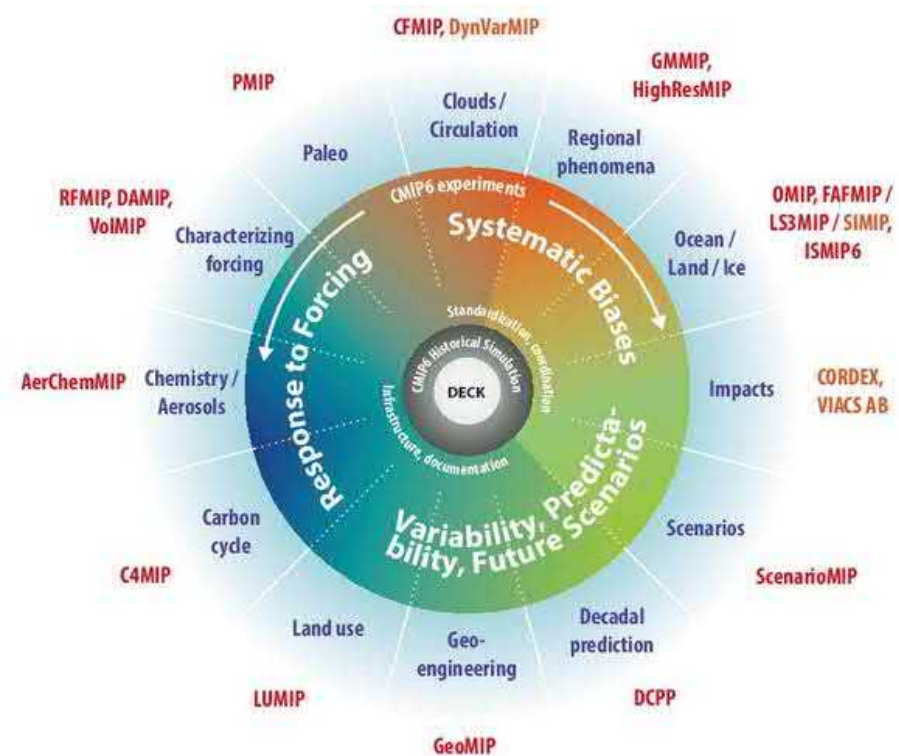
## Model input

Shared Socioeconomic Pathways  
SSP/RCP matrixes



## Experimental design

DECK-simulations (control, historical, 4xCO<sub>2</sub>, 1%CO<sub>2</sub>)  
23 endorsed Model Intercomparison Projects (MIPs)



# Mitigation challenges

Socioeconomic dimension



SSP = Shared Socioeconomic Pathway. Source: Rogelj et al (2018).

CB



# Amount of CMIP data has increased roughly by a factor of 50

• CMIP Phase Models		Data amount	
• CMIP1 (TAR)	<20	1 Gb	➤ More models
• CMIP2 (TAR)	>20	500 Gb	➤ Higher resolution
• CMIP3 (AR4)	~35	30–40 Tb	➤ More components
• CMIP5 (AR5)	>50	2–3 Pb	➤ More experiments
• CMIP6 (AR6)	109	20–70 Pb	

# Summary

- Using highly coupled Earth System Models (ESMs) in studying history and future pathways of chemistry-climate-biosphere-atmosphere-ocean system
- Limitations due to technical implementations (computer and data resources), fundamental understanding, and unavailable globally applicable parameters
- Big data allows from tens of models allows novel steps towards enhanced understanding of underlying uncertainties in processes, interactions and feedbacks