Progress on integrating an atmospheric chemistry model and aerosol model: Approximations and current results

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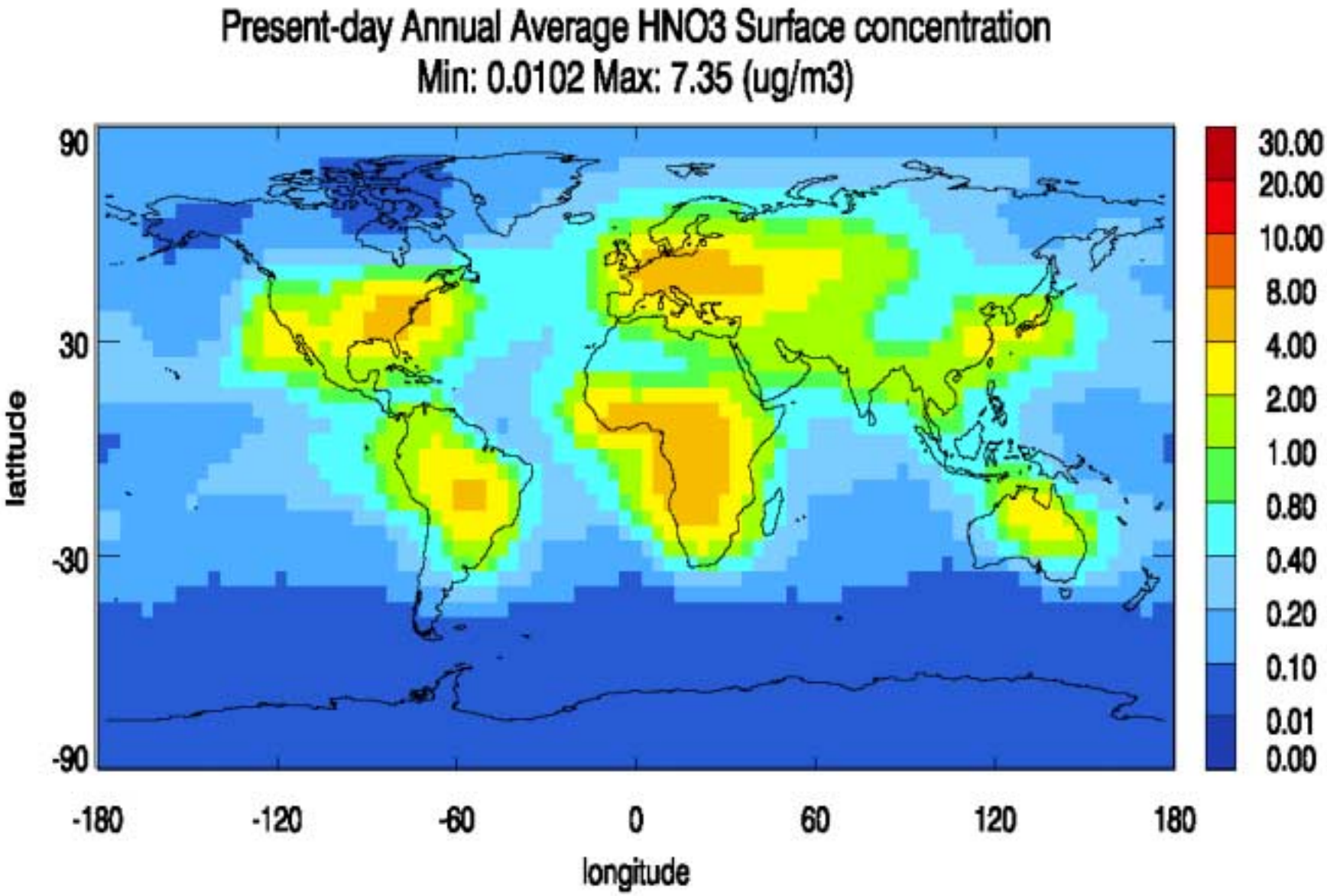
Goal: understand aerosol/oxidant interactions

- ¥ Depletion of H_2O_2 by reaction with SO_2 in drops
- ¥ Absorption of HNO_3 and reaction within aerosols
- ¥ Reactions within sea salt aerosols that release chlorine atoms
- ¥ Formation of organic aerosols formed as a result of the oxidation of gas phase precursors

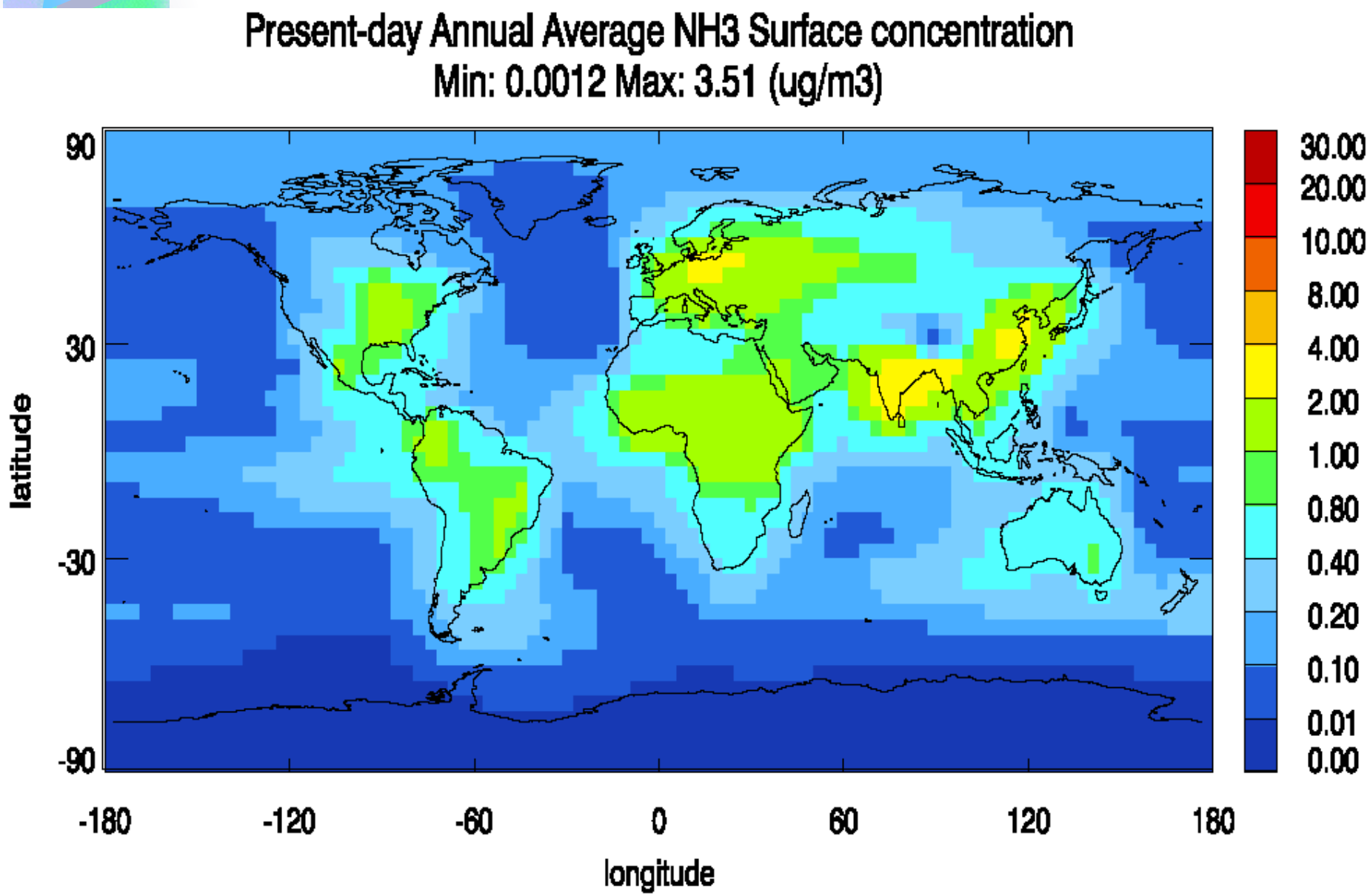
Outline

- Estimates of effects of nitrate and ammonium on aerosol forcing
- Development of a method to treat dust/sea salt phase interactions in the global model
- Progress on developing a prognostic capability for aerosol size
- Progress in developing a fast gas and aerosol global model

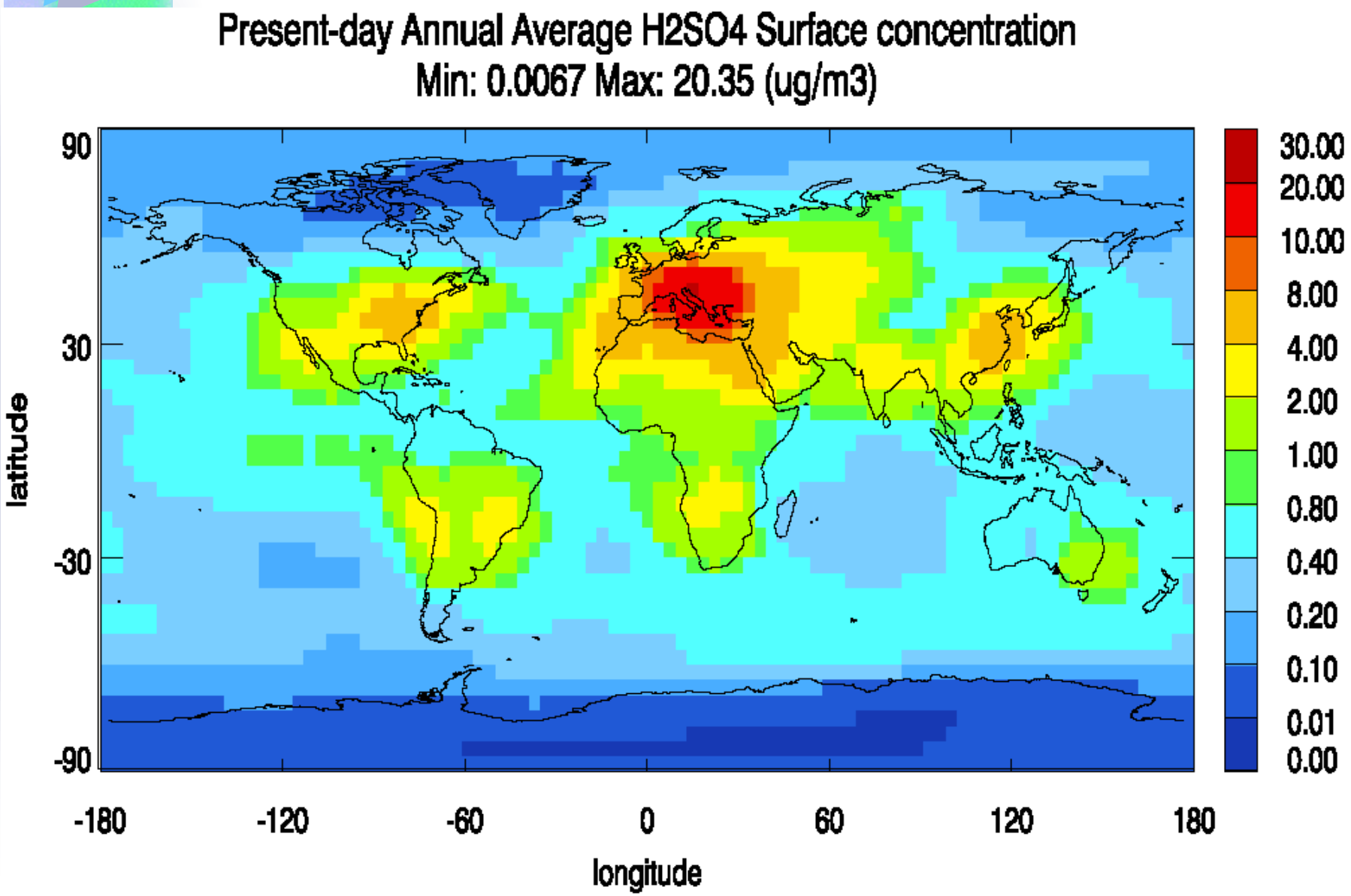
Estimates of Nitrate and Ammonium in Aerosols:



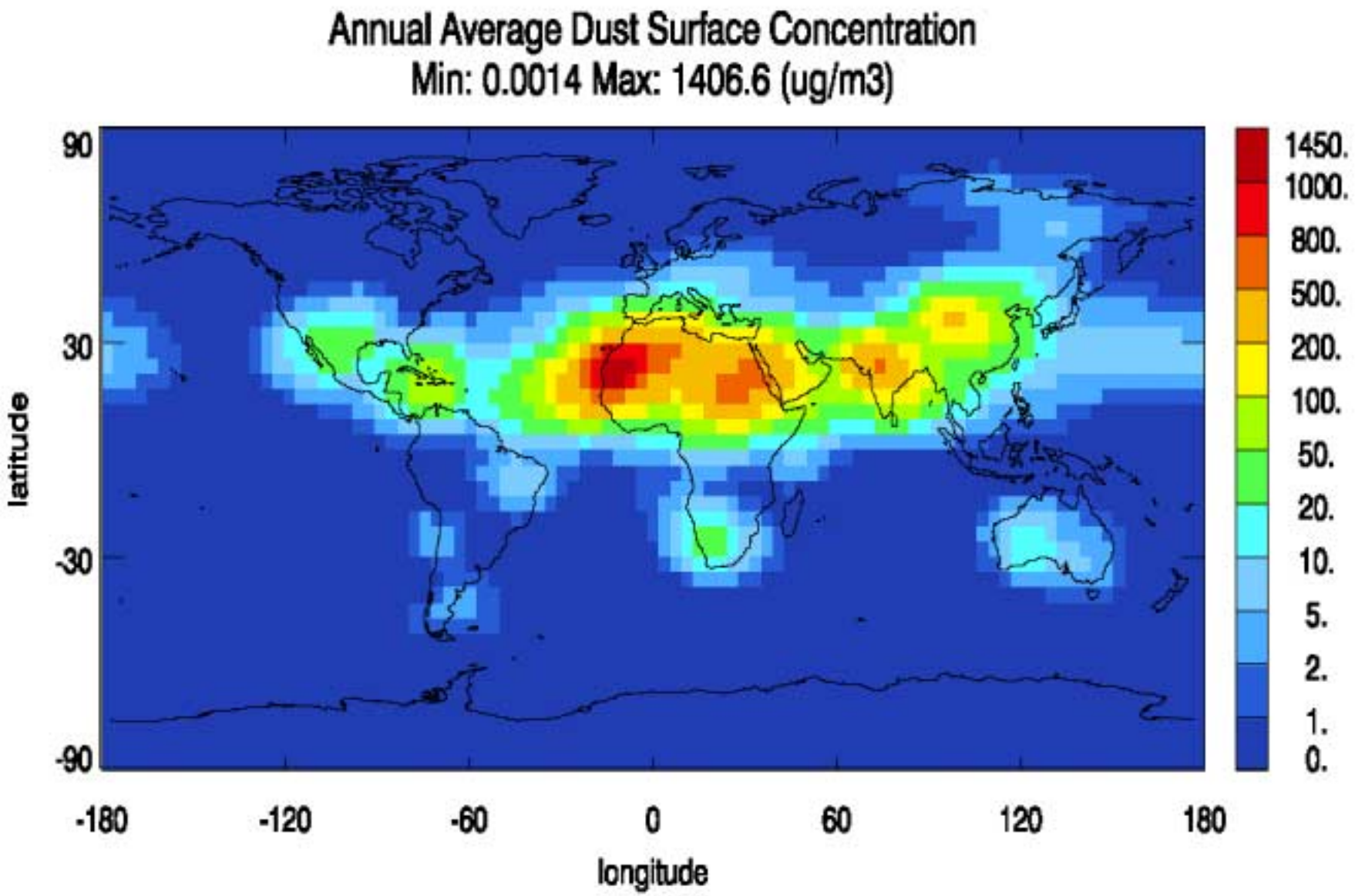
Initial Ammonium in Aerosols:



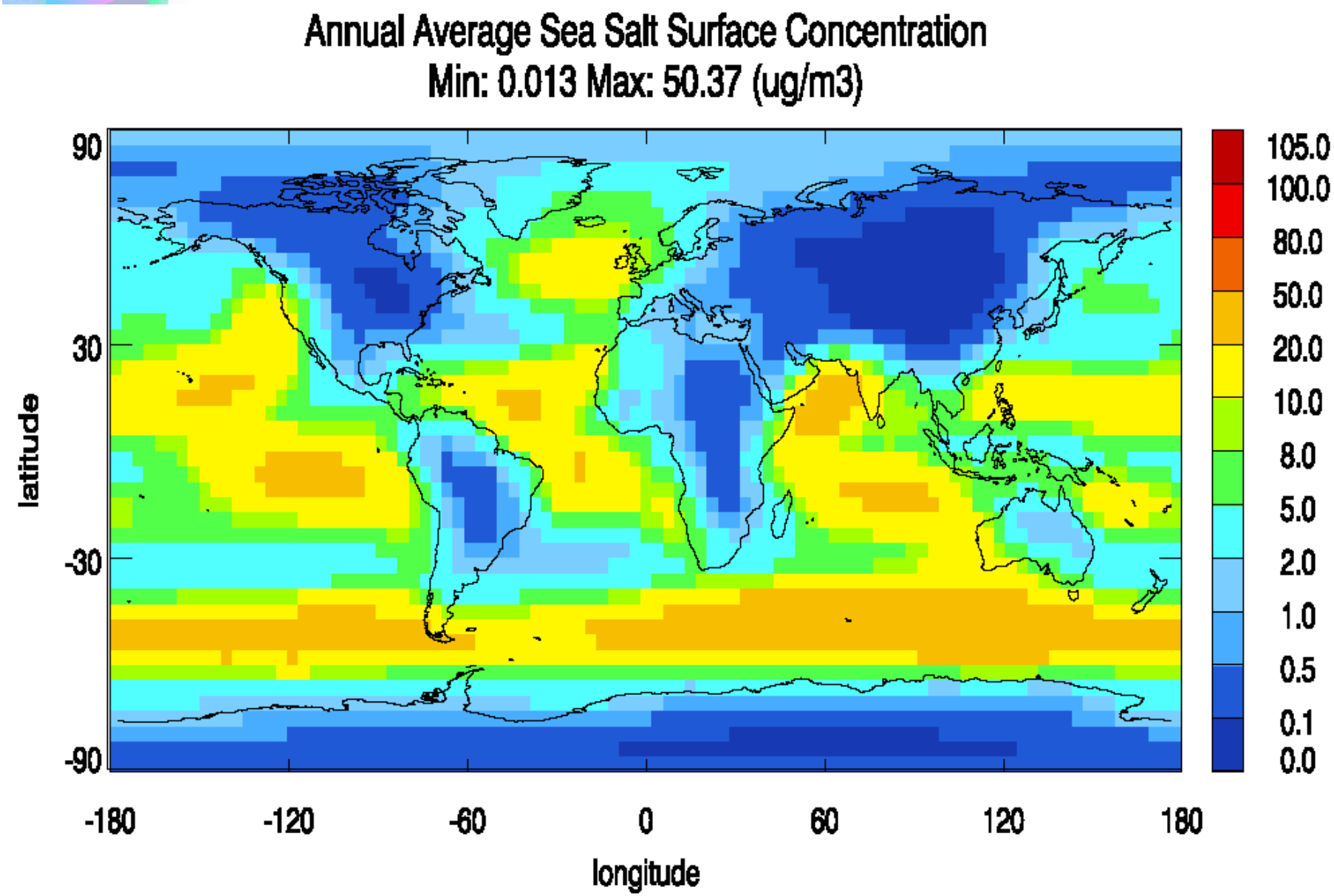
Initial H_2SO_4 in Aerosols:



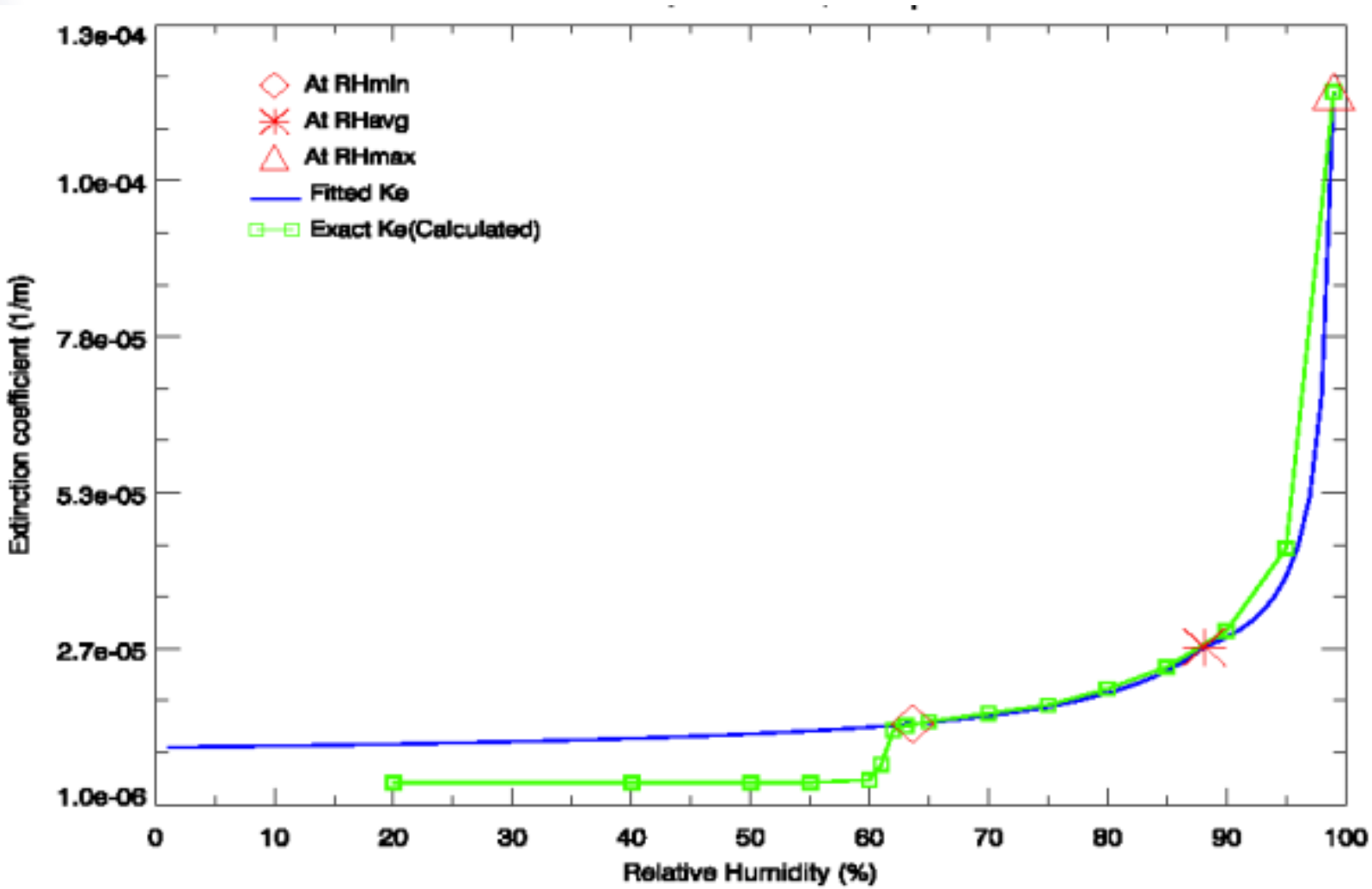
Importance of dust



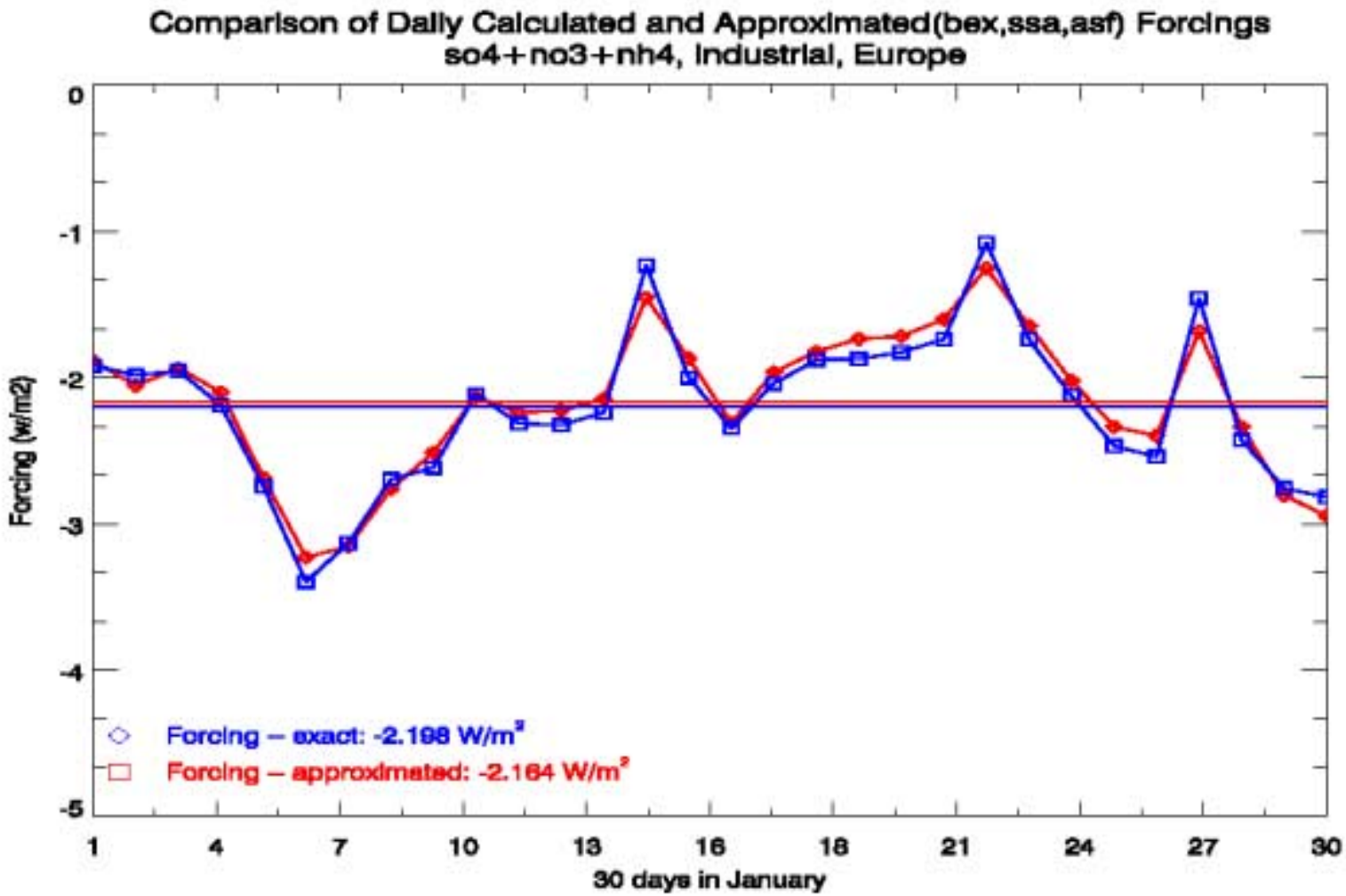
Importance of sea salt



Procedure to calculate forcing



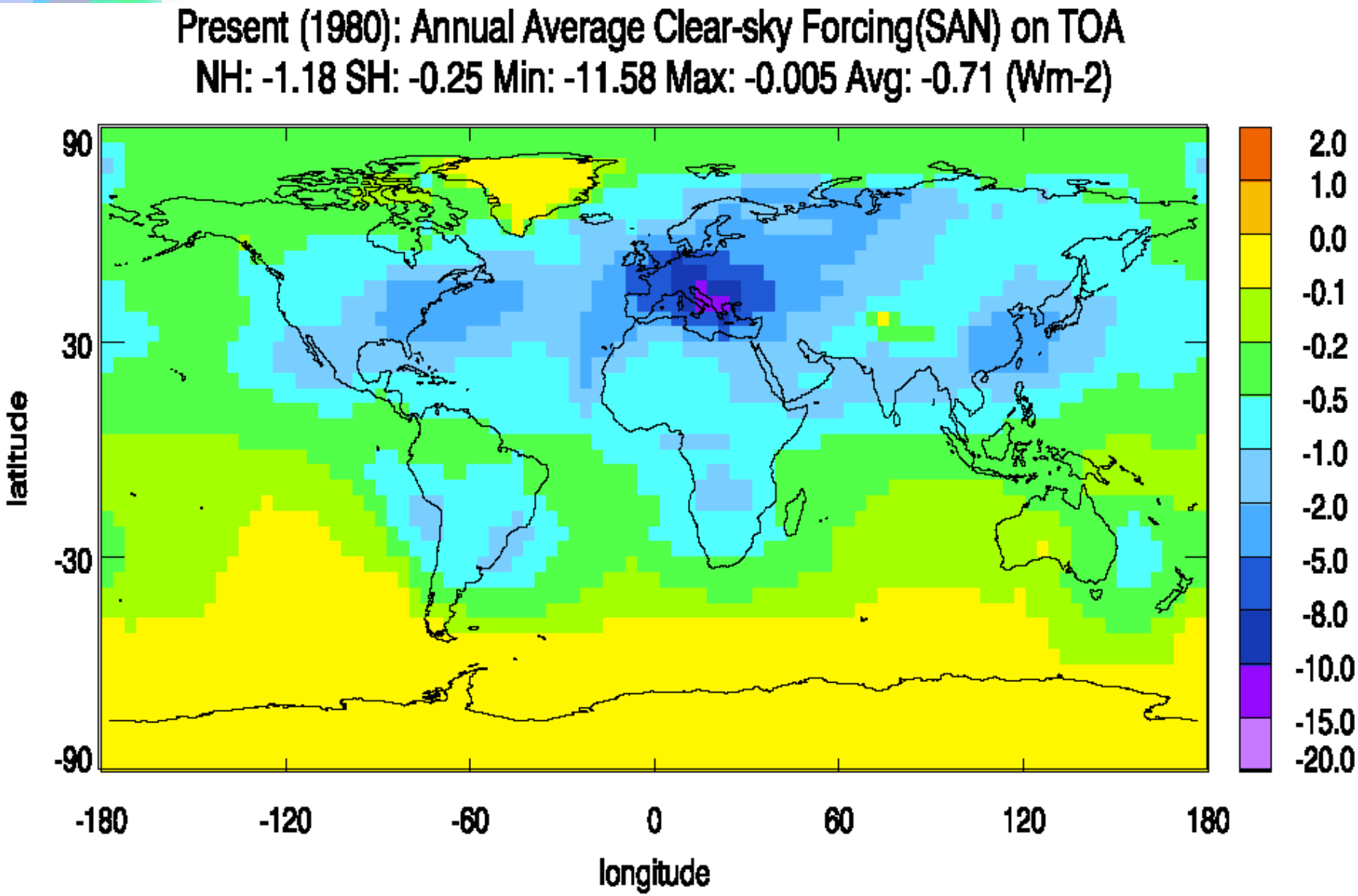
Accuracy of forcing calculation



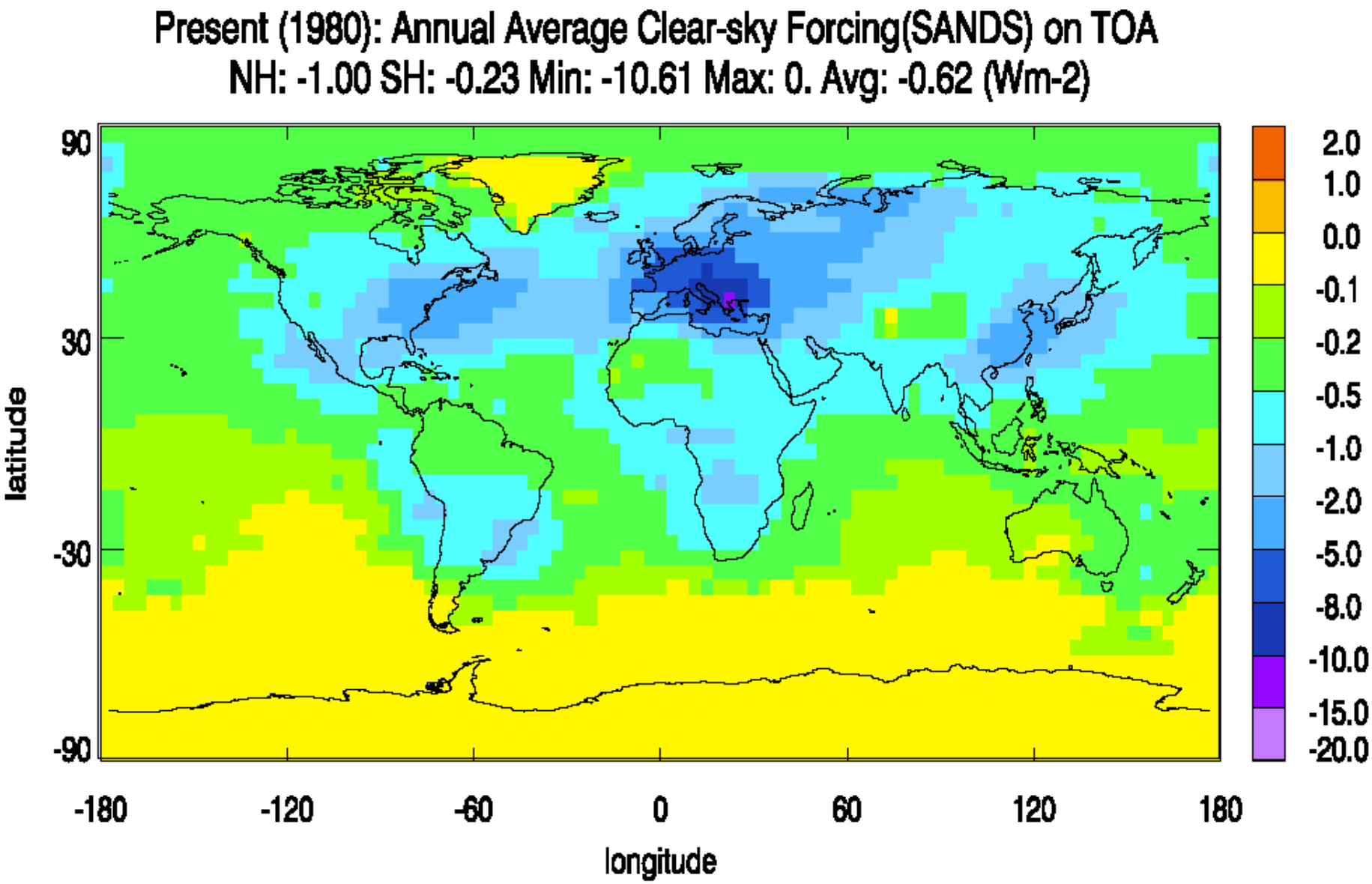
Clear-sky Short Wave Forcing by Present day (1980) Industrial and 2100 Aerosols

		Max RHs	Avg RHs	Min RHs	RH adjustment
Present:	SAN	-1.23	-0.65	-0.52	-0.71
Present:	SANDS	-1.03	-0.57	-0.46	-0.62
2100:	SAN	-1.75	-0.80	-0.61	-0.92
2100:	SANDS	-3.44	-1.74	-1.10	-1.91

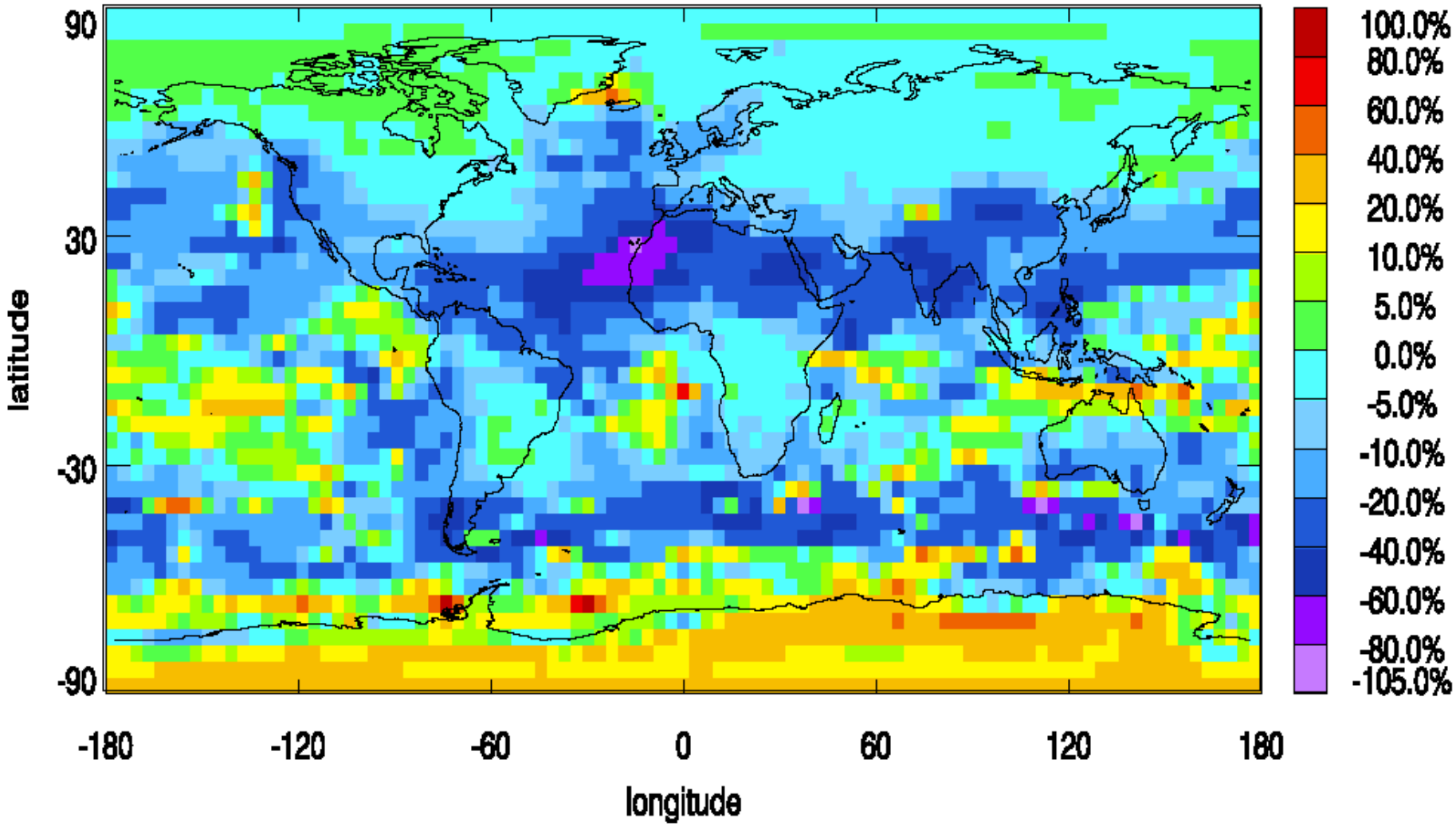
Present day forcing case with sulfate, ammonia and nitrate



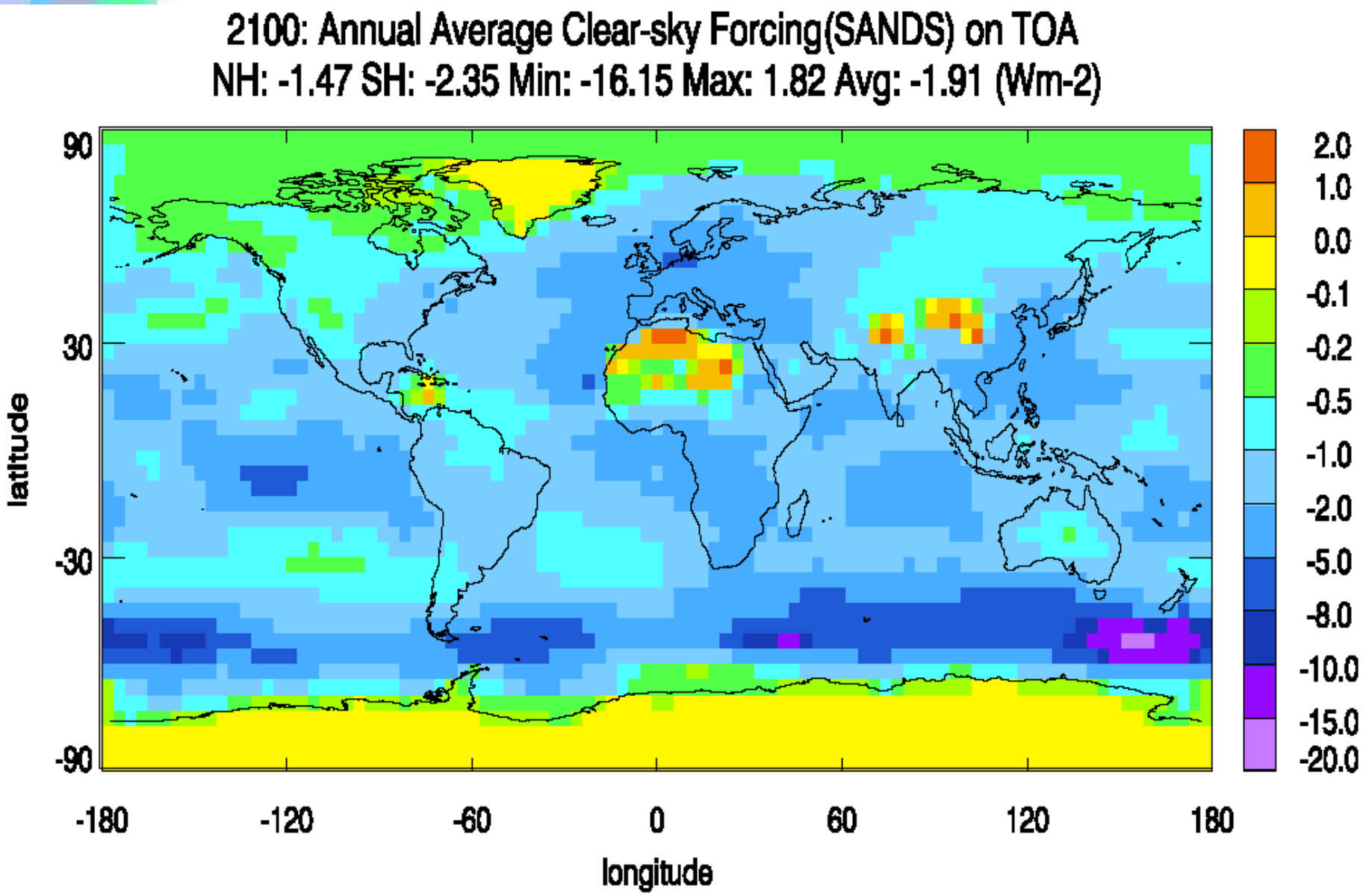
Present day forcing with dust and sea salt



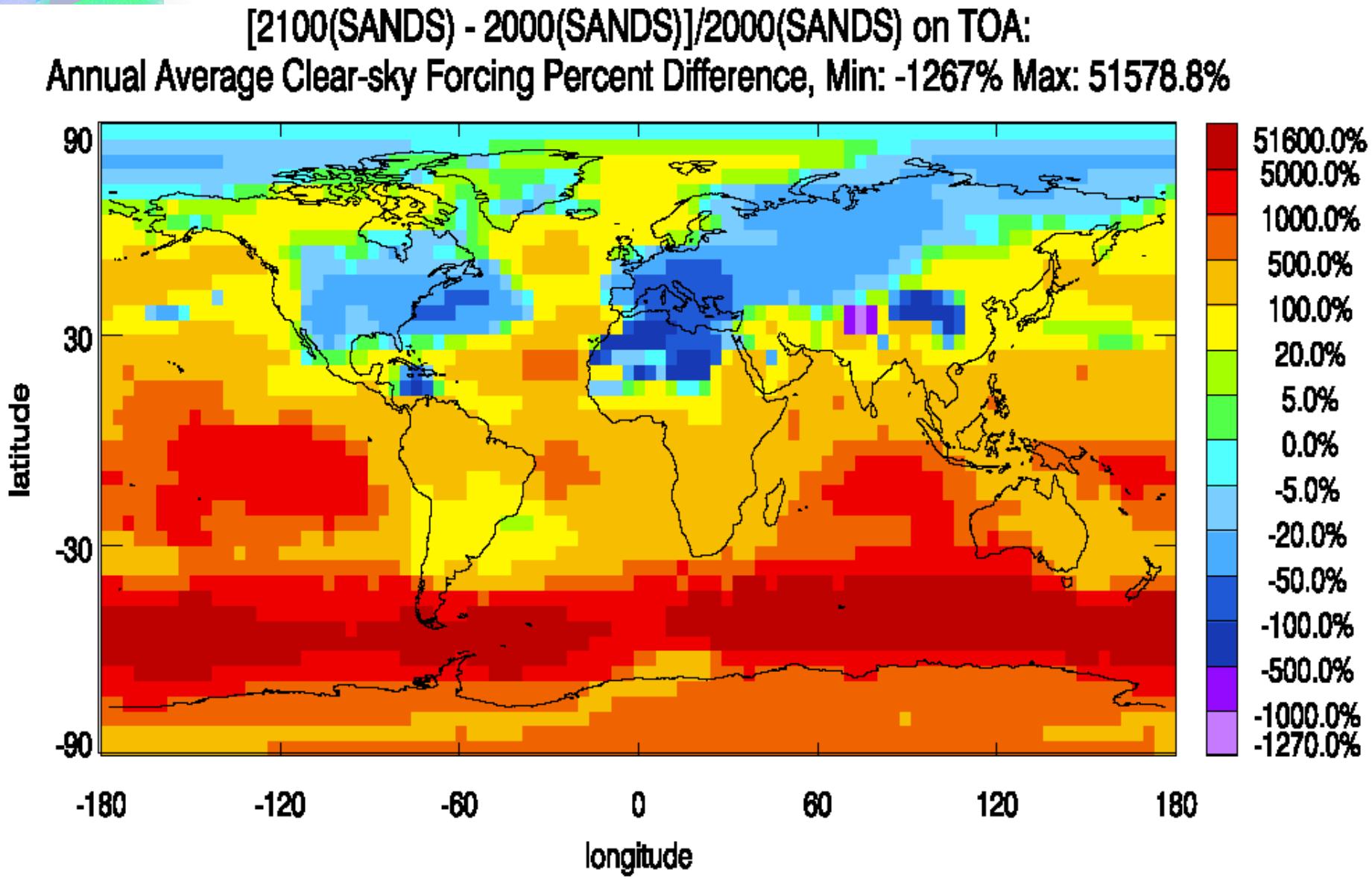
Percentage change in forcing when dust and sea salt are considered



Forcing in 2100



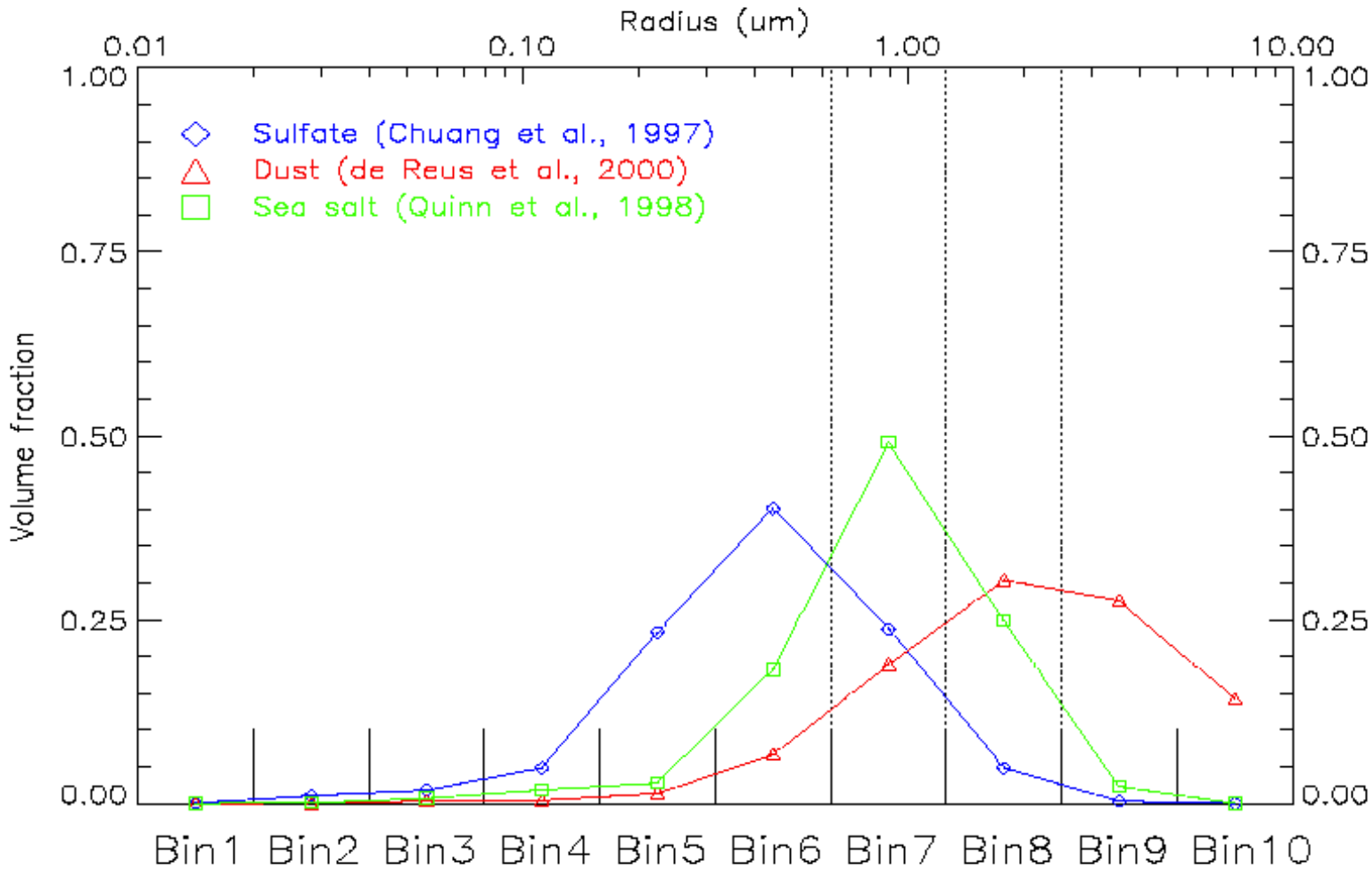
Percentage change in forcing 2100 and 2000

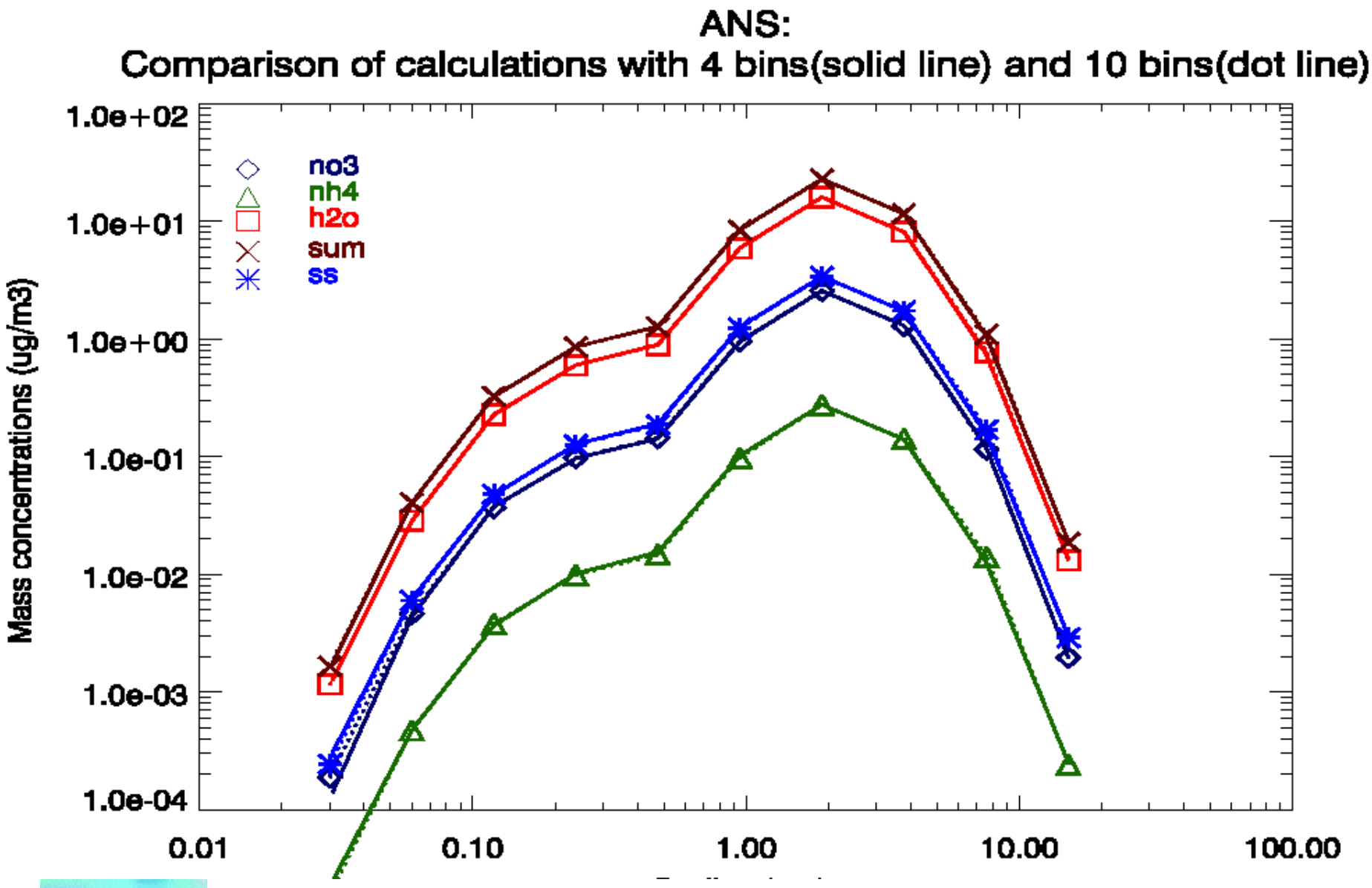


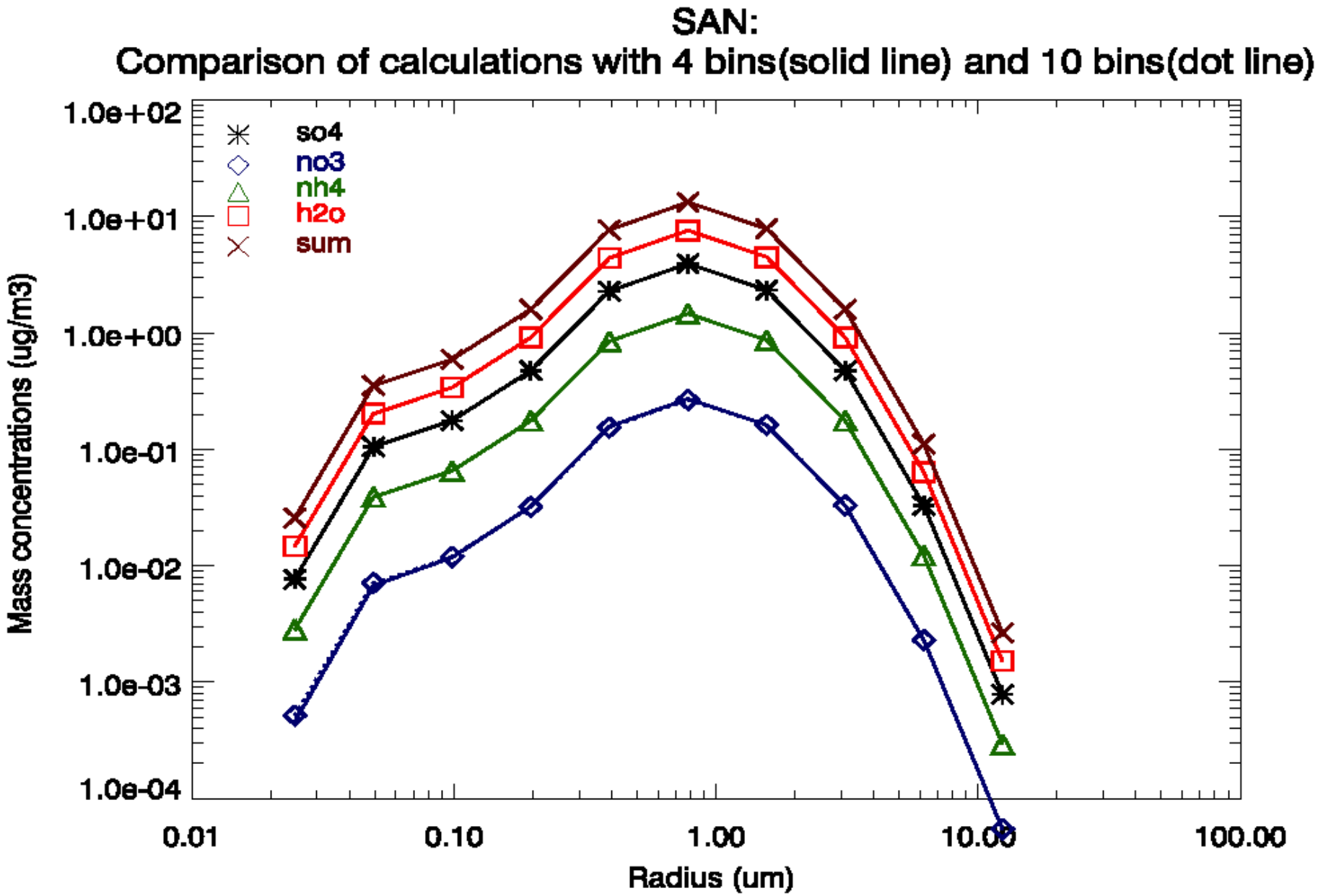
Comparison with other calculations:

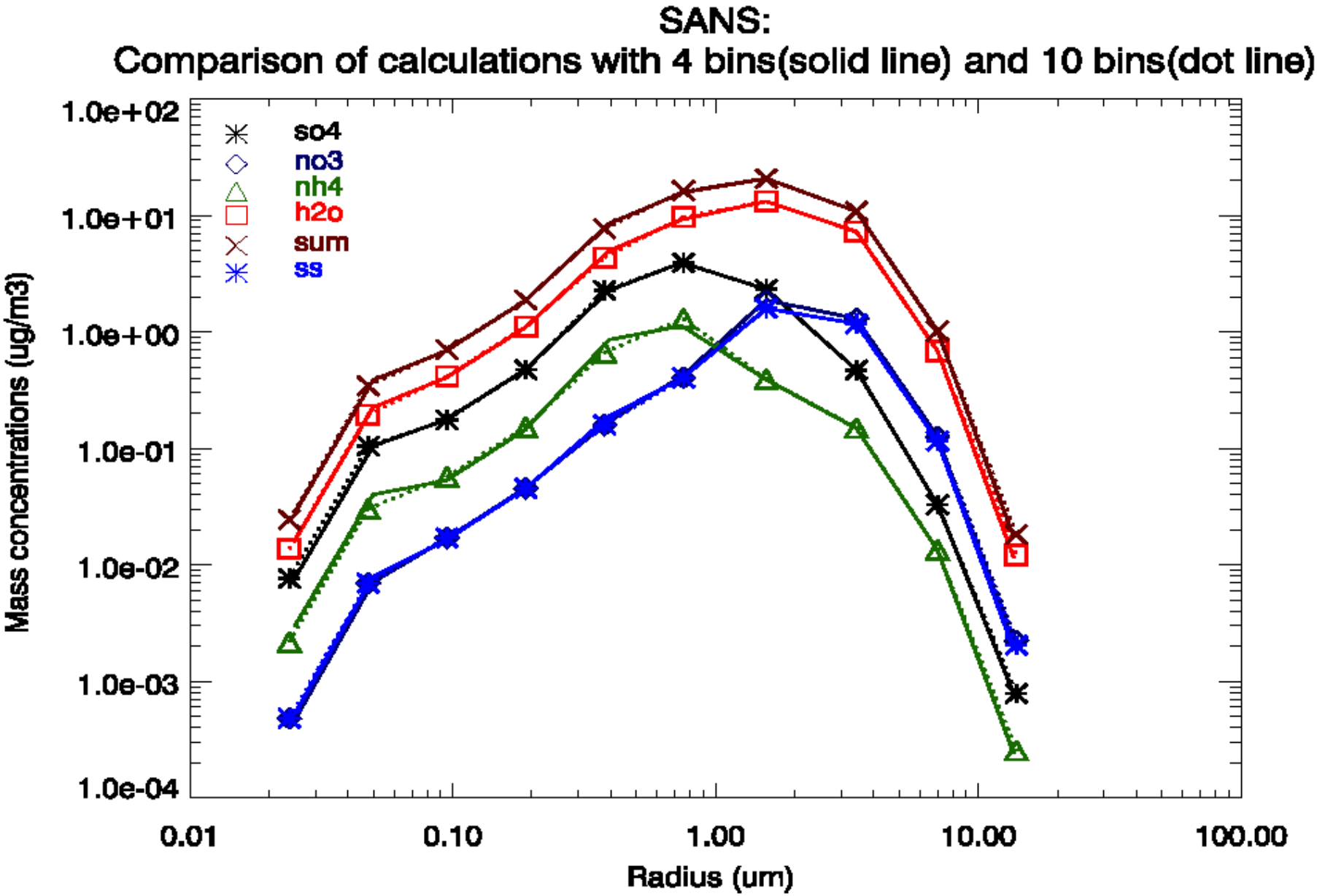
		Pre-industrial (SAN)	Present: SAN	Present: SANDS	2100: SAN	2100: SANDS
Burden	SO_4^{2-}	0.78	1.86	1.86	1.83	1.83
	NH_4^+	0.17	0.35	0.28	0.74	0.62
	NO_3^-	0.20	0.29	1.06	1.35	2.90
	H_2O	0.69	1.76	11.58	1.12	18.53
Forcing	This work (whole sky)		-0.38	-0.32	-0.43	-0.82
	Adams et al.		-1.14		-2.13	

Development of a method to treat dust/sea salt phase interactions in the global model




ANS:
Comparison of calculations with 4 bins(solid line) and 10 bins(dot line)
no3
nh4
h2o
sum
ss
Mass concentrations (ug/m3)
1.0e+02
1.0e+01
1.0e+00
1.0e-01
1.0e-02
1.0e-03
1.0e-04
0.01
0.10
1.00
10.00
100.00


SAN:
Comparison of calculations with 4 bins(solid line) and 10 bins(dot line)
so4
no3
nh4
h2o
sum
Mass concentrations (ug/m3)
1.0e+02
1.0e+01
1.0e+00
1.0e-01
1.0e-02
1.0e-03
1.0e-04
0.01
0.10
1.00
10.00
100.00
Radius (um)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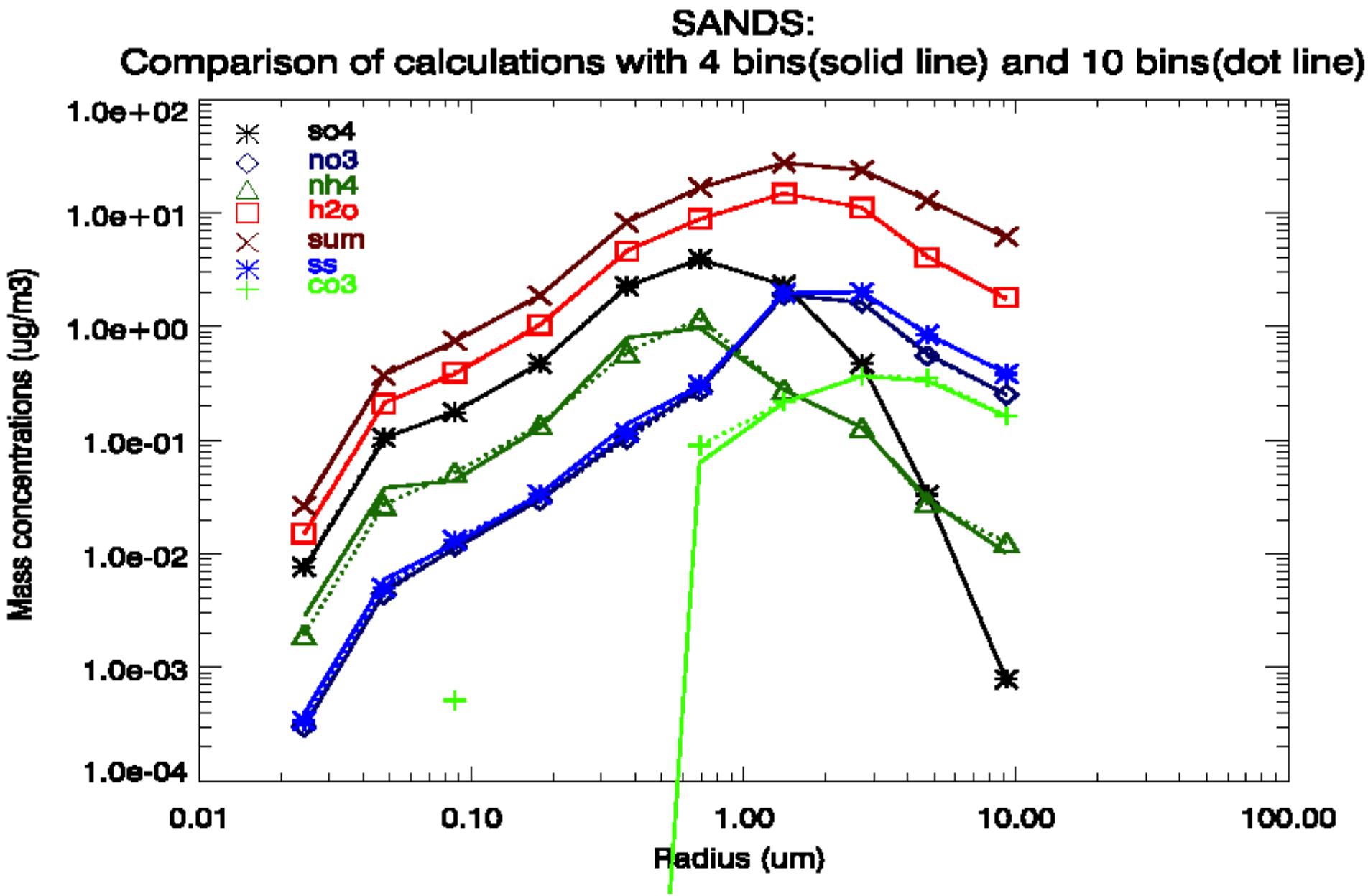
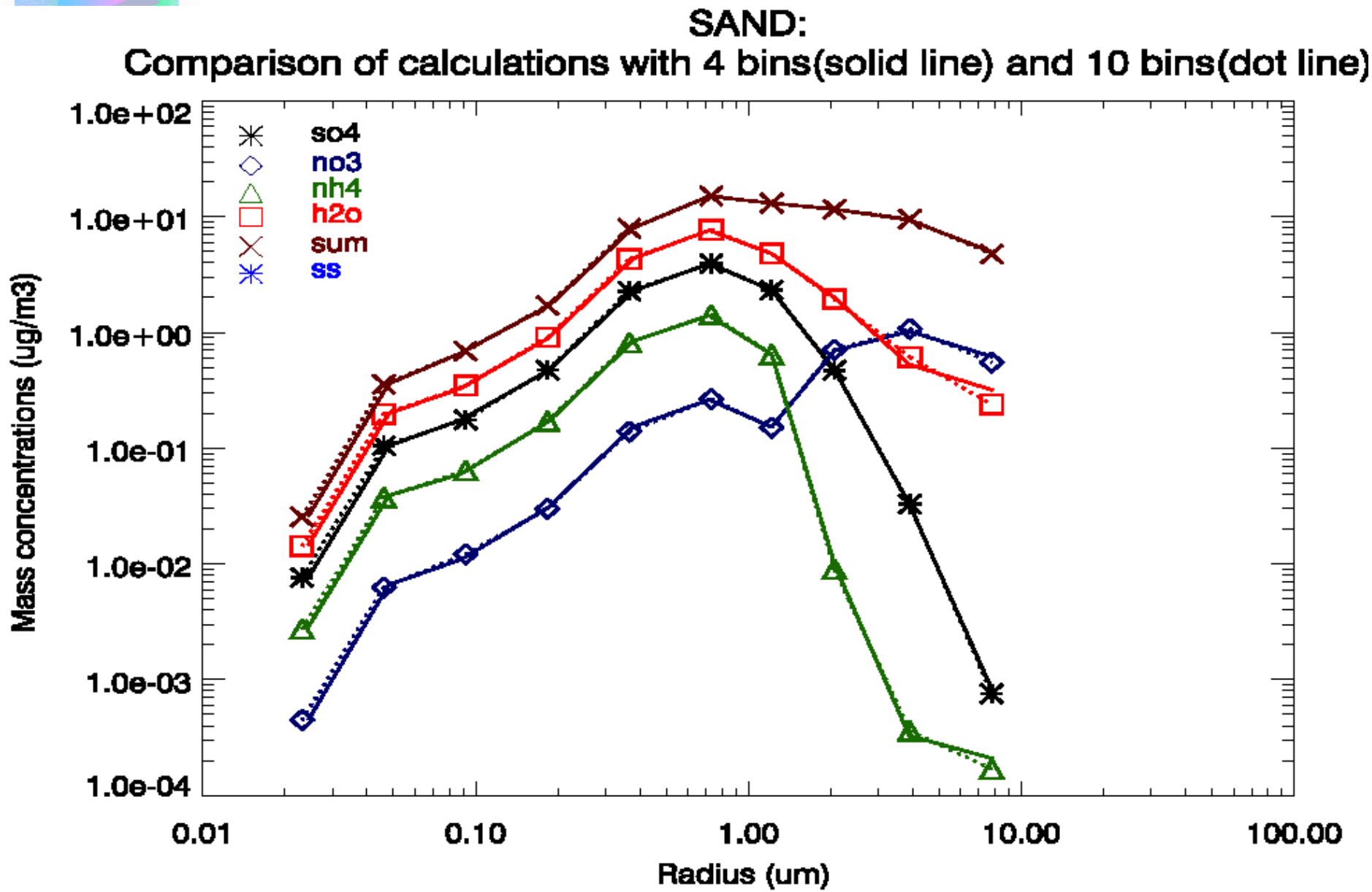
1.0e-03
1.0e-04
0.01
0.10
1.00
10.00
100.00
Radius (um)


SANDS:
Comparison of calculations with 4 bins(solid line) and 10 bins(dot line)
so4
no3
nh4
h2o
sum
ss
co3
Mass concentrations (ug/m3)
1.0e+02
1.0e+01
1.0e+00
1.0e-01
1.0e-02
1.0e-03
1.0e-04
0.01
0.10
1.00
10.00
100.00
Radius (um)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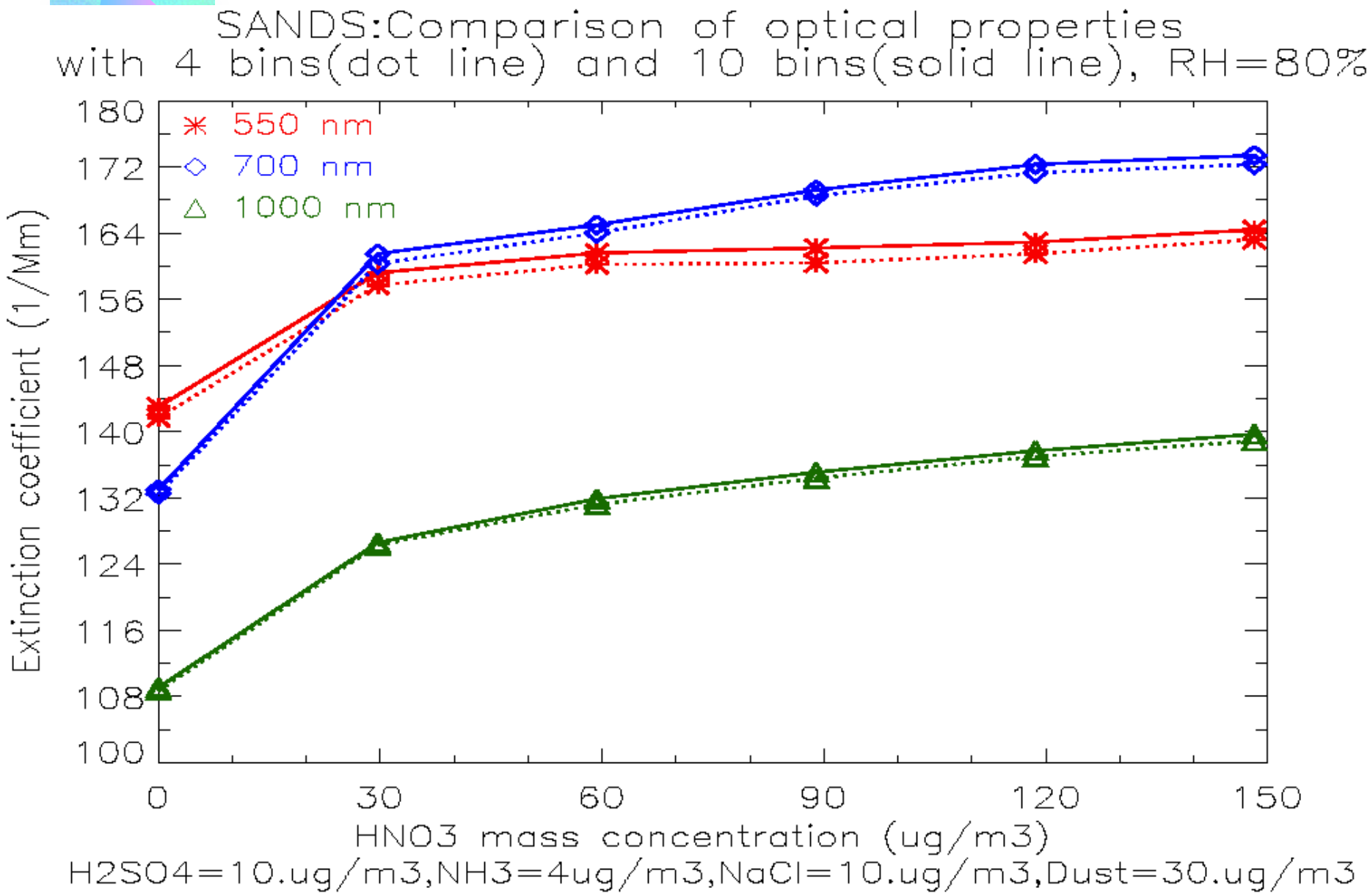
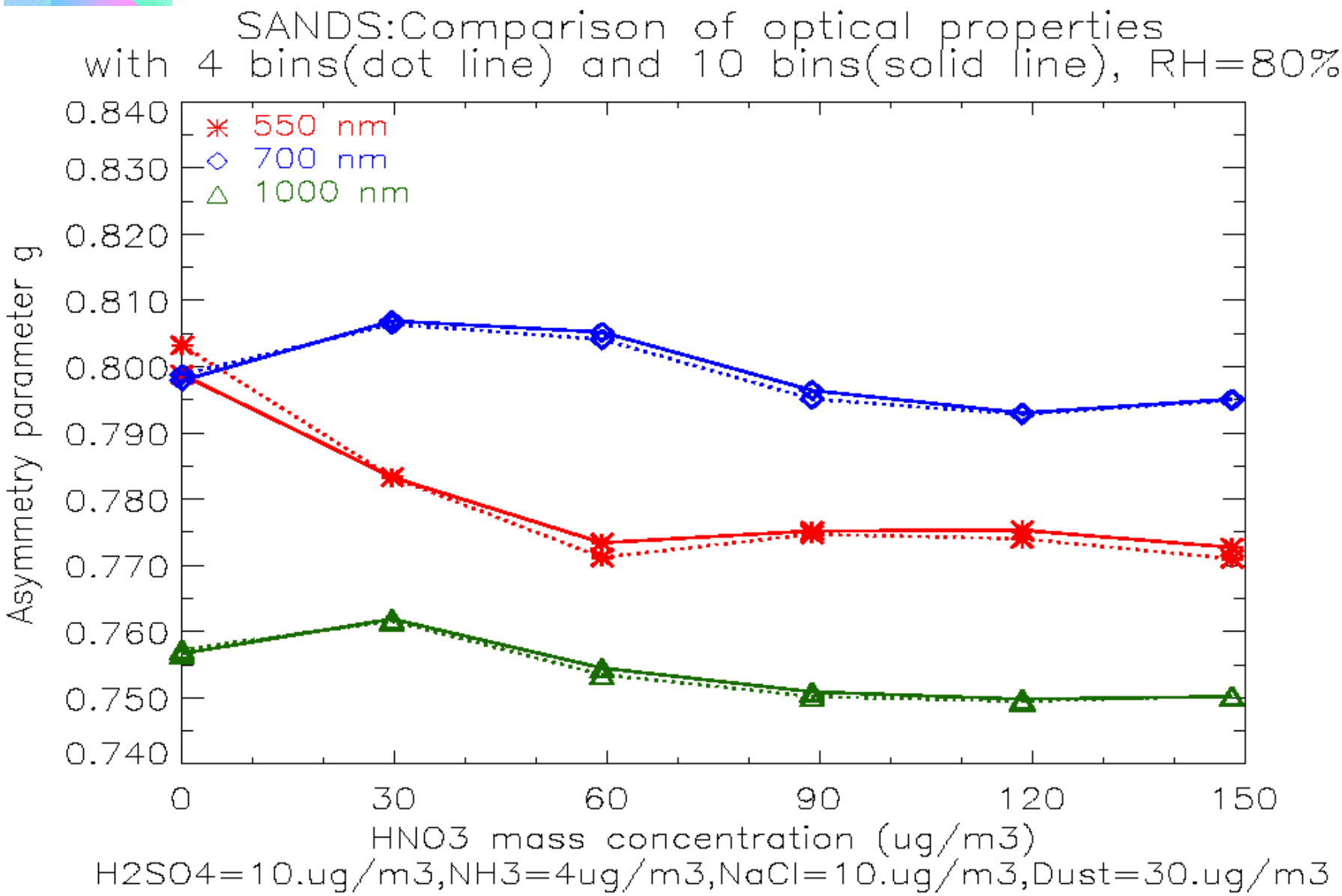
Comparison of calculations with 4 bins(solid line) and 10 bins(dot line)
so4
no3
nh4
h2o
sum
ss
Mass concentrations (ug/m3)
1.0e+02
1.0e+01
1.0e+00
1.0e-01
1.0e-02
1.0e-03
1.0e-04
0.01
0.10
1.00
10.00
100.00
Radius (um)

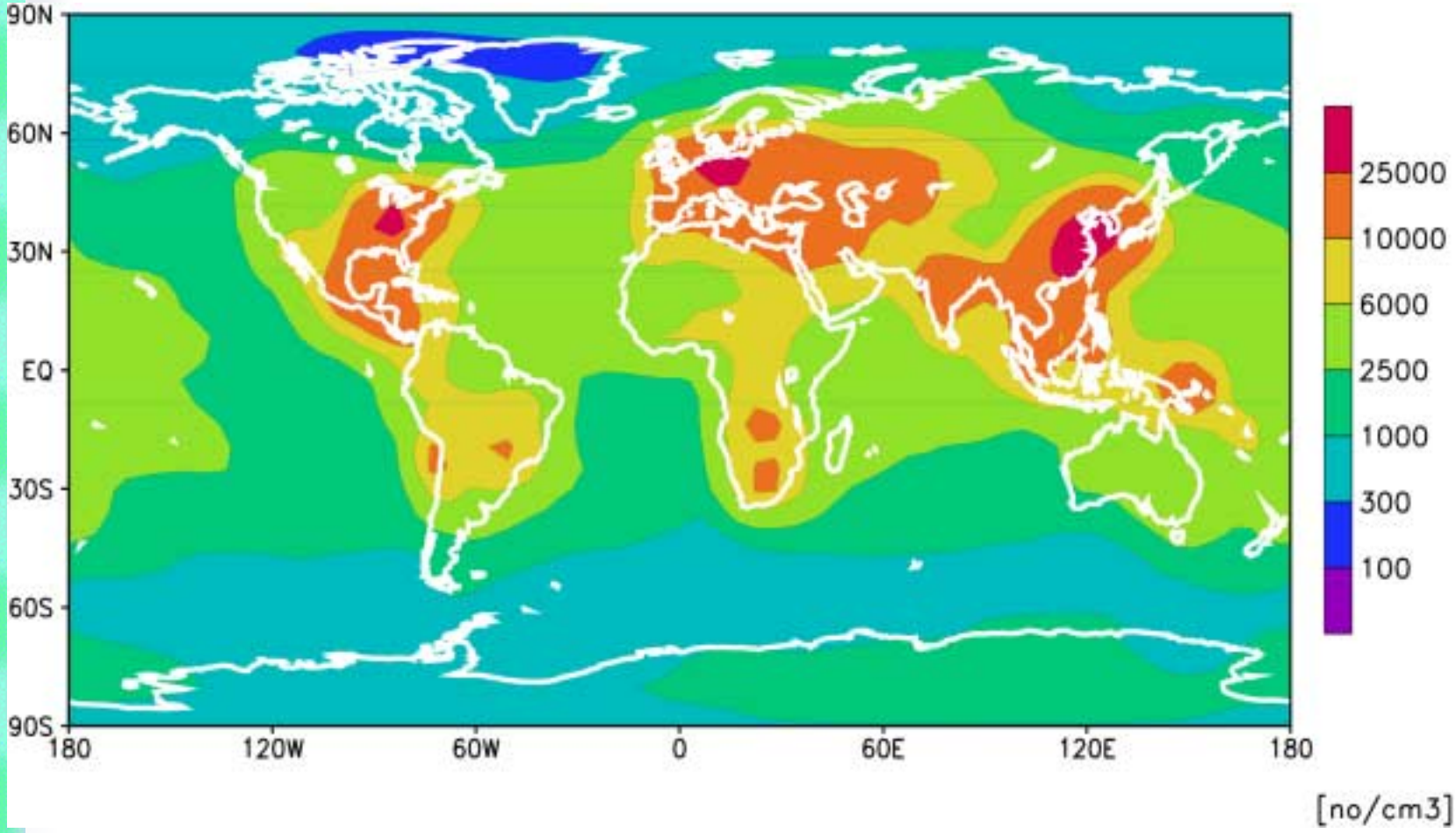

SANDS:Comparison of optical properties
with 4 bins(dot line) and 10 bins(solid line), RH=80%
550 nm
700 nm
1000 nm
Extinction coefficient (1/Mm)
180
172
164
156
148
140
132
124
116
108
100
0
30
60
90
120
150
HNO3 mass concentration (ug/m3)
H2SO4=10.ug/m3,NH3=4ug/m3,NaCl=10.ug/m3,Dust=30.ug/m3


SANDS:Comparison of optical properties
with 4 bins(dot line) and 10 bins(solid line), RH=80%
550 nm
700 nm
1000 nm
Asymmetry parameter g
0.840
0.830
0.820
0.810
0.800
0.790
0.780
0.770
0.760
0.750
0.740
0
30
60
90
120
150
HNO3 mass concentration (ug/m3)
H2SO4=10.ug/m3,NH3=4ug/m3,NaCl=10.ug/m3,Dust=30.ug/m3

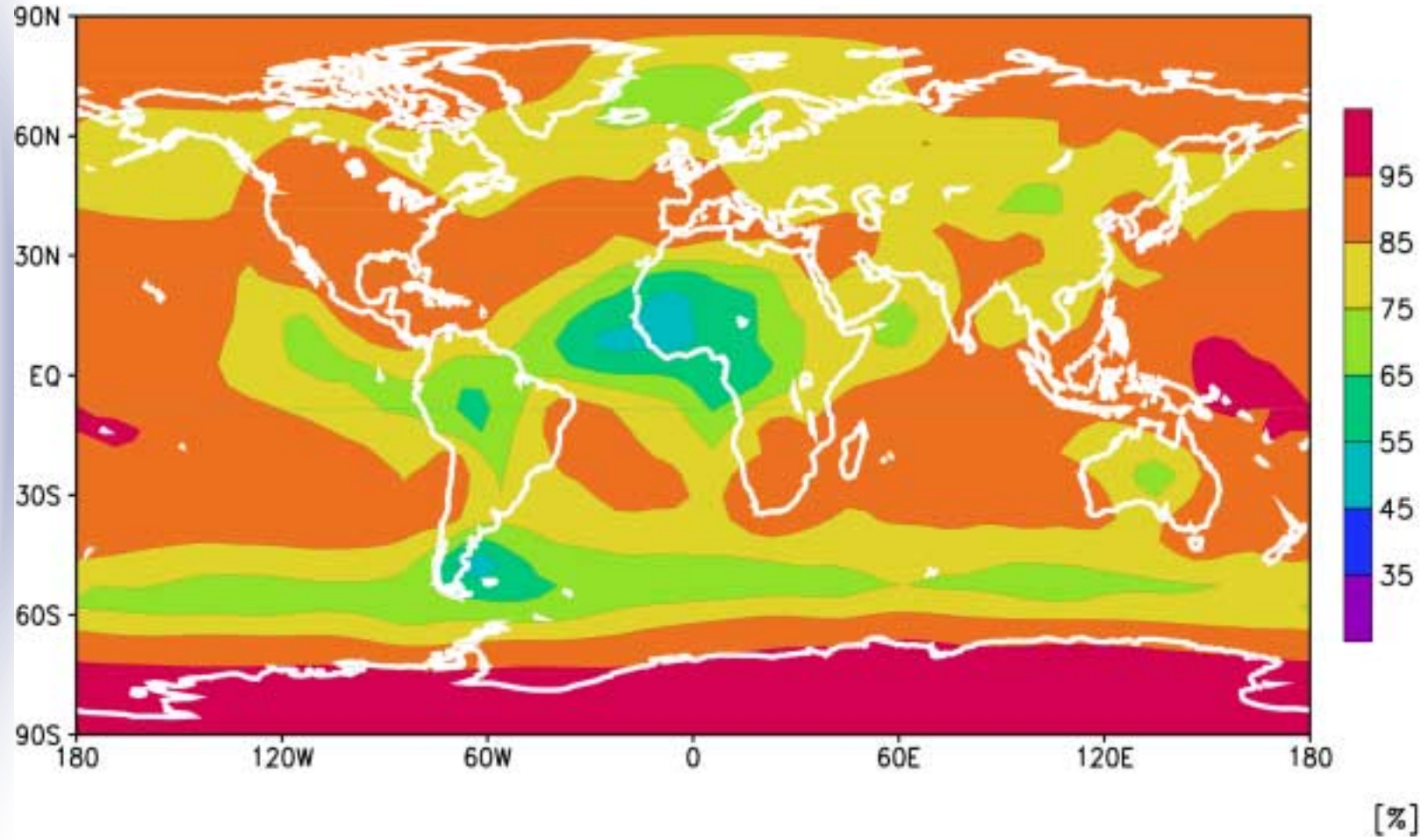
Progress on developing a prognostic capability for aerosol size

- Developed multi-mode, multi-moment aerosol nucleation and coagulation model
- Compared method in off-line mode with a full size-resolved aerosol model (Weisenstein-AER)
- Added model with both classical and Kulmala nucleation parameterization to Grantour

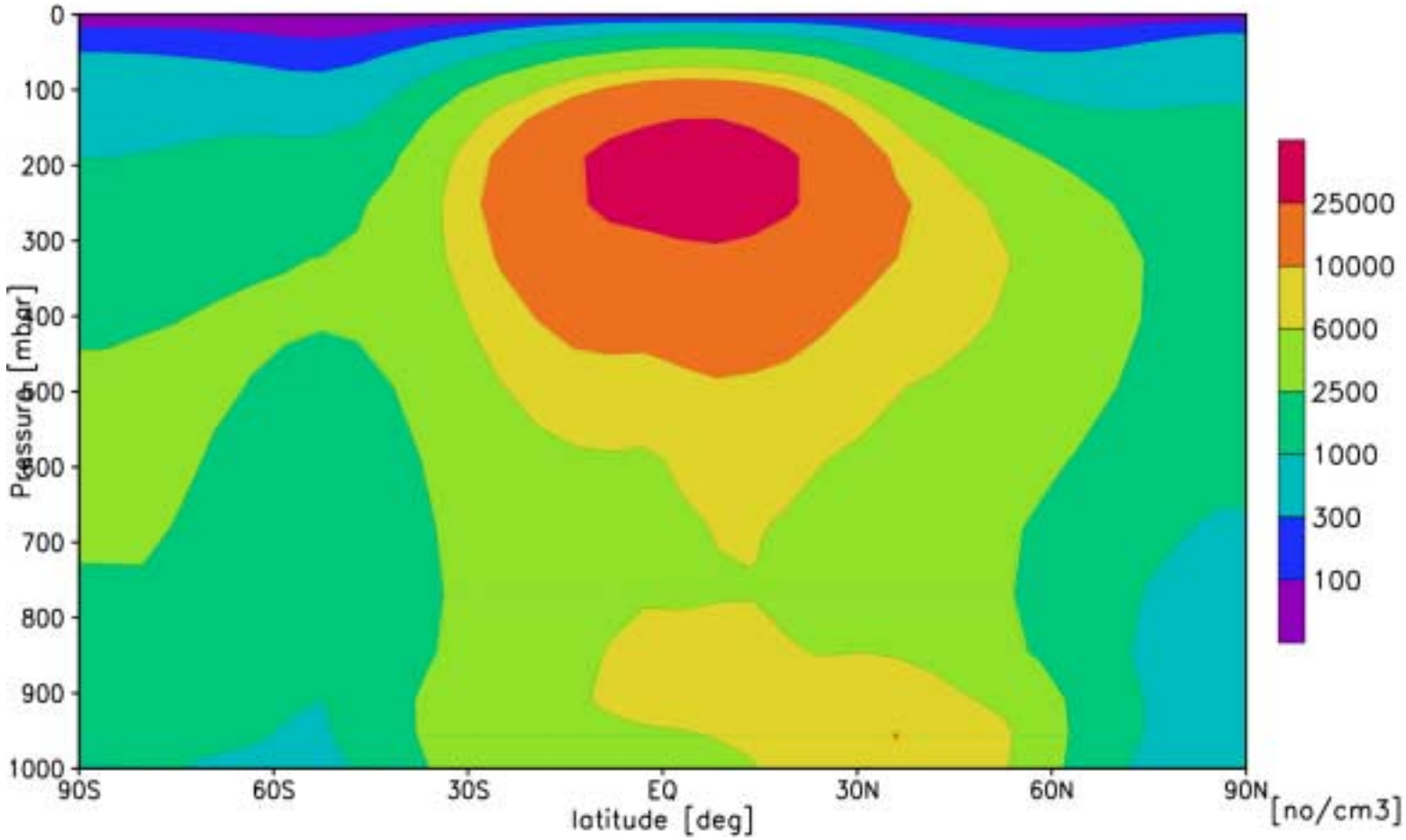
Preliminary prediction of surface aerosol number concentration



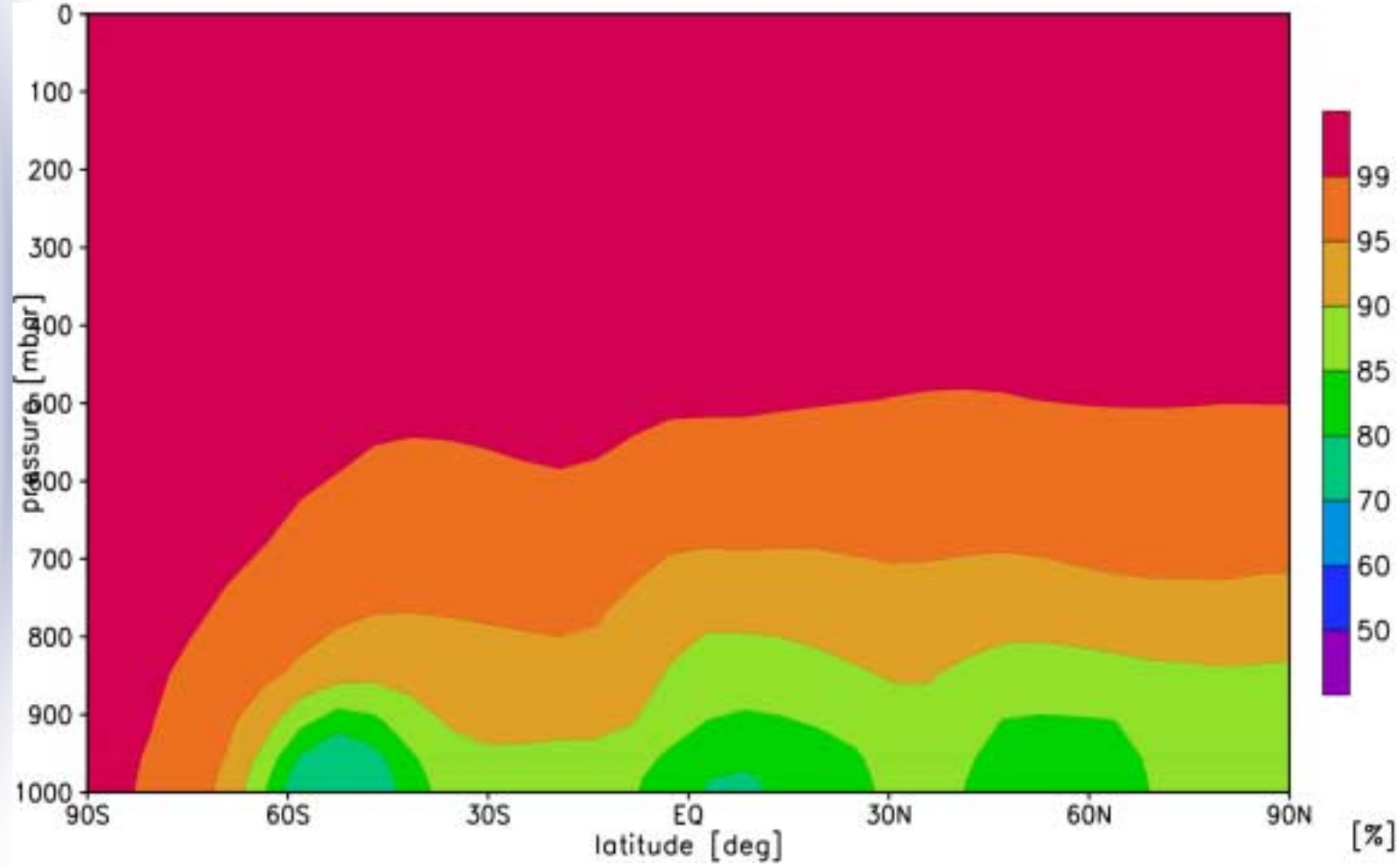
Fraction of aerosol number associated with sulfate aerosol



Zonal average total aerosol number (cm^{-3})



Fraction of particles that are sulfate



Progress in developing a fast gas and aerosol global model

- ¥ Developed mechanism that represents a full suite of VOCs
- ¥ Fast Sillman solution method
- ¥ Can use up to 4 hour chemical time steps

Condensed photochemical mechanism

- Contains NO_x, PANs, HNO_3, CO, CH_4, Lumped anthropogenic VOCs (fast-reacting and slow-reacting), biogenic,VOC,
  OH, HO_2, and RO_2 radicals. (38 species)

- Tested versus full mechanism based on updated Lurmann et al. (1986) (200 species)

Numerical solution

- ¥ Iterative procedure, fully implicit solution

- ¥ Uses equation for radical sources and sinks to obtain solution for OH and HO_2 in place of matrix inversion

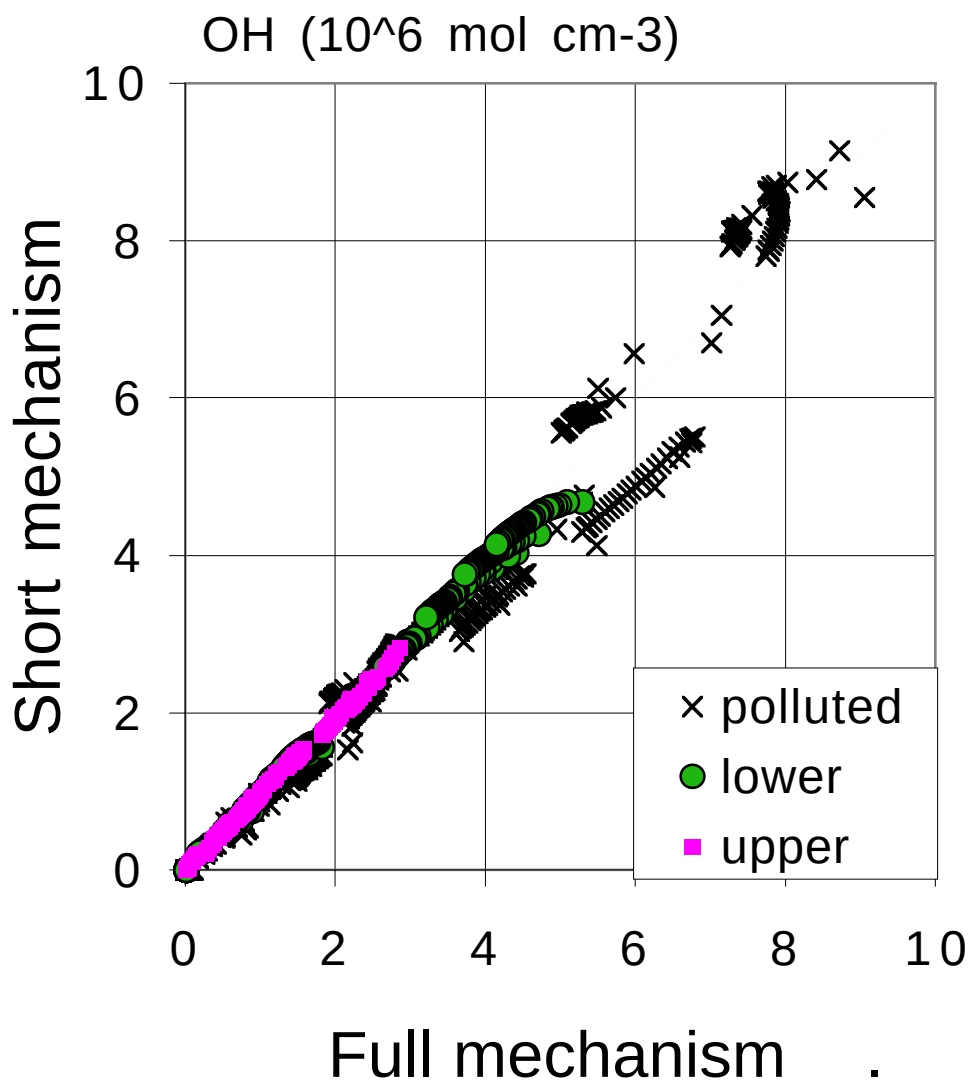
- ¥ Tested in intercomparisons for gas-phase and aqueous-phase tropospheric chemistry

Preliminary test of condensed photochemistry

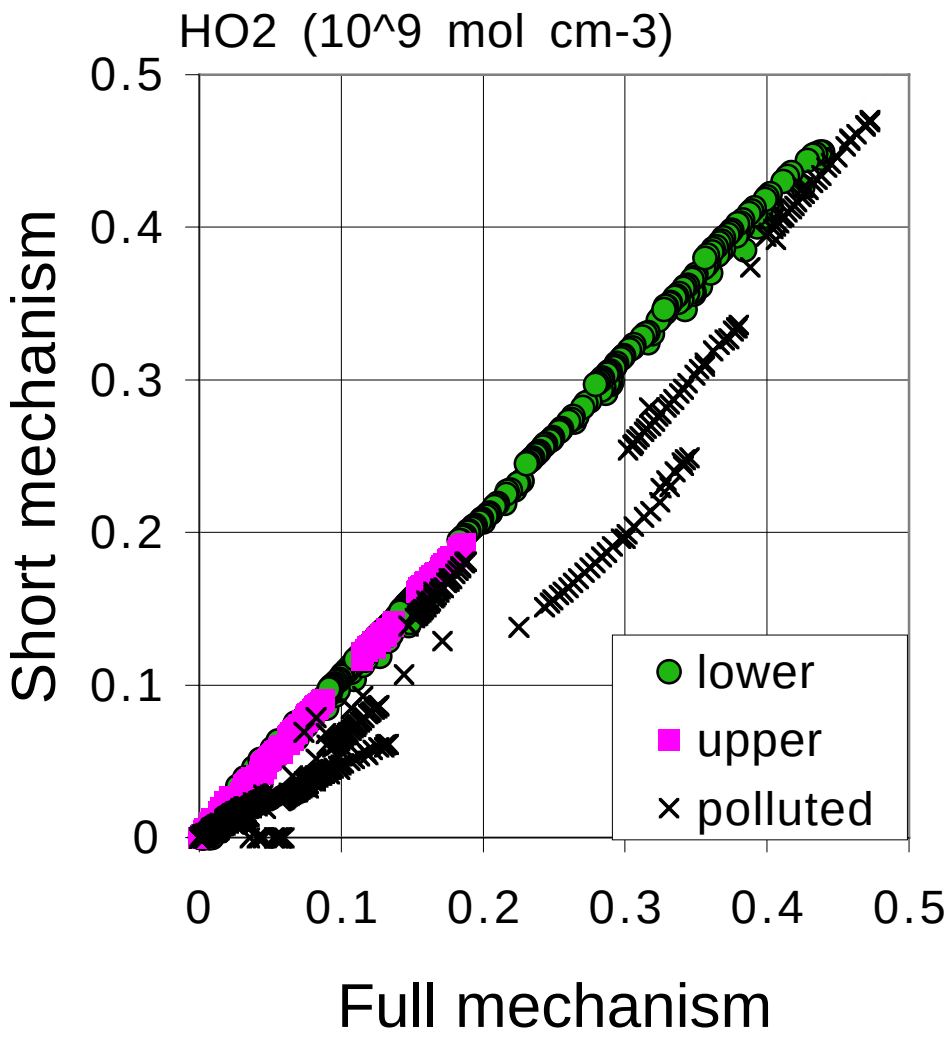
- 1-d (vertical) model for tropospheric chemistry/transport at 40 N, including sub-sections representing urban and polluted rural regions

- Identical calculations: short versus full photochemistry

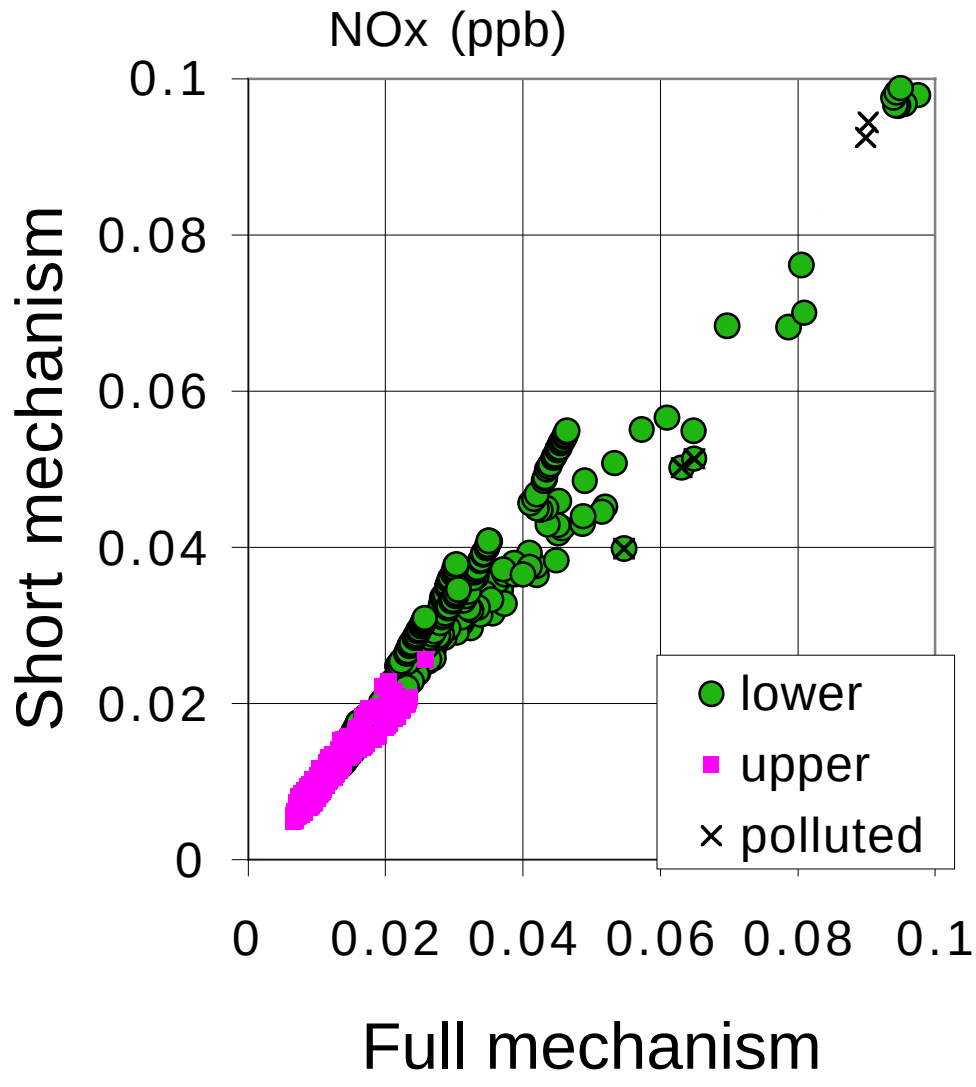
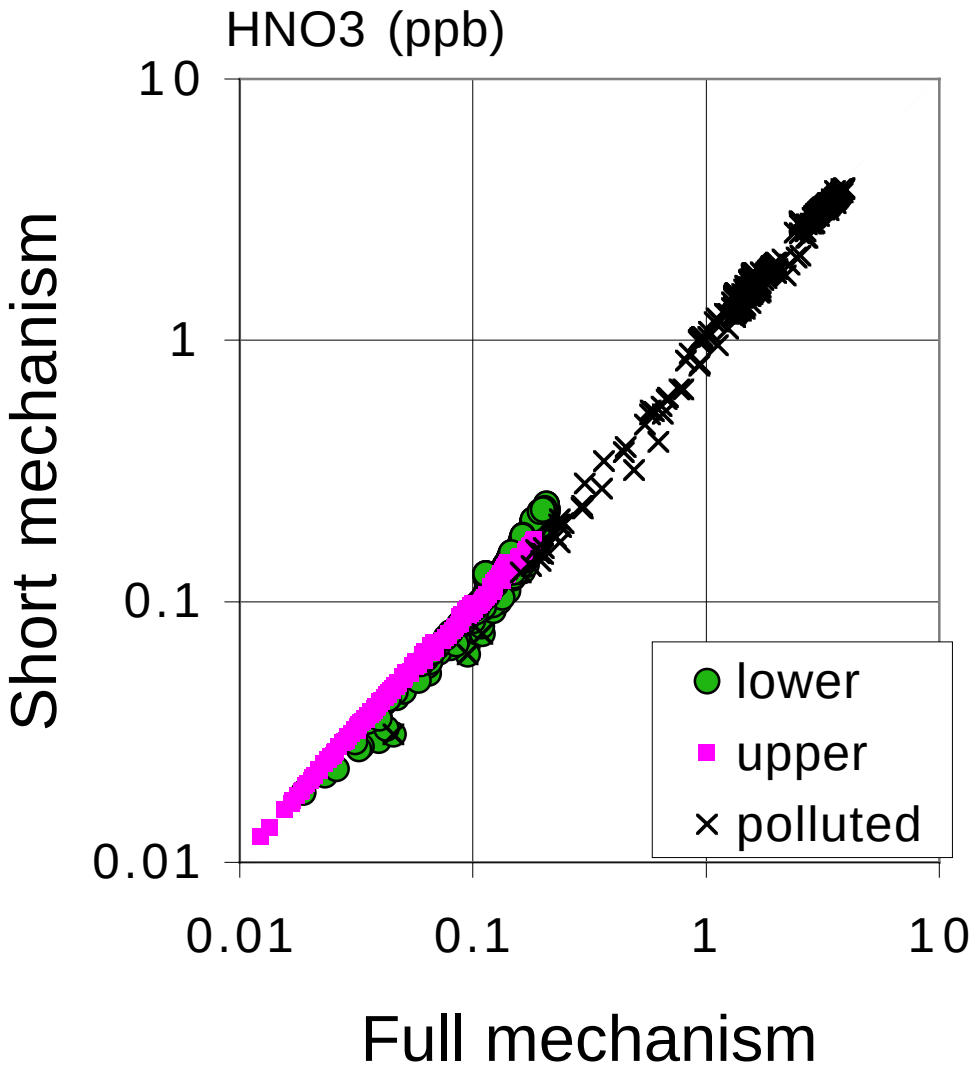
OH: Short vs full chemistry



HO2: Short vs full chemistry



NOx: Short vs full chemistry



HNO3: Short vs full chemistry