

# A statistical framework to quantify model uncertainty

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National Centre for  
Atmospheric Science  
NATURAL ENVIRONMENT RESEARCH COUNCIL



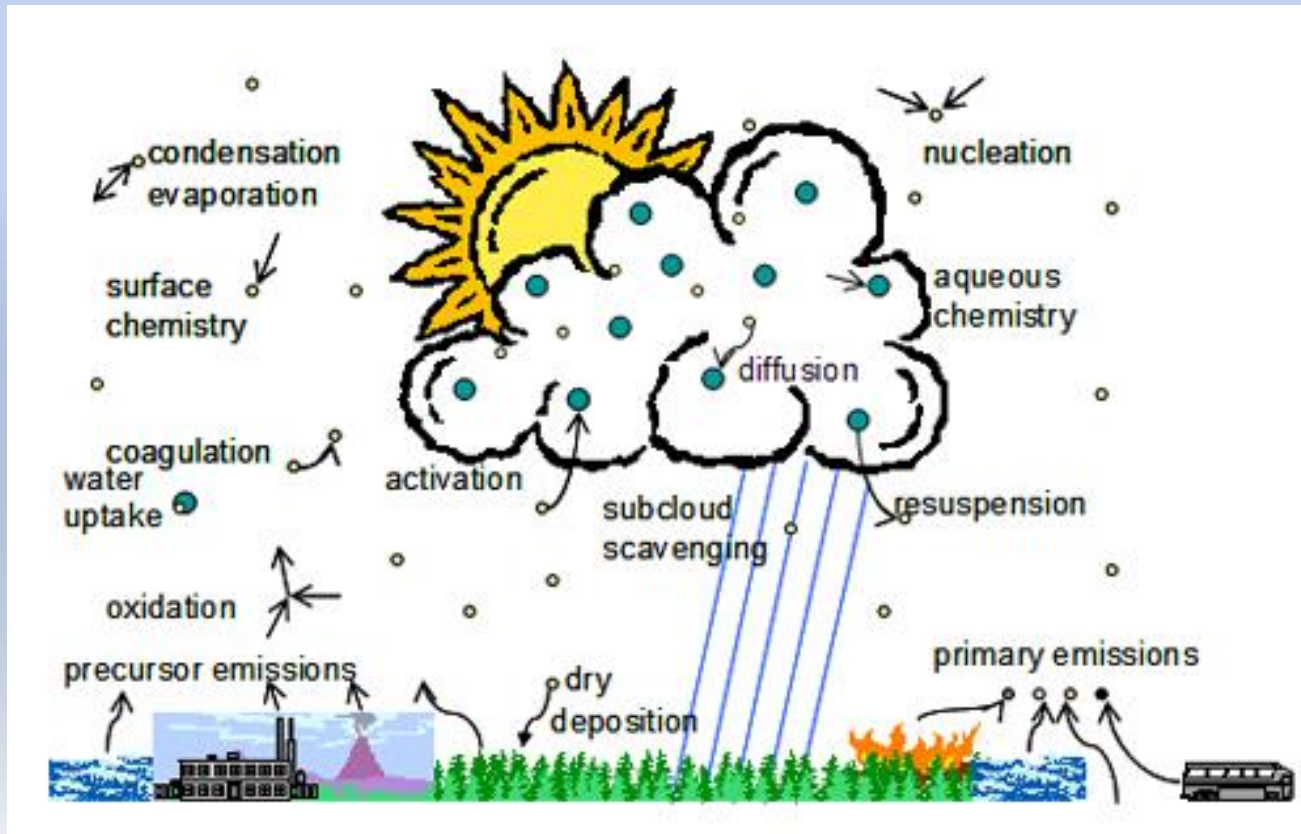
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# 1. GLOMAP



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- We use the global aerosol model **GLOMAP** (Mann et al. 2010)
- A microphysical modal model simulating the evolution of global aerosol including sulphate, sea-salt, dust and black carbon



## 2. Uncertainty in modelling



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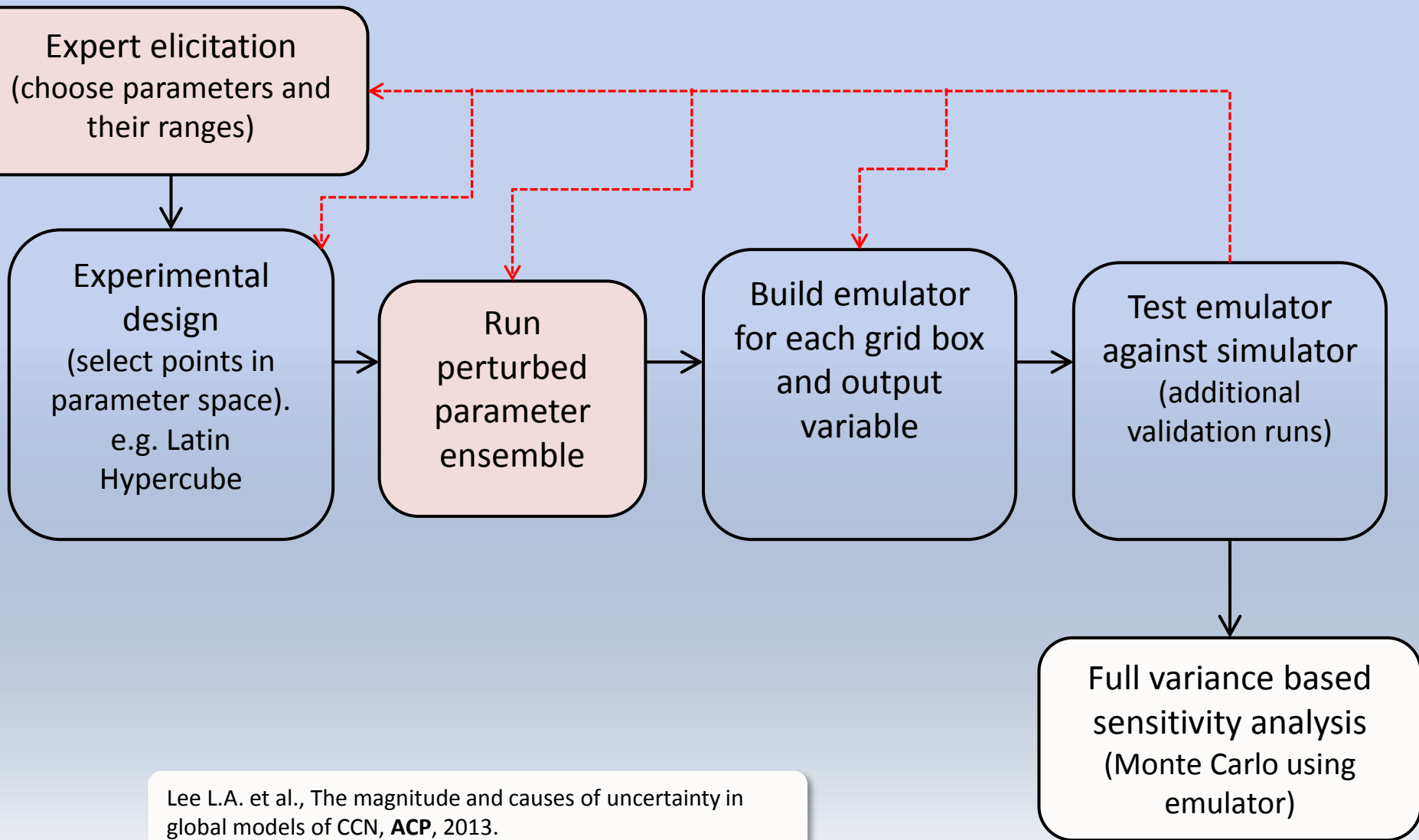
- Structural uncertainty
  - Compare multiple models of the same type
  - Compare model to observations

AEROCOM

- Parametric uncertainty
  - Compare runs of the same model with perturbed parameters
  - Compare model to observations

AEROS

# 3. The procedure



Lee L.A. et al., The magnitude and causes of uncertainty in global models of CCN, *ACP*, 2013.

## 4. Expert elicitation



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- Discussion
- Variety of views

‘We think these are the uncertain parameters and their values are very unlikely to fall outside of these ranges’

- Broaden the range of any single expert
- Potentially already too anchored?

# 5. Biogenic SOA and BL nucleation



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- Design an experiment to look at just two parameters and their relationship to CCN
- Uncertainty scaled with usual values
- BIO\_SOA: 0.2 – 20  
$$\text{EMTERP}(I,K) = \text{EMTERP}(I,K) * \text{AEROS\_BIO\_SOA}$$
- BL\_NUC: 0.01 – 100  
$$\text{JBLN} = \text{JBLN} * \text{AEROS\_BLN\_RATE}$$

## 6. Experimental design



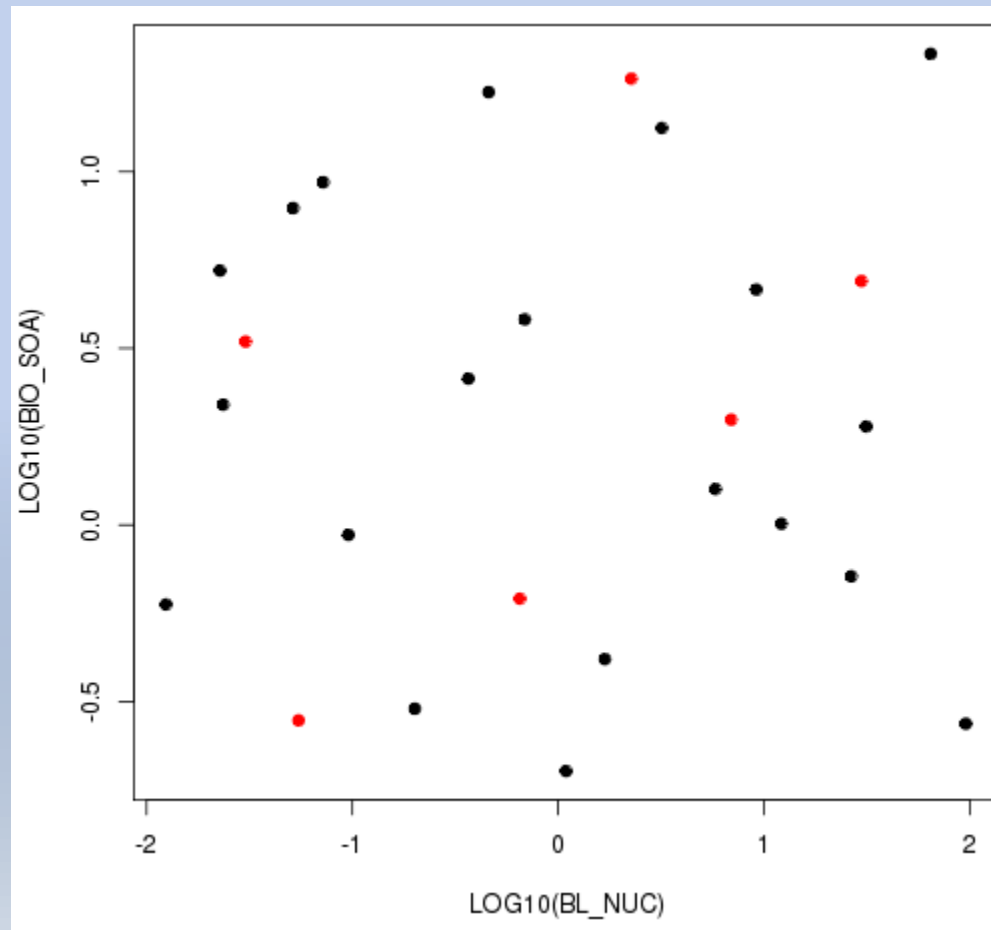
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- Need **maximum information** in **fewest runs**
- Maximin Latin Hypercube used
  - good marginal coverage
  - good space-filling properties
- Number of runs?
  - depends on ‘active’ parameters and function smoothness
- Validation crucial to highlight design issues
  - may need to sequentially design
  - could identify discontinuities/regime shifts

# 7. BIO\_SOA / BL\_NUC design



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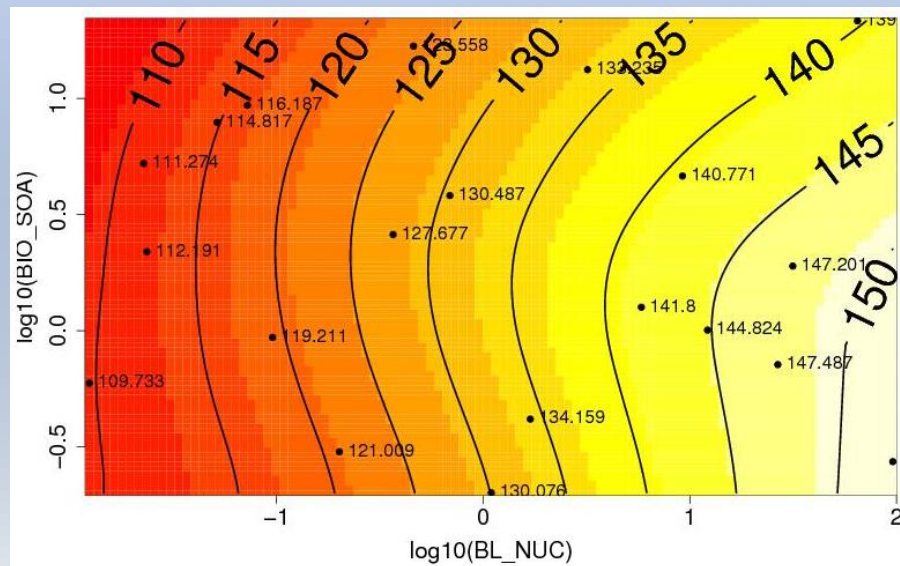


## 8. Filling in the gaps - emulation



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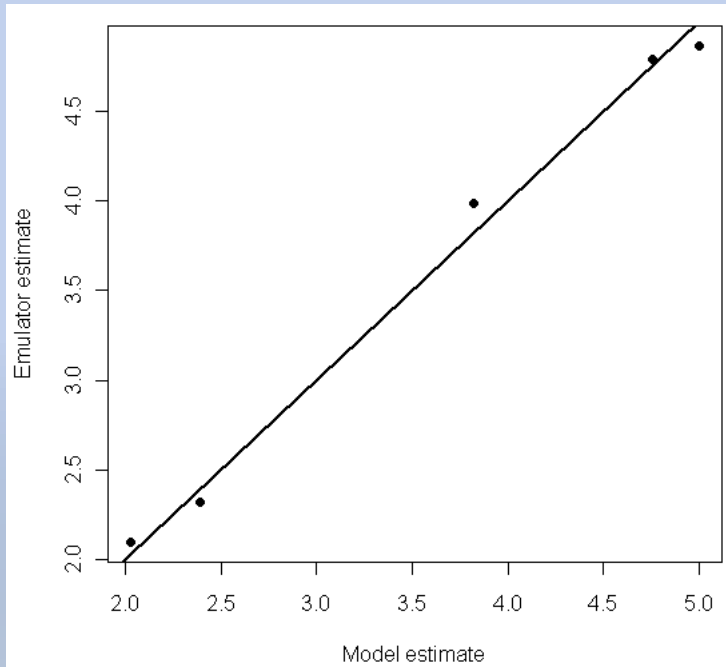
- Interpolate well-space model runs to estimate at untried points
- Bayesian method exploiting conditional probability
- Non-parametric



# 9. Emulator validation



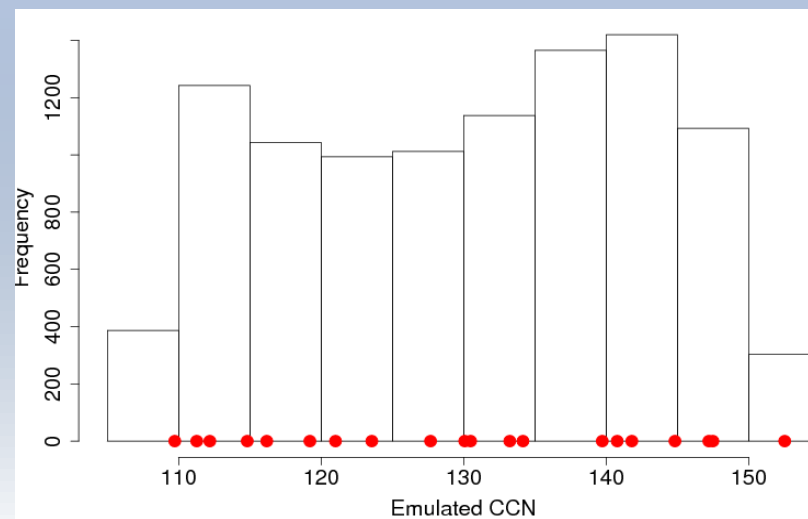
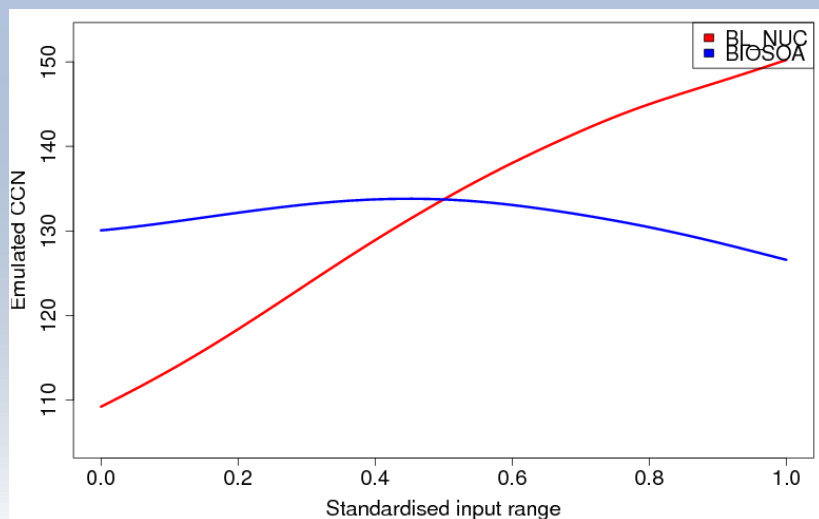
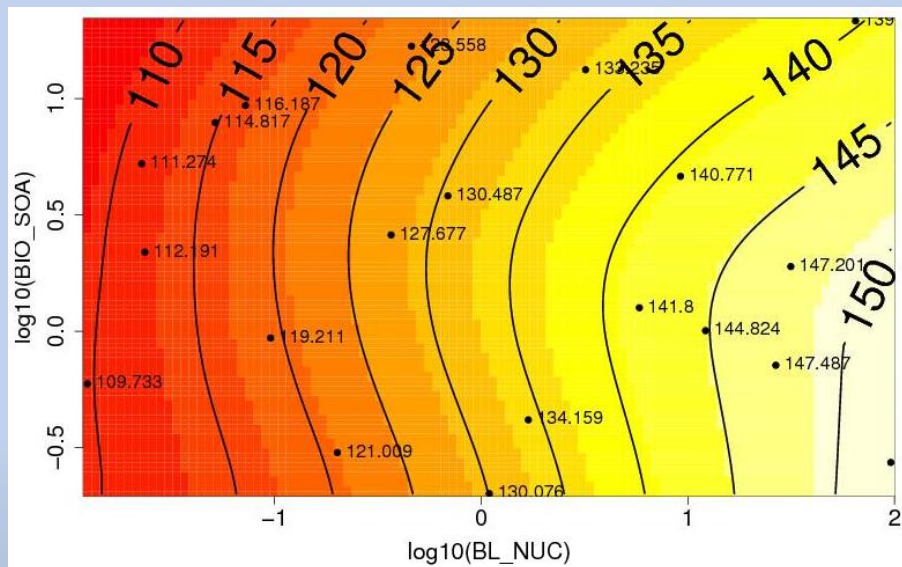
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Is the emulator output a good approximate of the model output?

YES – use the emulator mean instead

# 10. Filling in the gaps - emulation



# 11. Variance-based sensitivity analysis



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**Variance decomposition:**

$$Var(Y) = \sum_{i=1} V_i + \sum_{i<j} V_{ij} + \dots + V_{12\dots p}$$

Variance due to each parameter:

$$V_i = Var_{X_i} (E(Y | X_i)), V_{ij} = Var_{X_{ij}} (E(Y | X_{ij}))$$

**Main effect sensitivity:**

$$S_i = \frac{V_i}{Var(Y)}$$

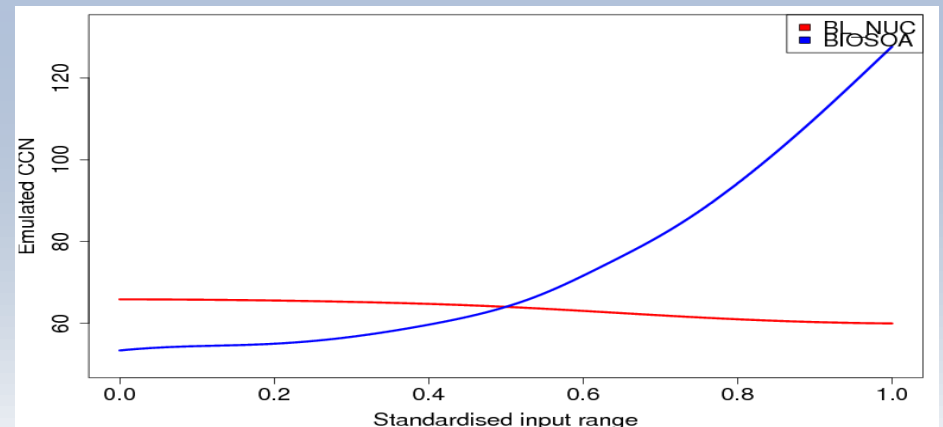
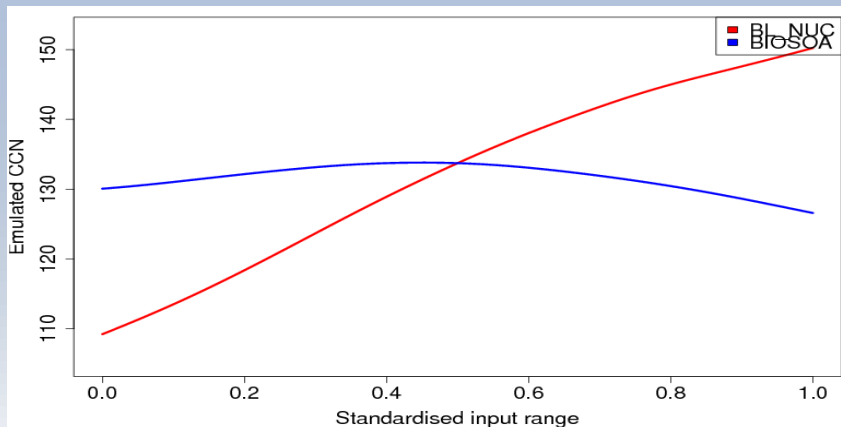
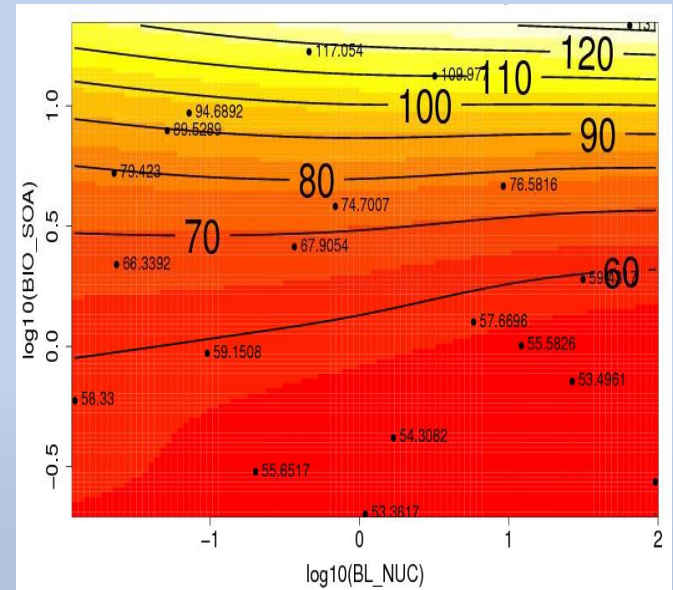
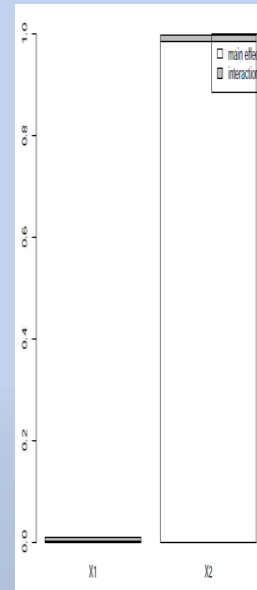
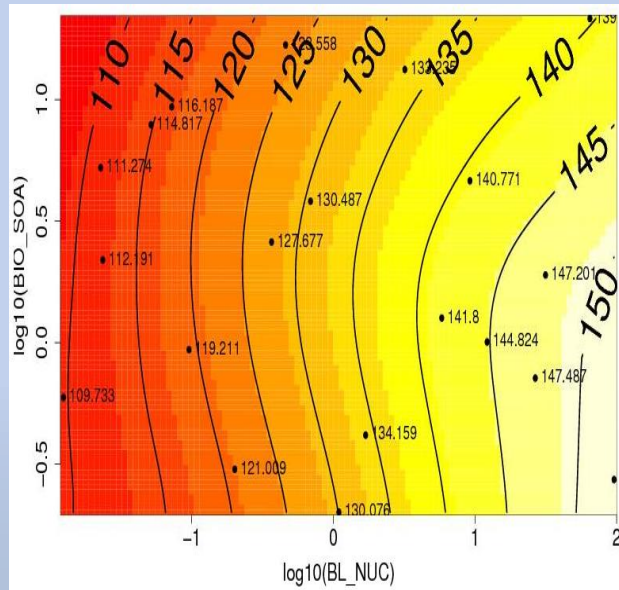
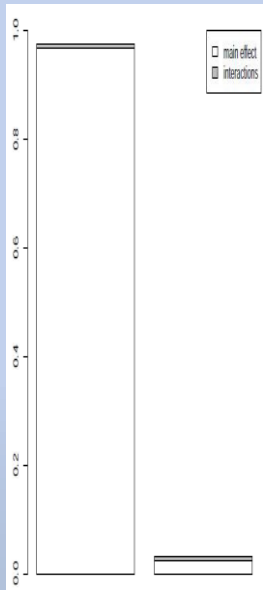
Main effects + Interactions:

$$\sum_{i=1} S_i + \sum_{i<j} S_{ij} + \dots + S_{12\dots p} = 1$$

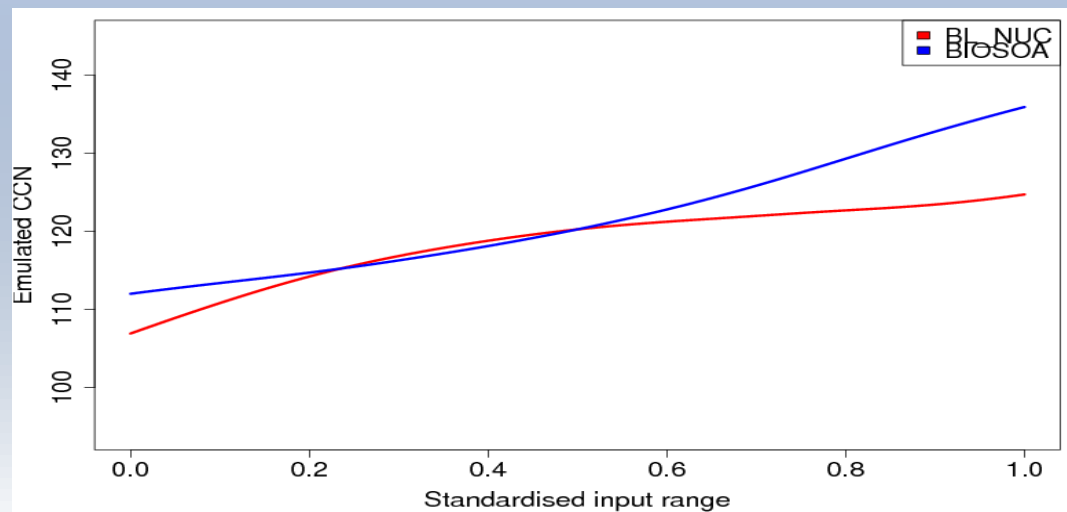
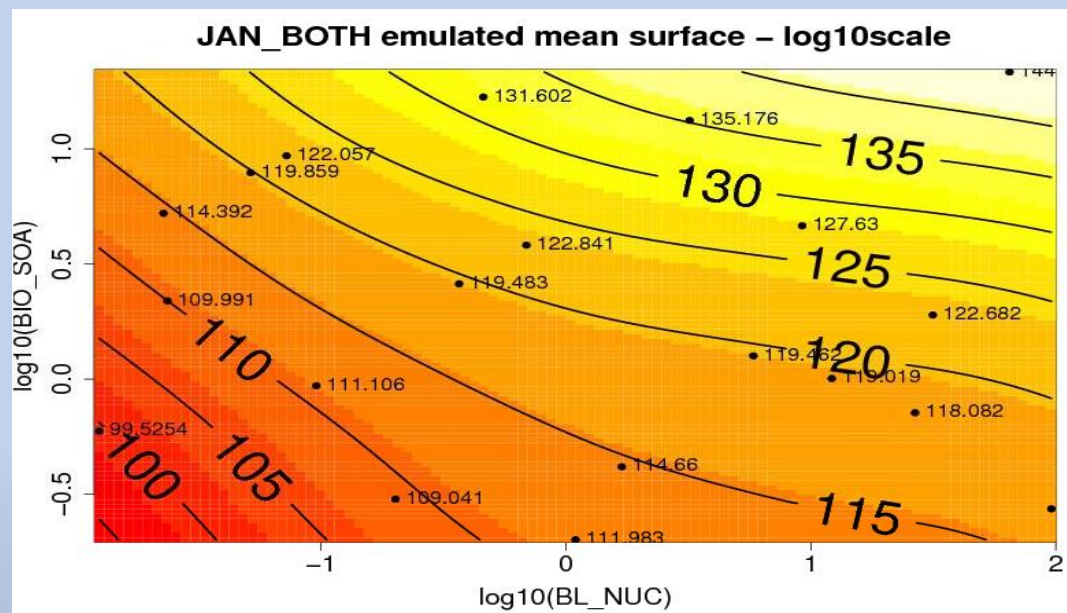
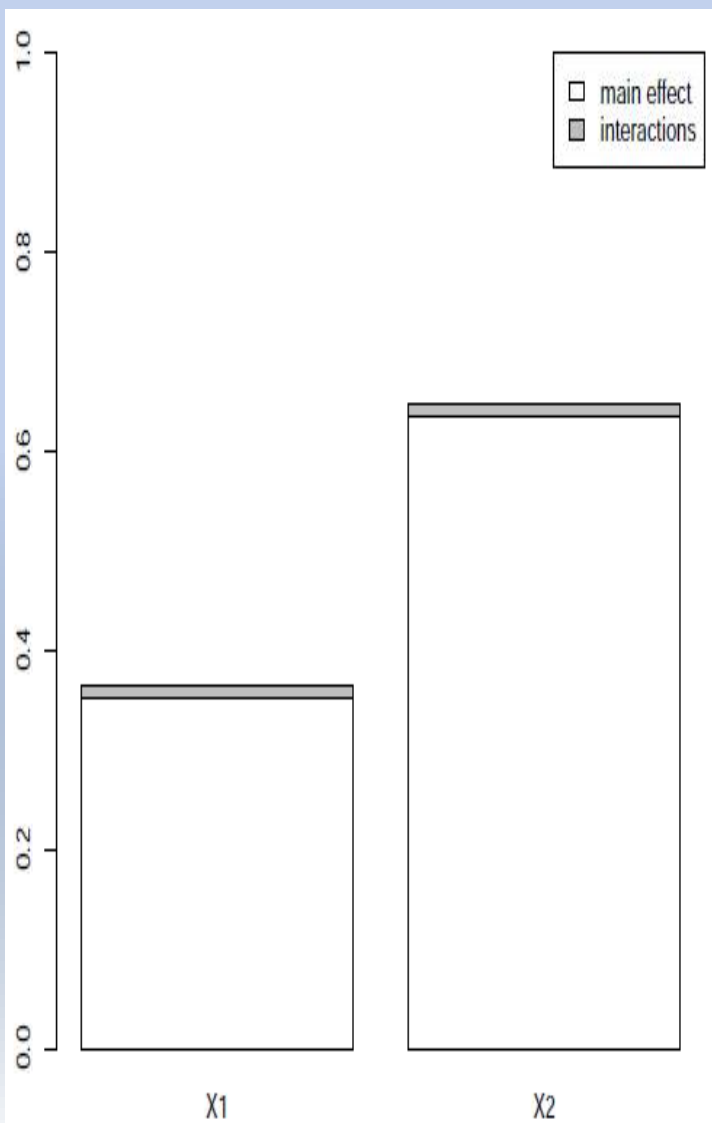
# 12. Main effects



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# 13. Main effects

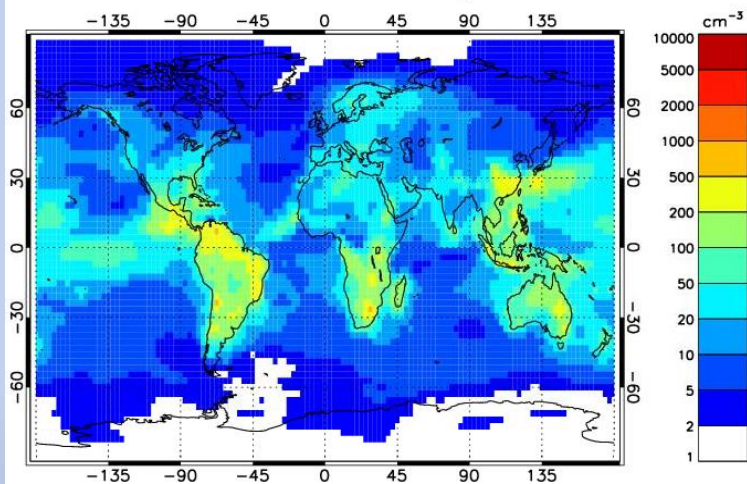


# 14. Global main effects

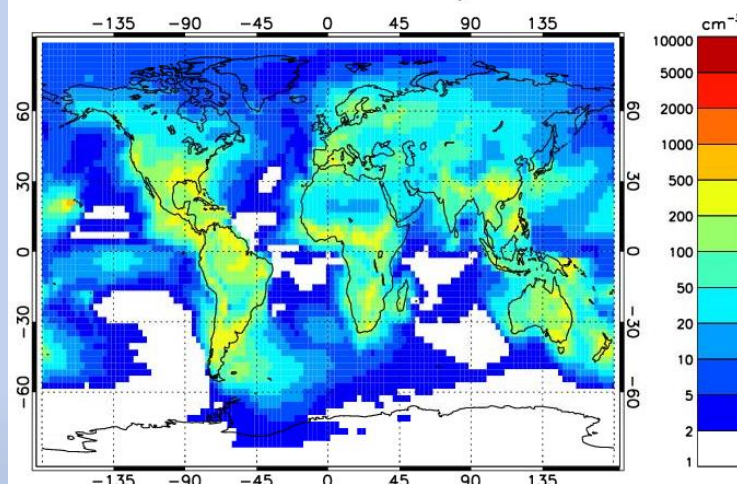


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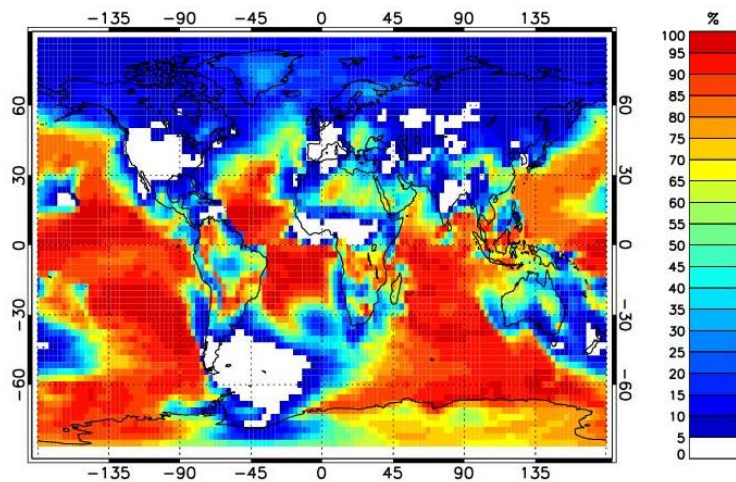
CCN JAN Absolute\_uncertainty BL\_NUC



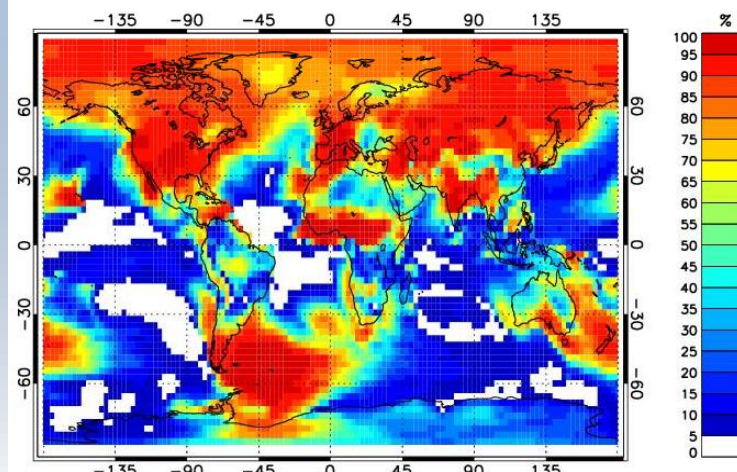
CCN JAN Absolute\_uncertainty BIO\_SOA



CCN JAN Main\_effect BL\_NUC



CCN JAN Main\_effect BIO\_SOA



# 15. 28 parameter elicitation



Elicitation:  
Ask the experts

Parameter	Lower	Upper
BCOC mass emission rate (fossil fuel)	0.5	2.0
BCOC mass emission rate (biomass burning)	0.25	4.0
BCOC mass emission rate (biofuel)	0.25	4.0
Sea spray mass flux (coarse/acc)	0.2x	5.0x
SO2 emission flux (anthropogenic)	0.6x	1.5x
SO2 emission flux (volcanic)	0.5x	2.0x
Biogenic monoterpene production of SOA	5 Tg/a	360Tg/a
Anthropogenic VOC production of SOA	3Tg/a	160Tg/a
DMS mass flux	0.5x	
BCOC mode diameter (fossil fuel)	30 nm	
BCOC mode diameter (biomass burning)	50 nm	
BCOC mode diameter (biofuel)	50 nm	
Subgrid conversion of SO2 to SO4 ("primary SO4")	0%	
Mode diameter of "primary SO4"	20 nm	

Mass emission rates

Microphysics  
Model properties

Parameter	Lower	Upper
BL nucleation rate k[H2SO4]	1E-10	2E-04
FT nucleation rate (BHN)	x0.01	X10
Ageing "rate" from insol to sol (monolayer)	0.3	5
Modal width (accumulation)	1.2	1.8
Modal width (Aitken)	1.2	1.8
Mode separation diameter (nucleation/Aitken)	9nm	20nm
Mode separation diameter (Aitken/accumulation)	x1.5	x3

Parameter	Lower	Upper
Cloud drop activation dry diameter	30	100
Reaction SO2 + O3 in cloud water (clean)	pH=4	pH=6.5
Reaction SO2 + O3 in cloud water (polluted)	pH=3.5	pH=5

Cloud processing

Dry and wet deposition

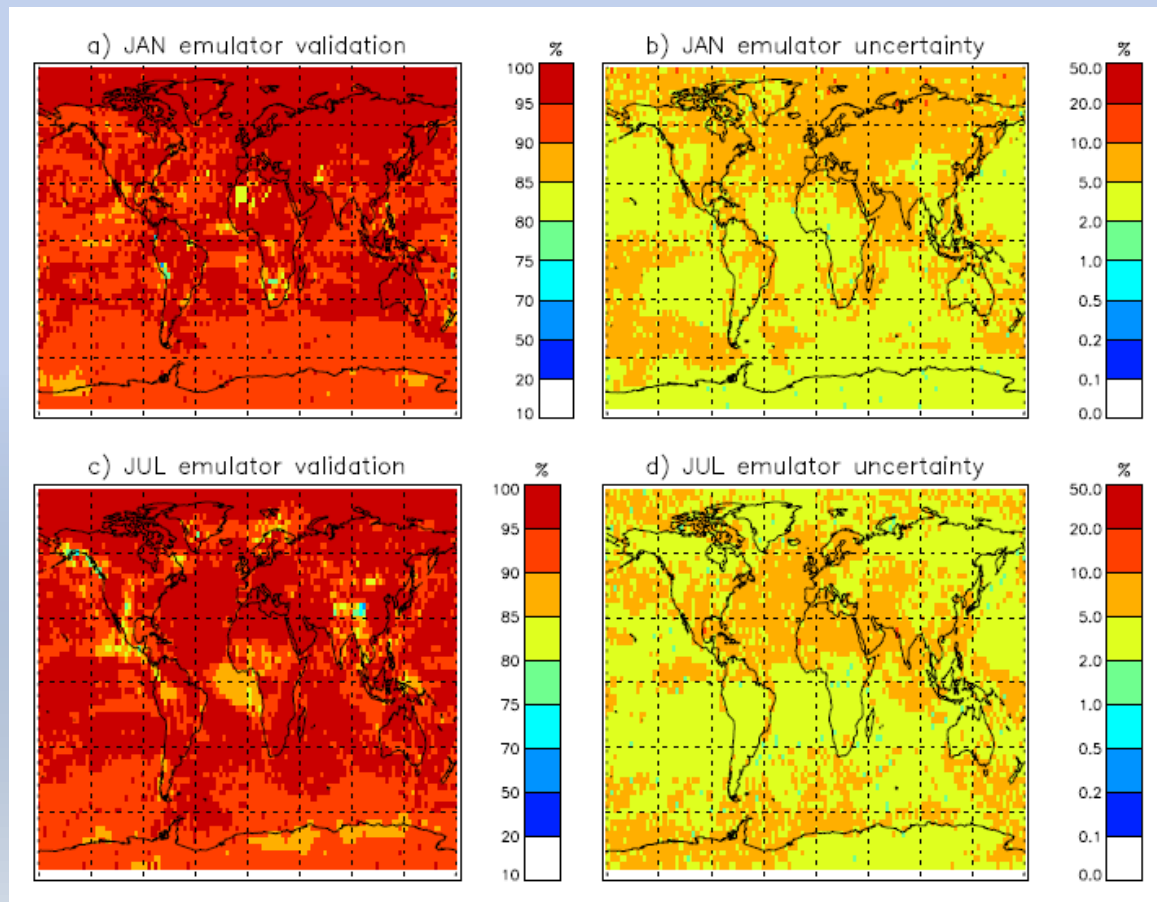
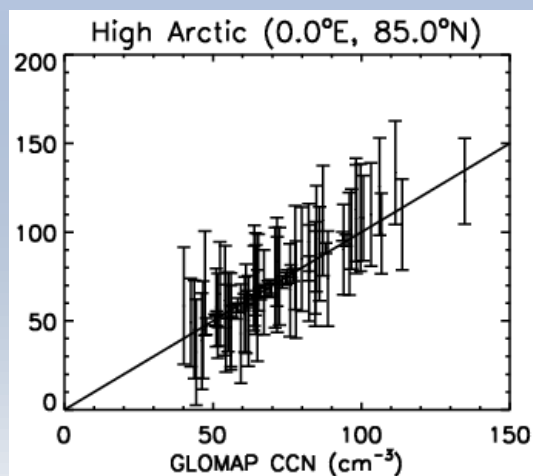
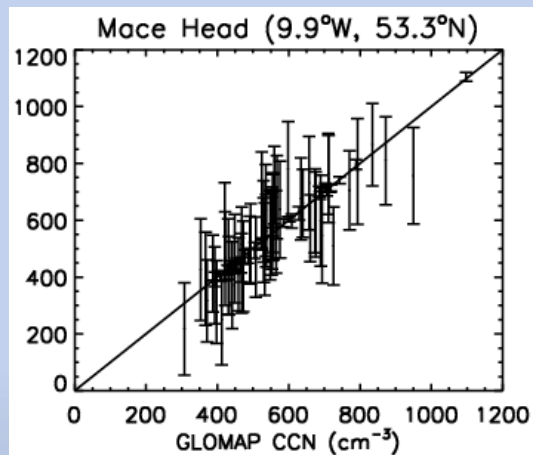
Parameter	Lower	Upper
Nucleation scavenging dry D (above activation)	0	100
Nucleation scavenging fraction (T< -15C)	0.05	0.75
Dry deposition velocity (Aitken)	x0.5	X2.0
Dry deposition velocity (accumulation)	X0.1	X10.0
Dry deposition velocity (SO2)	X0.5	X2.0



# 16. 28 parameter validation



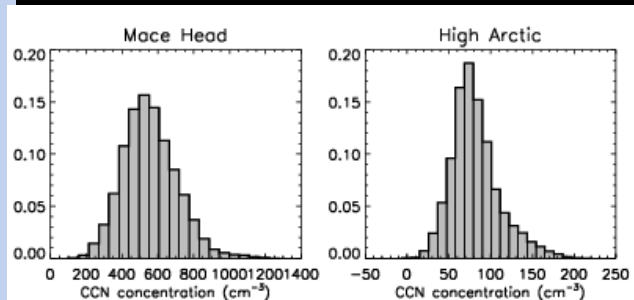
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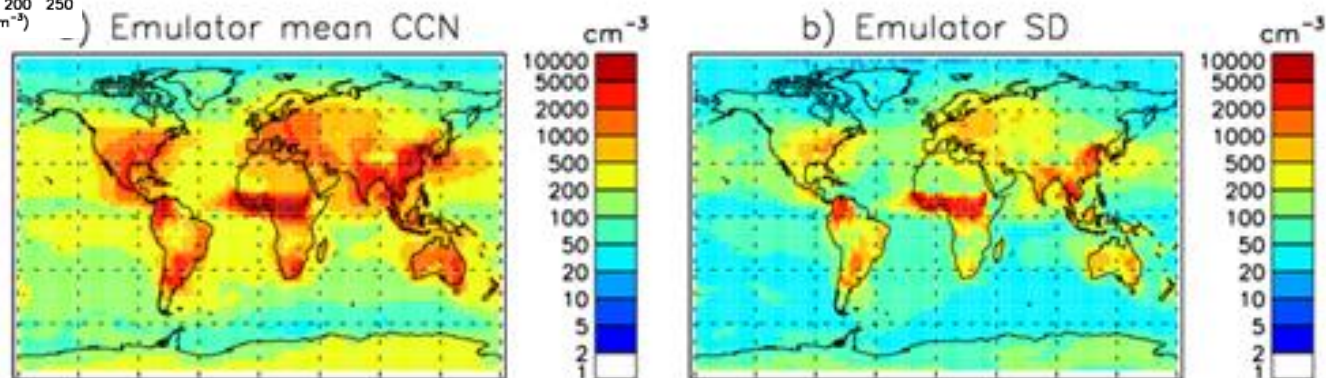
# 17. Estimated CCN and its uncertainty concentration in every surface grid box



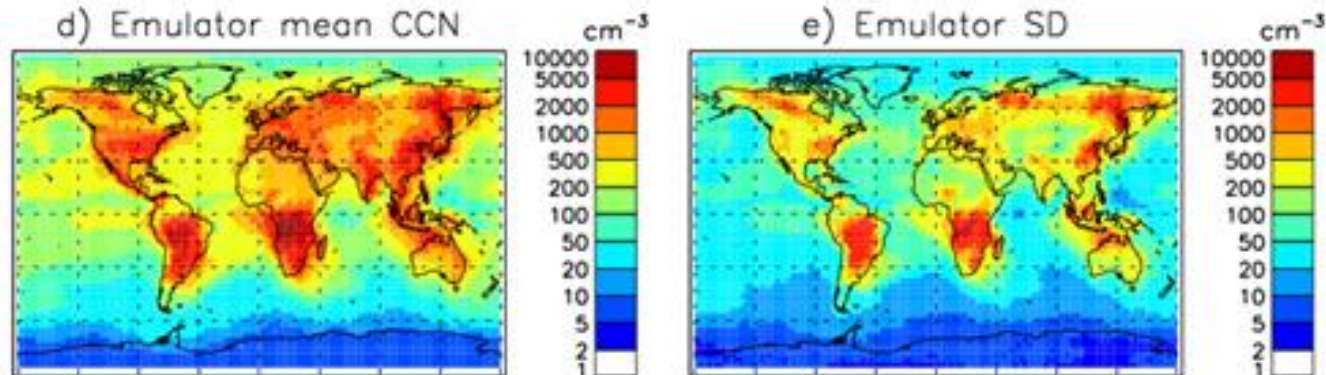
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January



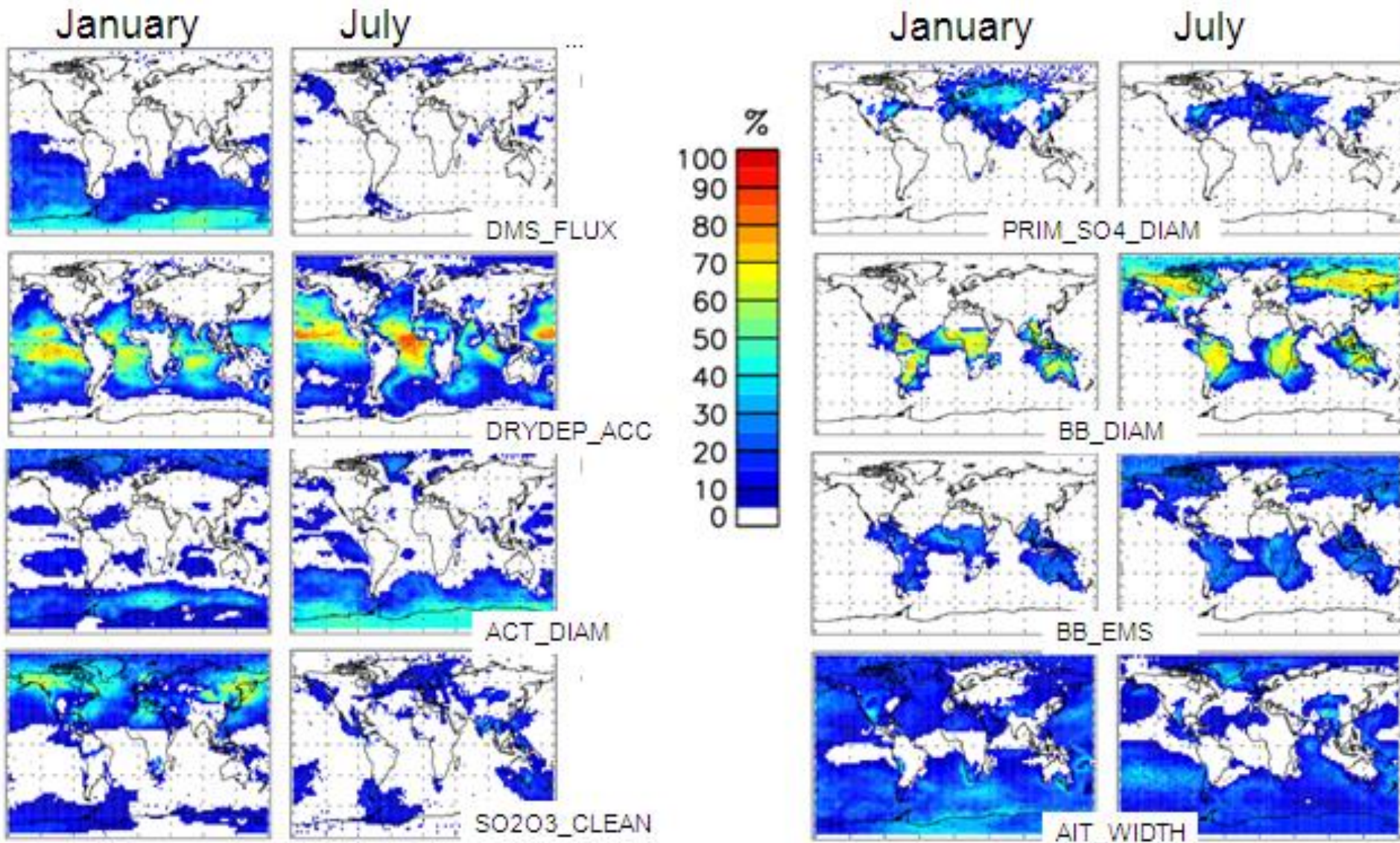
July



# 18. Surface parameter sensitivities



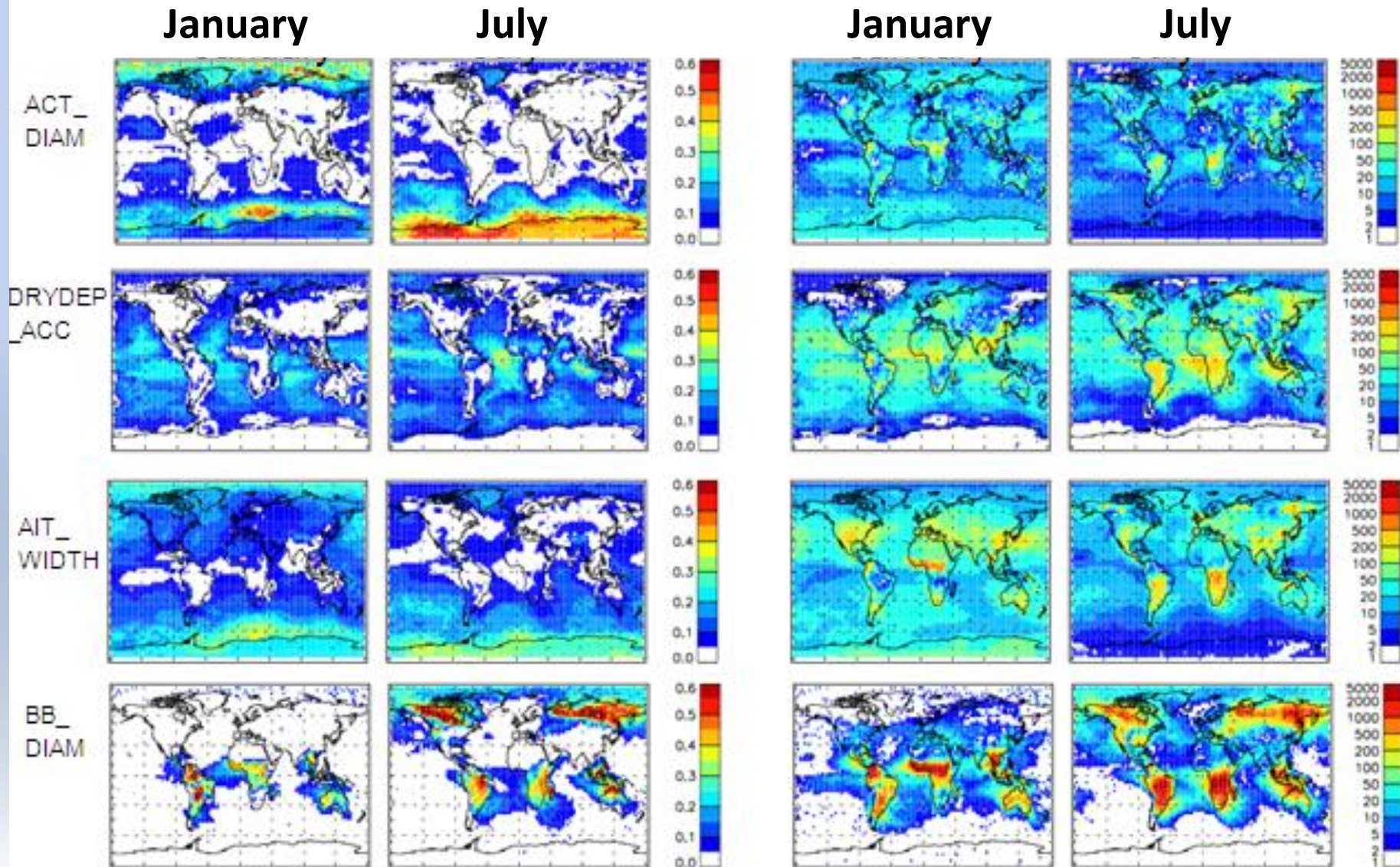
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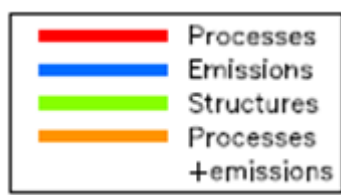
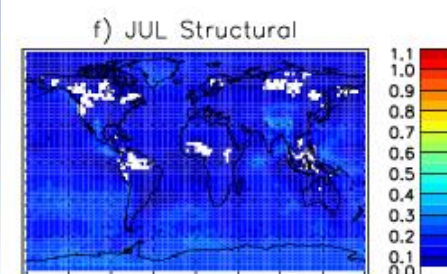
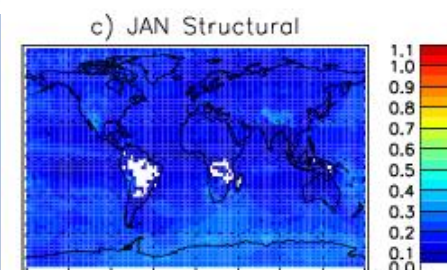
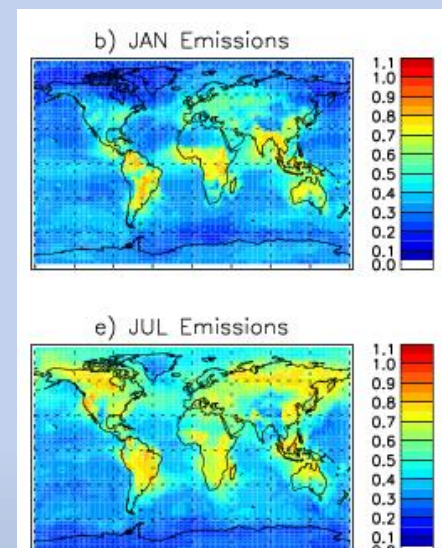
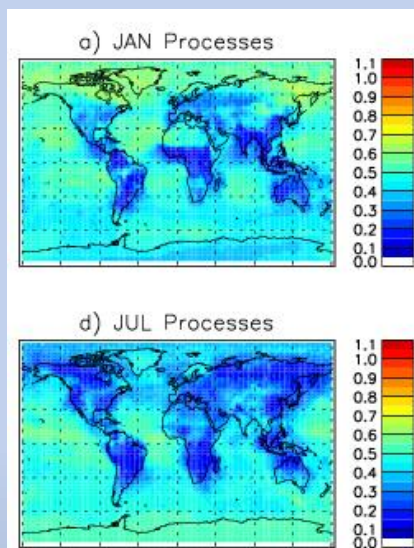
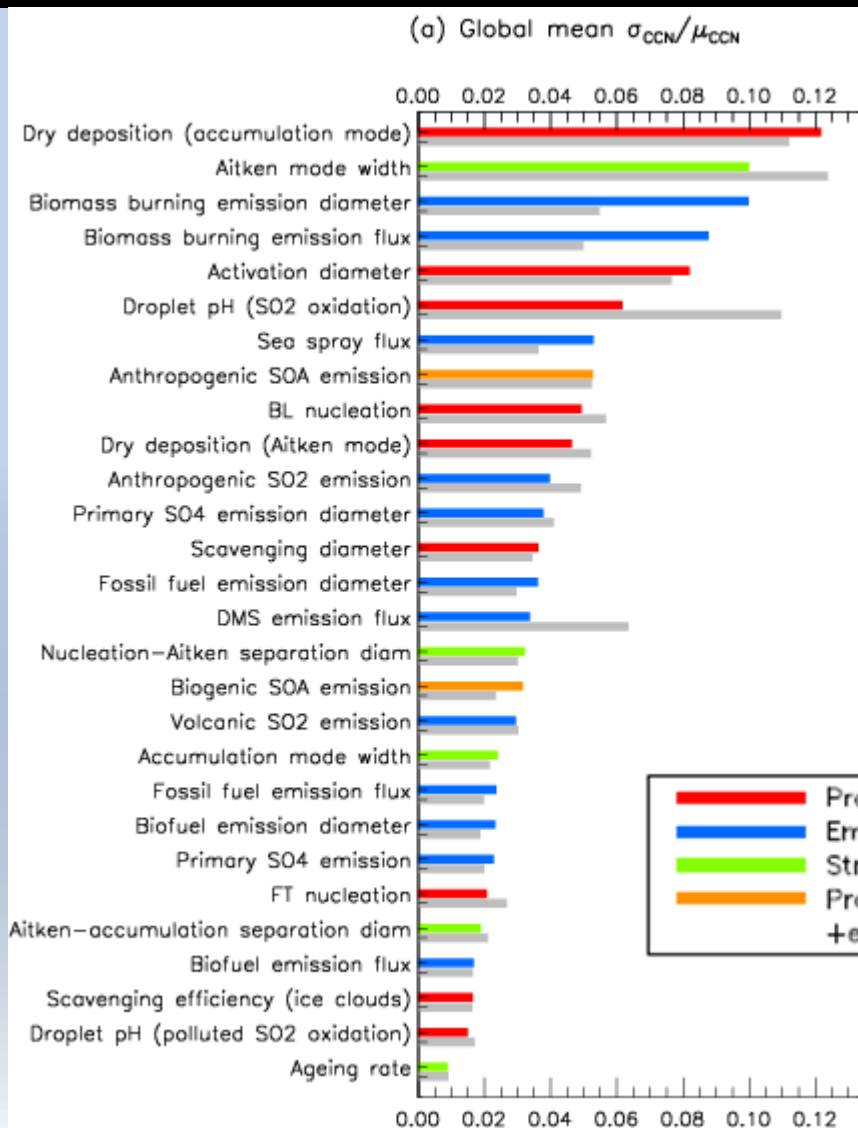
# 19. LHS: $\sigma_{\text{CCN}}/\mu_{\text{CCN}}$ and RHS: absolute $\sigma_{\text{CCN}}$



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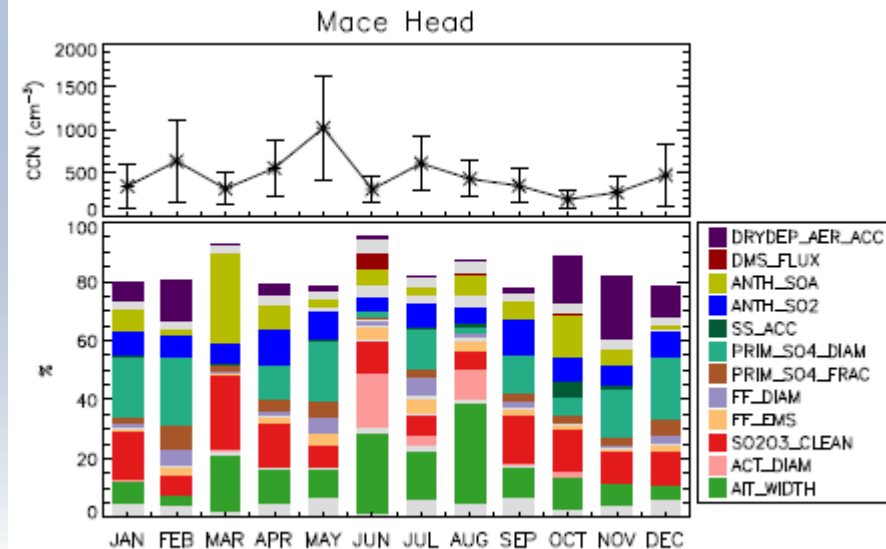
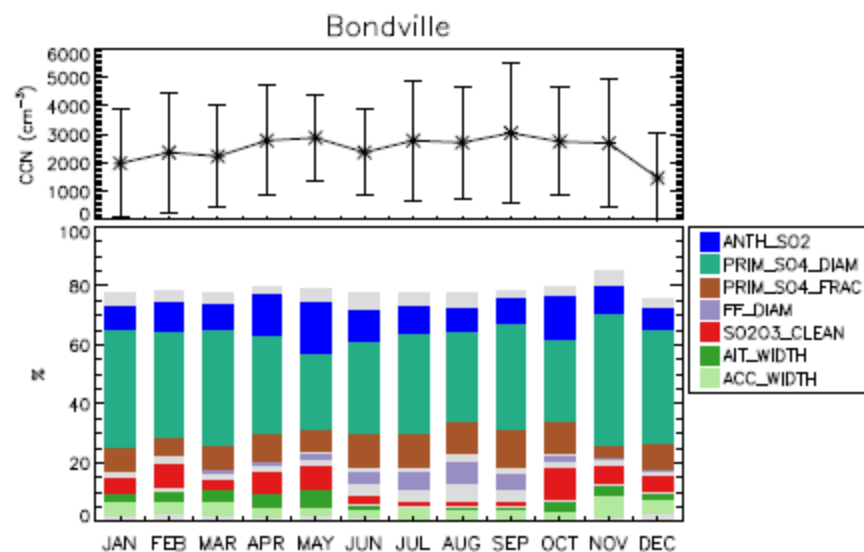
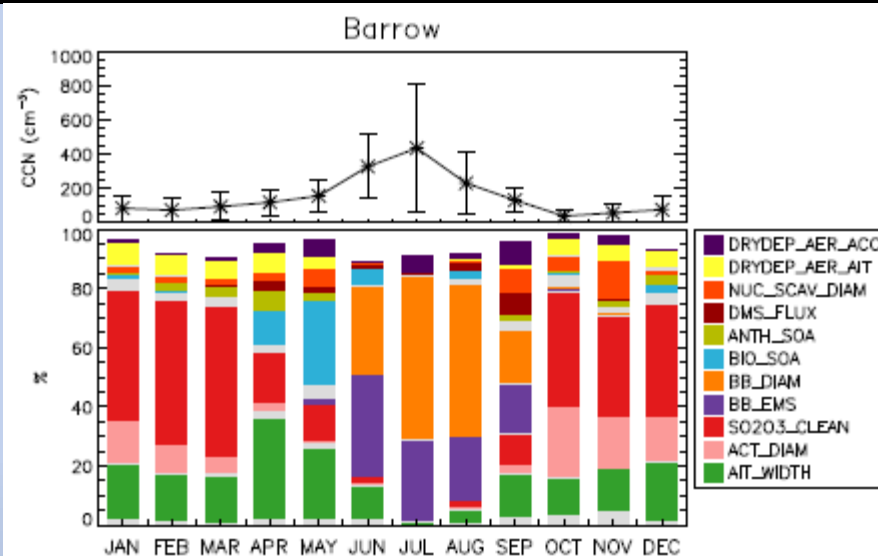
# 20. Summarising global maps



# 21. Seasonal parameter sensitivities



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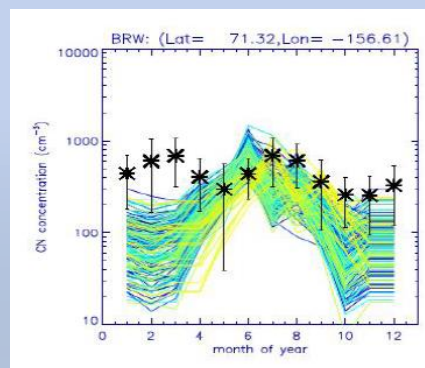
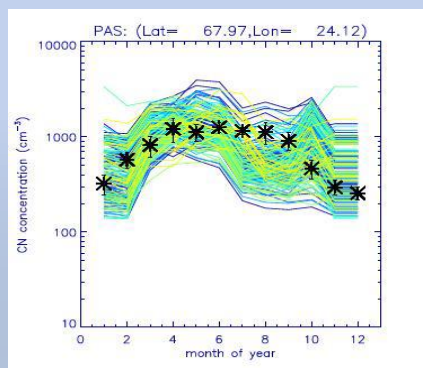


## 22. Structural uncertainty



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- Structural uncertainty
  - Considering the model uncertainty is any model configuration near to observations



- How do sensitivities in different models compare?
  - AEROCOM joint proposed experiments (presented by Ken Carslaw)



- Lee, L. A., Carslaw, K. S., Pringle, K. J., Mann, G. W., and Spracklen, D. V.: Emulation of a complex global aerosol model to quantify sensitivity to uncertain parameters, *Atmos. Chem. Phys.*, 11, 12253-12273, doi:10.5194/acp-11-12253-2011, 2011.
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