



Norwegian
Meteorological
Institute

AeroTab (NorESM2) : **look-up table code for aerosol optics** **and size-info, e.g. for CCN activation**

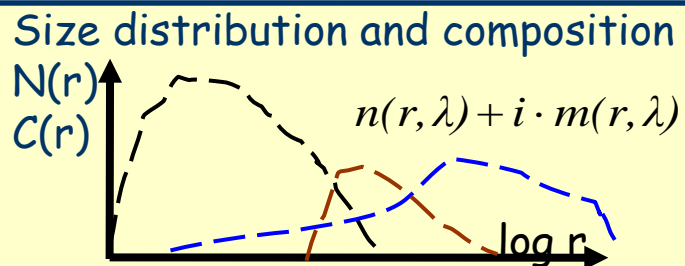
Alf Kirkevåg

13.01.2020

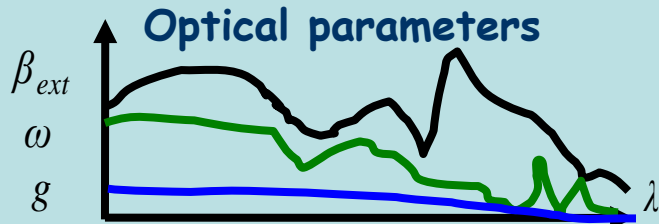
KL planning Meeting 15/1 2020

From life cycle calculations:
DU, SS and process specific SO_4 , BC, OC
+ relative humidity RH

Cond., coag. + cloud processing
(solve continuity eq.)



Mie theory



In CAM6-Nor

Optics
look-up
tables

Principle: Scheme
for parameterized
optical parameters

SW:

kcomp0.out
kcomp1.out
...

kcomp10.out

LW:

lwcomp0.out
lwcomp1.out
...

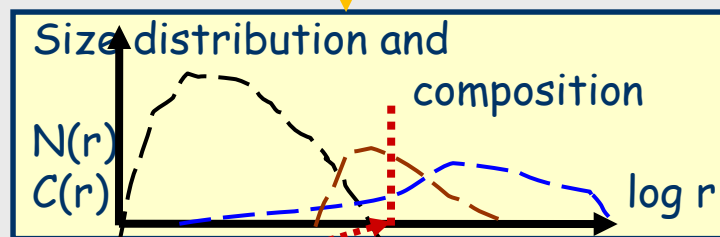
lwcomp10.out

+ aerocomk*.out
& aerodryk*.out
only with AeroCom set-up

Radiative
transfer code

From life cycle calculations:
DU, SS and process specific SO_4 , BC, OC

Cond., coag. + cloud processing
(solve continuity eq.)



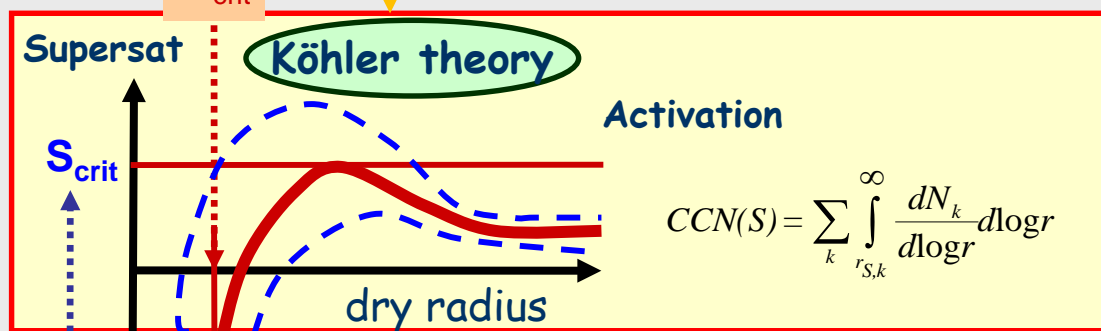
Principle: Scheme
for sizes used as input
to cloud droplet number
concentrations (CDNC)
calculations

Look-up tables:
lognormally fitted $N(r)$

logntilp0.out
logntil1.out

...
logntilp10.out

In CAM6-Nor



Calculated/realized S:
from adiabatic lifting, assuming
equilibrium between the
particles and the environment
(Abdul-Razzak and Ghan, 2000)

$CCN(S) \rightarrow$ source for CDNC

effective droplet radii,
liquid water content

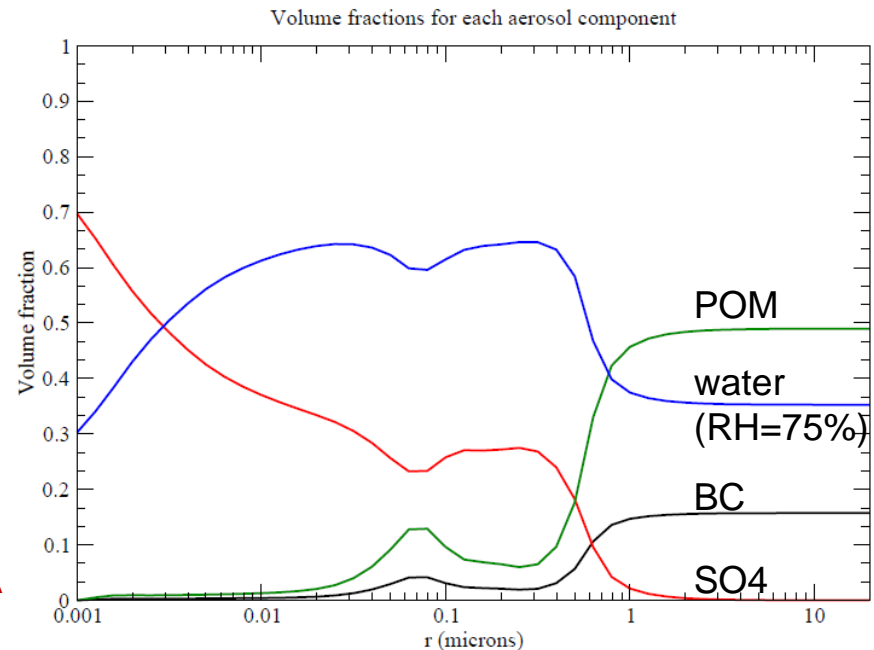
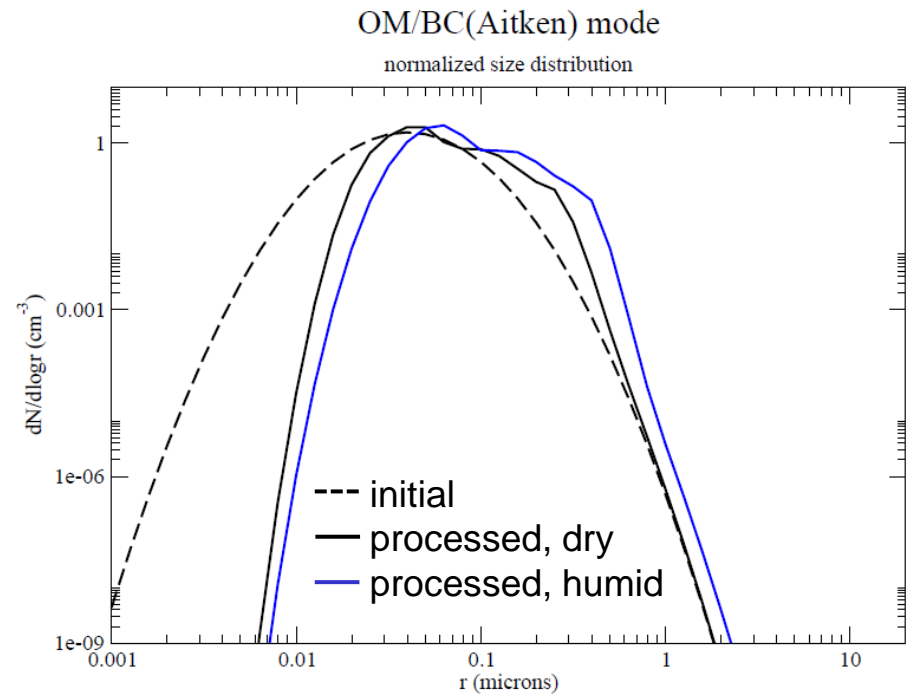
Radiative
forcing, W/m^2

Aerosol growth by:

- condensation of H_2SO_4 or SOA
- coagulation of Aitken particles onto larger pre-existing particles
- cloud-processing/wet phase chemistry
- hygroscopic growth

$$\ln\left(\frac{e_r}{e_{s,w}}\right) = \frac{2M_w\sigma_{s/r}}{RT\rho_w r} - \frac{M_w}{\rho_w} \left[\left(\frac{r}{r_0}\right)^3 - 1 \right] \sum_{\kappa} \nu_{\kappa} \Phi_{\kappa} \frac{\rho_{\kappa} \nu_{\kappa,k}(r_0)}{M_{\kappa}}$$

Ex. from
old version
without SOA



[20] We describe the size distribution with 44 size-bins along a logarithmic r -axis, with a bin-width of $\Delta \log(r/\mu\text{m}) = 0.1$. A discrete form of the continuity equation for $N_k(r,t)$;

$$\frac{\partial}{\partial t} \left[\frac{\partial N_k(r,t)}{\partial \log r} \right] + \frac{\partial}{\partial \log r} \left[\frac{D \log r}{Dt} \frac{\partial N_k(r,t)}{\partial \log r} \right] = 0, \quad (2)$$

Continuity equations for particle number concentrations

(see Kirkevåg and Iversen, 2002)

and similar equations for constituent mass concentrations are solved using a positive definite (anti-diffusive up-wind) advection scheme by Smolarkiewicz (1983) (*Mon. Wea. Rev.* 111, 479-486.)

[22] Following *Chuang and Penner* [1995],

$$\delta V_{aq}(r) = \frac{\Delta V_{aq}}{I_{max}} \theta(r - r_c) \left(\int \frac{dN(r)}{d \log r} \theta(r - r_c) d \log r \right)^{-1}$$

$$\delta V_{con}(r) = \frac{\Delta V_{con}}{I_{max}} r D'(r) \left(\int \frac{dN(r)}{d \log r} r D'(r) d \log r \right)^{-1}$$

and assuming coagulation of small particles onto larger size-modes:

$$\delta V_{coag}(r) = \frac{\Delta V_{coag}}{I_{max}} K_{1,2}(r, r_2) \left(\int \frac{dN(r)}{d \log r} K_{1,2}(r, r_2) d \log r \right)^{-1}$$

Hygroscopic growth of size distributions is also solved with the Smolarkiewicz scheme, but here with known growth factors, $f(r)$ (from Köhler Eq.), instead of known process mass (e.g. condensate, from CAM-Oslo life-cycle scheme).

**Not a part of AeroTab,
but related assumptions which are
needed in CAM-Oslo, in the
subroutine modalapp:**

(from Kirkevåg and Iversen, 2002):

[26] Let $\Delta V_{k,aq}$, $\Delta V_{k,con}$, and $\Delta V_{k,coag}$ denote the integrated added volumes per volume of dry air for mode k . Integrating equations (6–8) multiplied with the total size distribution or only mode k , yields the apportionment between the modes:

$$\Delta V_{k,con} = \Delta V_{con} \left[\int r D'(r) \frac{dN_k(r)}{d \log r} d \log r \right] \cdot \left[\int r D'(r) \frac{dN(r)}{d \log r} d \log r \right]^{-1}, \quad (9)$$

$$\Delta V_{k,coag} = \Delta V_{coag} \left[\int K_{1,2}(r, r_2) \frac{dN_k(r)}{d \log r} d \log r \right] \cdot \left[\int K_{1,2}(r, r_2) \frac{dN(r)}{d \log r} d \log r \right]^{-1}, \quad (10)$$

$$\Delta V_{k,aq} = \Delta V_{aq} \left[\int \theta(r - r_c) \frac{dN_k(r)}{d \log r} d \log r \right] \cdot \left[\int \theta(r - r_c) \frac{dN(r)}{d \log r} d \log r \right]^{-1}. \quad (11)$$

To reduce computational costs by table look-up and interpolation, we approximate equations (9–11) by using the initial size distribution in the integrands. We therefore only need to evaluate the modal apportionments for the first iteration. This approximation may displace the size-distributions, the effect of which is examined more closely in section 4, but is necessary in order to avoid solving equation (2) for the whole size distribution $N(r)$. Figure 1 shows an example of the effect of this approximation on a contaminated marine aerosol. The differences are negligible except for the smallest particles. For continental aerosol modes, the differences are even smaller.

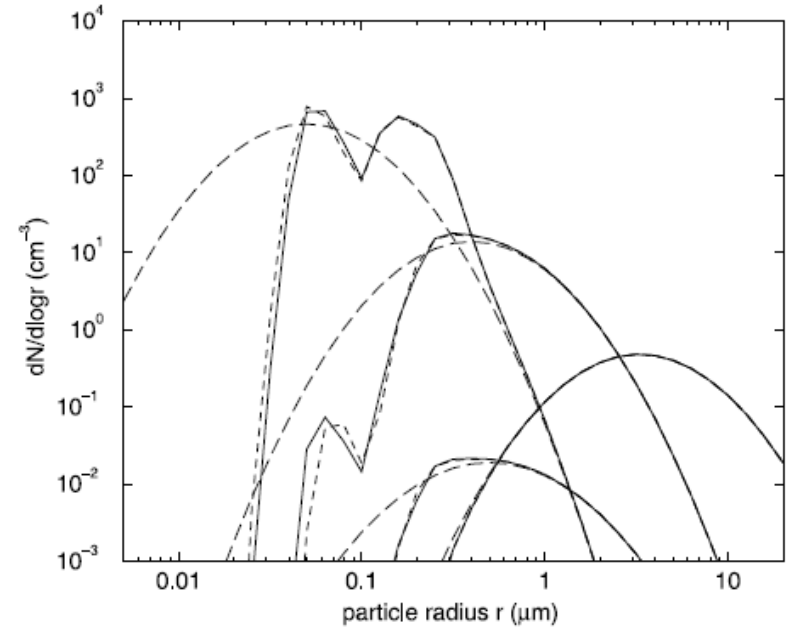
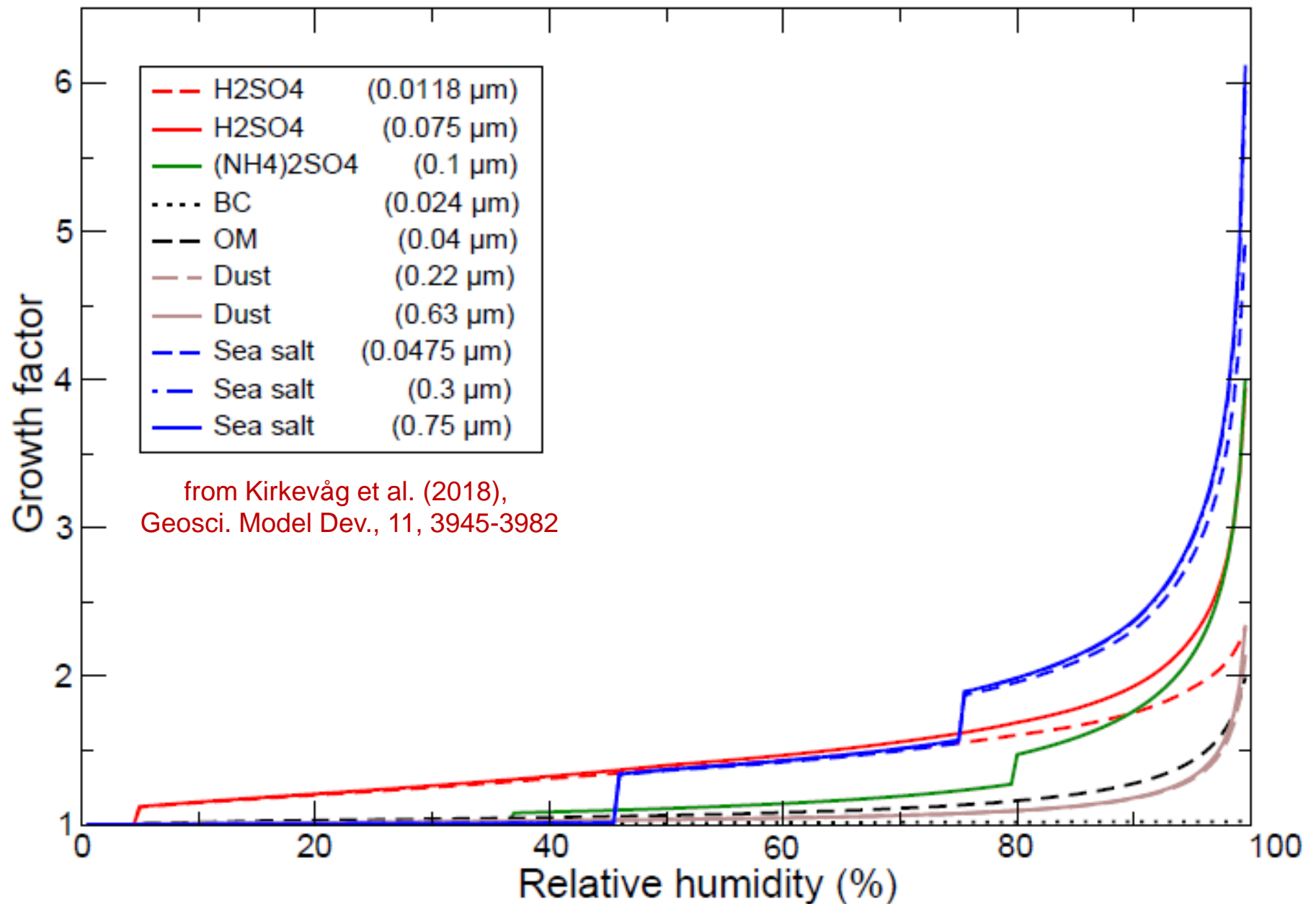


Figure 1. Example of the effects of condensation, coagulation and cloud processing on 4 modes of a marine size distribution, where $C^a = 10 \mu\text{g cm}^{-3}$, $f_{bc} = 0.1$, and $f_{aq} = 0.75$. The long-dashed curves are pure background size distributions, while the dashed and solid curves are parameterized and nonparameterized internally mixed modes.

Hygroscopic growth



The AeroTab code for producing look-up tables (LUT) (on NorESM git)

<u>AeroTab</u>	Main program, loops over a predefined input parameter space to make LUT
specbands	Define spectral bands, and sub-bands for Chandrasekhar averaging
constsize	Define physical constants and necessary aerosol parameters
modepar	Define log-normal size parameters and grids for use in the LUT
drydist	Calculate dry log-normal background number size distributions
condsub	Calculate diffusion coefficients
coagsub	Calculate coagulation coefficients
tabrefind	Read in and interpolate refractive indices for the used spectral bands
openfiles	Open files for output (LUT for use in CAM6-Nor)
tableinfo	Add relevant header info to the LUT (mode/mixture dependent)
hygro	Calculate hygroscopicity for each pure component (not always a constant)
conteq -> smolar	Find process-modified size distributions of number and constituent mass by use of the Smolarkiewicz advection scheme
rhsub -> koehler -> mixsub -> smolar	Calculate hygroscopic growth by numerically solving the Köhler equation for all externally and internally mixed components, and find new size distributions after hygroscopic swelling
sizemie -> refind -> miev0 -> chandrav	Calculate gross optical properties (integrated over all or some sizes) Calculate refractive indices for internal mixtures (volume / Maxwell-Garnett) Mie-calculations: qext, qsca, ggsc, sback Calculate chandrasekhar averaged optical properties sub-bands -> bands
modetilp	Find log-normal fits to the process-modified number size distributions

Setting up AeroTab.f to produce the required choice of lookup-tables

- c Modify the following input to create different sets of look-up tables:
- c Let iopt=1 for optics tables (CCN look-up tables for CAM-Oslo with diagnostic CDNC is no longer available), or iopt=0 for size distribution calculations (used in CCN activation in CAM4/5-Oslo and CAM6-Nor with prognostic CDNC):

iopt=1

- c Lognormal mode fitting (itilp=1, iopt=0) --> logntilp*.out (and nkcomp.out for dry, modified size distributions).

itilp=1-iopt

- c Outout for iopt=1 --> lwkcomp*.out or kcomp*.out, aerodryk*.out, aerocomk*.out, and nkcomp*.out (for size distributions for all RH).
- c SW: ib=29 (ave.=>12) SW "bands" (CAMRT), or
- c SW: ib=31 (ave.=>14) (RRTMG) (Added November 2013), or
- c LW: ib=19 (ave.=>16) (RRTMG) (Added November 2013):

ib=31

Let ib=31 for
SW optics,
and ib=19
for LW optics

...Loop over all modes/mixtures:

do kcomp=0,10 : for look-up tables, kcomp=0,10 (only kcomp=1-10 needed for logntilp*.out)

(... calculation for each mixture kcomp)

end do

Aerosol tracers and mixtures

some tracers are lumped in the look-up tables (LUT)

MODE/MIXTURE INDEX	Tracer 1	Tracer 2	Tracer 3	Tracer 4	Tracer5	Tracer 6	Tracer 7
0 (BC_AX)	BC_AX						
1 (SO4 COAT)	SO4_NA	SOA_NA	SO4_A1	SOA_A1			
2 (BC COAT)	BC_A	SO4_A1	SOA_A1				
3 (NO LONGER USED)							
4 (OM/BC COAT)	OM_AI	BC_AI	SO4_A1	SO4_A2	SOA_A1		
5 (SO4 PRIMARY)	SO4_PR	BC_AC	OM_AC	SO4_A1	SO4_AC	SO4_A2	SOA_A1
6 (DST A2)	DST_A2	BC_AC	OM_AC	SO4_A1	SO4_AC	SO4_A2	SOA_A1
7 (DST A3)	DST_A3	BC_AC	OM_AC	SO4_A1	SO4_AC	SO4_A2	SOA_A1
8 (SALT A1)	SS_A1	BC_AC	OM_AC	SO4_A1	SO4_AC	SO4_A2	SOA_A1
9 (SALT A2)	SS_A2	BC_AC	OM_AC	SO4_A1	SO4_AC	SO4_A2	SOA_A1
10 (SALT A3)	SS_A3	BC_AC	OM_AC	SO4_A1	SO4_AC	SO4_A2	SOA_A1
11 (NO LONGER USED)							
12 (BC NUCL)	BC_N						
13 (NO LONGER USED)							
14 (BC NUCL)	OM_NI	BC_NI					

these need LUT

= clean 2

= clean 4

Tracers contributing to number concentration in green.

New tracers since CAM4-Oslo in red.

_AC = coagulation
 _A1 = condensation
 _A2 = cloud processing

Do Loop:

The Index represents:

do kcomp = 0, 10

mode/mixture **kcomp**

do 540 irelh = irelh1, irelh2

ambient relative humidity **relh**

do 540 ifombg = ifombg1, ifombg2

mass fraction of OM (as SOA) in the OM & SO₄ backgr. of mixture 1, **fombg**

do 540 ifbcbg = ifbcbg1, ifbcbg2

mass fraction of BC in the OM & BC backgr. of mixture 4, **fbcbg**

do 540 ictot = ictot1, ictot2

total added mass ($\mu\text{g}/\text{m}^3$ per particle per cm^3) from cond.& coag.,
and wet phase chemistry/cloud processing for kcomp = 5-10, **ctot**

do 540 ictote = ictote1, ictote2

total added mass ($\mu\text{g}/\text{m}^3$ per particle per cm^3) from cond.& coag.,
and wet phase chemistry/cloud processing, for kcomp = 1-2, **ctote**

do 540 ifac = ifac1, ifac2

OM+BC mass fraction of total added process mass, **fac**

do 540 ifbc = ifbc1, ifbc2

BC fraction of added OM and BC, **fbc**

do 540 ifaq = ifaq1, ifaq2

wet phase SO₄ to total SO₄ added, **faq**

(... code ...)

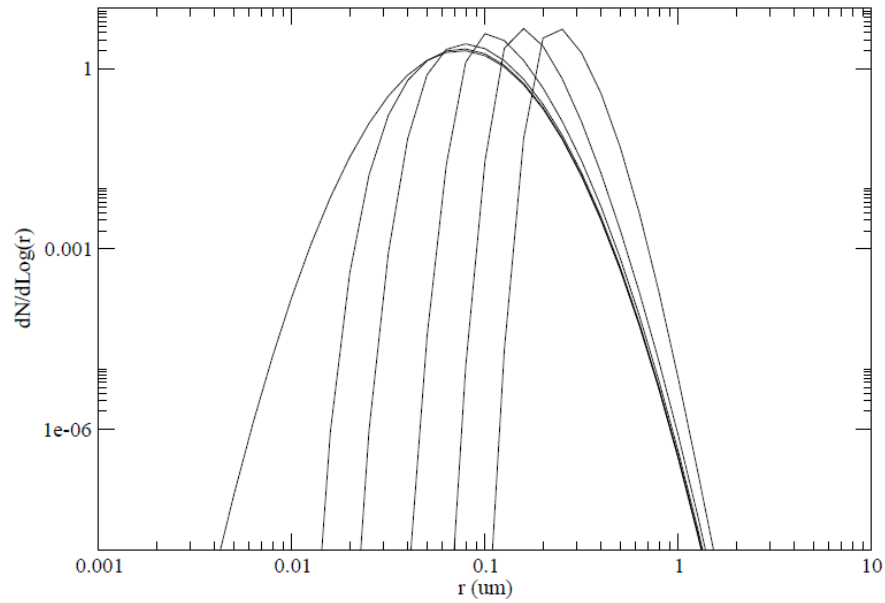
540 continue ! ifaq, ifbc, ifac, ictot/ictote, ifombg, ifbcbg, irelh

enddo ! kcomp

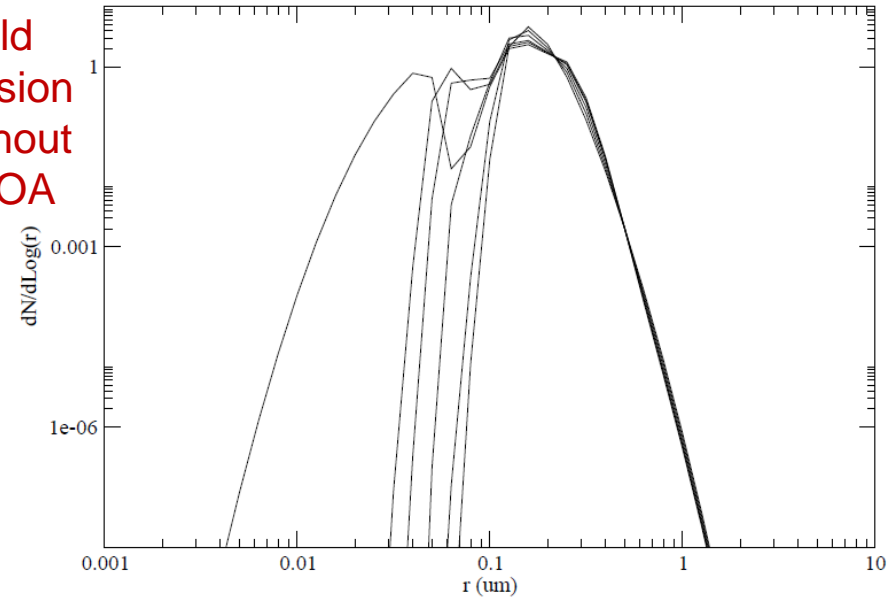
Note: «added» here means added onto an originally «log-normal background», i.e. addition of process-specific mass which causes changes in the size distributions.

Examples
from
old
version
without
SOA

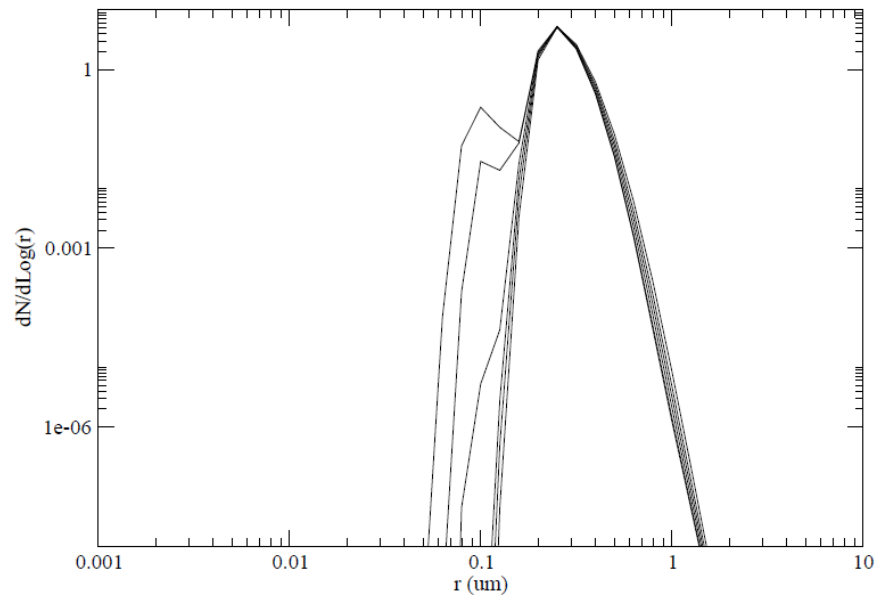
modified SO4(a) mode
with varying cat



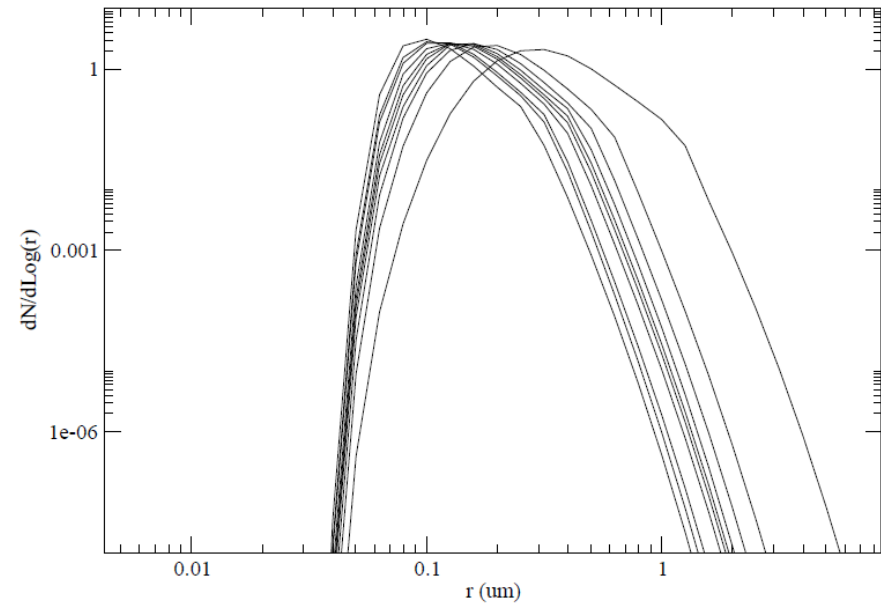
modified SO4(a) mode
with varying faq



modified SO4(a) mode
with varying fac



modified SO4(a) mode
with varying RH



Ex. optics look-up tables for normalized size-distribution (1 cm^{-3}):
 SO4_NA / SO4_A1 mode (without SOA), kcomp1.out

(+ fac, fbc, faq for full mixtures, i.e. for kcomp5-10.out)

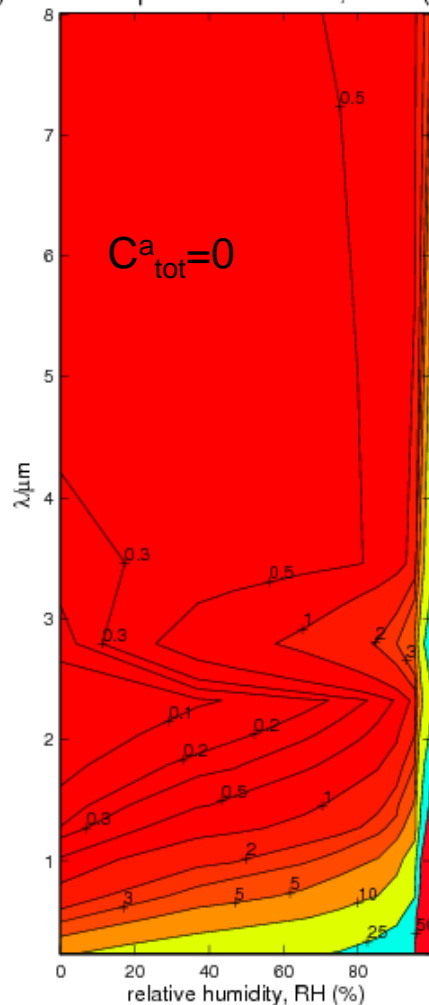
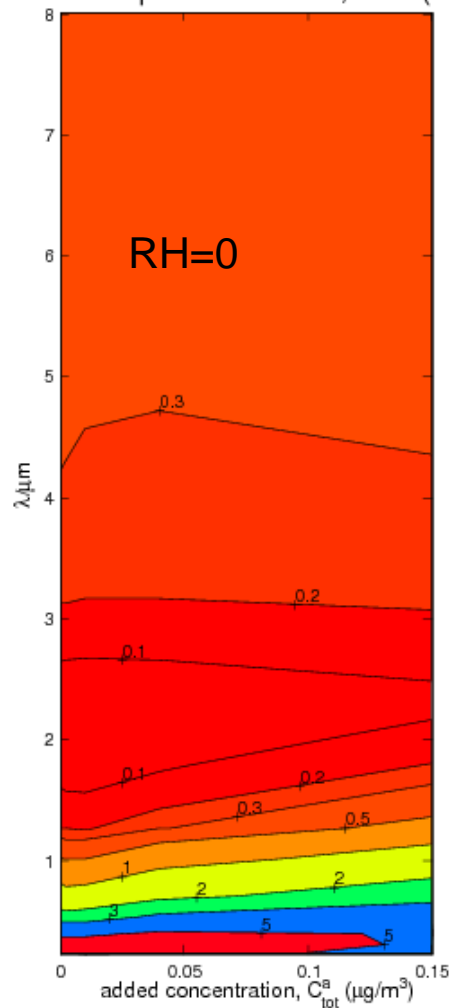
kcomp	λ -band	RH	catot ($\mu\text{g}/\text{m}^3$)	ω (SSA)	g (ASS)	β_{ext} (km^{-1})	k_{ext} (m^2/g)
1	1	0.000	0.100E-09	0.10000E+01	0.47359E+00	0.16628E-06	0.27715E+01
1	2	0.000	0.100E-09	0.10000E+01	0.39279E+00	0.71593E-07	0.11932E+01
1	3	0.000	0.100E-09	0.10000E+01	0.32032E+00	0.31281E-07	0.52137E+00
1	4	0.000	0.100E-09	0.10000E+01	0.23817E+00	0.11838E-07	0.19731E+00
1	5	0.000	0.100E-09	0.10000E+01	0.16972E+00	0.42962E-08	0.71605E-01
1	6	0.000	0.100E-09	0.99925E+00	0.10729E+00	0.13311E-08	0.22185E-01
1	7	0.000	0.100E-09	0.98957E+00	0.68222E-01	0.40892E-09	0.68156E-02
1	8	0.000	0.100E-09	0.89741E+00	0.54710E-01	0.26690E-09	0.44485E-02
1	9	0.000	0.100E-09	0.51139E+00	0.37973E-01	0.20475E-09	0.34126E-02
1	10	0.000	0.100E-09	0.17958E+00	0.28885E-01	0.29873E-09	0.49789E-02
1	11	0.000	0.100E-09	0.63999E-01	0.22469E-01	0.45194E-09	0.75325E-02
1	12	0.000	0.100E-09	0.16020E-02	0.15484E-01	0.71279E-08	0.11880E+00
1	13	0.000	0.100E-09	0.47779E-03	0.10429E-01	0.15419E-07	0.25700E+00
1	14	0.000	0.100E-09	0.23886E-04	0.17066E-02	0.26914E-07	0.44857E+00
1	1	0.000	0.100E-04	0.10000E+01	0.46974E+00	0.18902E-06	0.26923E+01
1	2	0.000	0.100E-04	0.10000E+01	0.38826E+00	0.81015E-07	0.11539E+01

etc...

Example from old
version without SOA

Example use of output from look-up tables for SO4(a) mode using MATLAB

Aerosol Specific Extinction, MEC (m^2/g) Aerosol Specific Extinction, MEC (m^2/g)



Mass specific extinction coefficient:

$$\text{MEC} = \beta_{\text{ext}} / C_{\text{tot}} \text{ (without water)}$$

Examples from old version without SOA

MEC's dependence on 2 of 5 input parameters (pluss λ):
total internally mixed mass, and RH

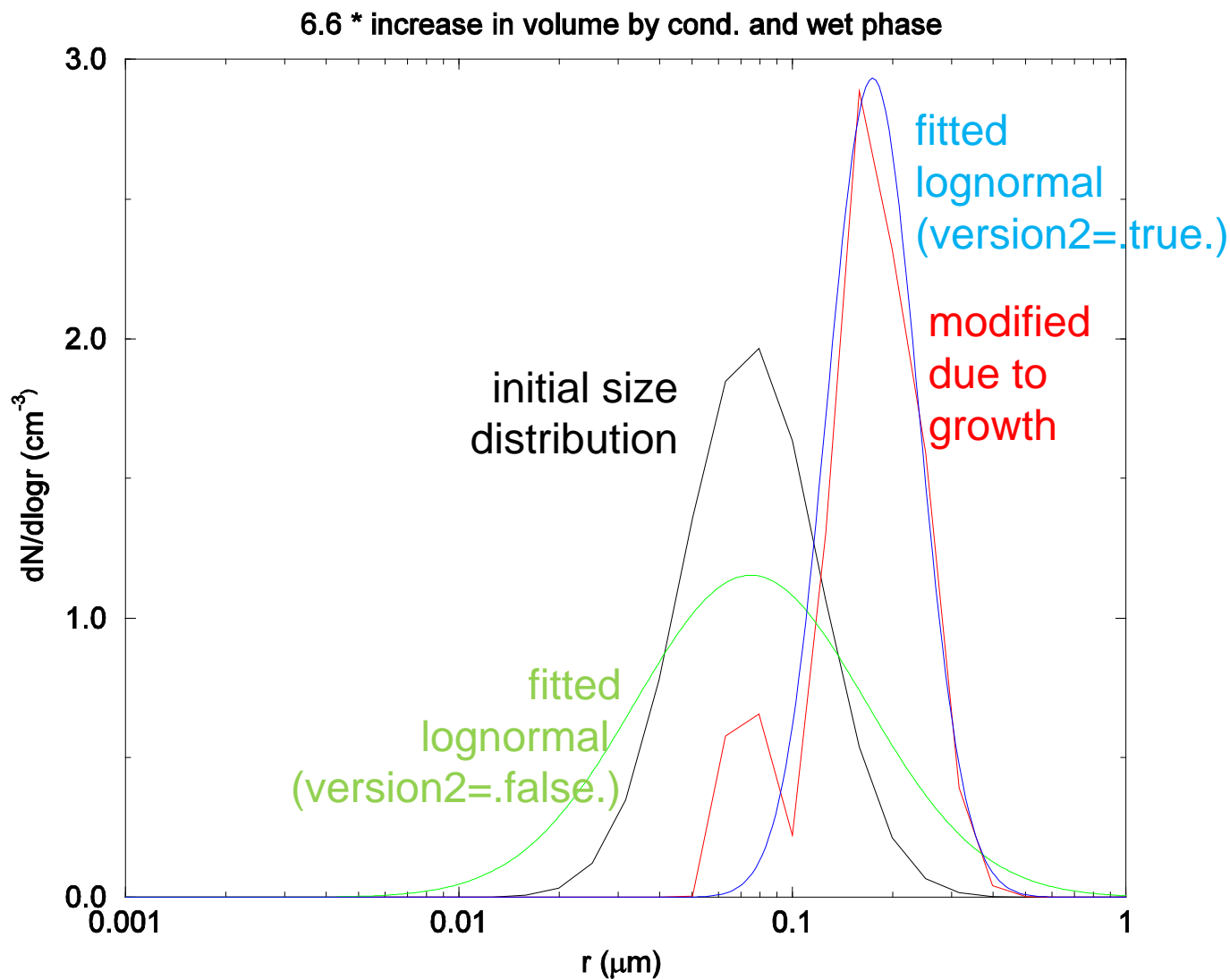
Ex. look-up tables for log-normal size parameters (dry aerosol):
 SO4(a) mode, logntilp5.out

catot ($\mu\text{g}/\text{m}^3$)	fac	fbc	faq	R (m)	$\log_{10}(\sigma)$	kcomp
0.10000E-09	0.00000E+00	0.00000E+00	0.00000E+00	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.00000E+00	0.25000E+00	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.00000E+00	0.50000E+00	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.00000E+00	0.75000E+00	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.00000E+00	0.85000E+00	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.00000E+00	0.10000E+01	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.10000E-01	0.00000E+00	0.75000E-01	0.20140E+00	5
0.10000E-09	0.00000E+00	0.10000E-01	0.25000E+00	0.75000E-01	0.20140E+00	5
etc...						
...						
0.15000E+00	0.99900E+00	0.70000E+00	0.50000E+00	0.23800E+00	0.11835E+00	5
0.15000E+00	0.99900E+00	0.70000E+00	0.75000E+00	0.23800E+00	0.11835E+00	5
0.15000E+00	0.99900E+00	0.70000E+00	0.85000E+00	0.23800E+00	0.11831E+00	5
0.15000E+00	0.99900E+00	0.70000E+00	0.10000E+01	0.23900E+00	0.11621E+00	5
0.15000E+00	0.99900E+00	0.99900E+00	0.00000E+00	0.23100E+00	0.11803E+00	5
0.15000E+00	0.99900E+00	0.99900E+00	0.25000E+00	0.23100E+00	0.11803E+00	5
0.15000E+00	0.99900E+00	0.99900E+00	0.50000E+00	0.23100E+00	0.11803E+00	5
0.15000E+00	0.99900E+00	0.99900E+00	0.75000E+00	0.23100E+00	0.11803E+00	5
0.15000E+00	0.99900E+00	0.99900E+00	0.85000E+00	0.23100E+00	0.11803E+00	5
0.15000E+00	0.99900E+00	0.99900E+00	0.10000E+01	0.23100E+00	0.11800E+00	5

Example from old
version without SOA

Example of lognormal fitting (LUT for r and σ) for use in the activation code

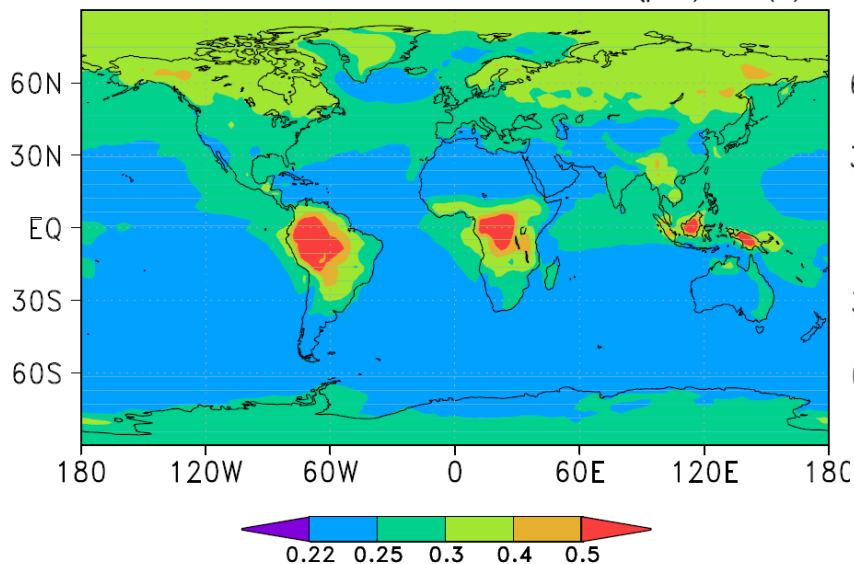
SO₄(a)



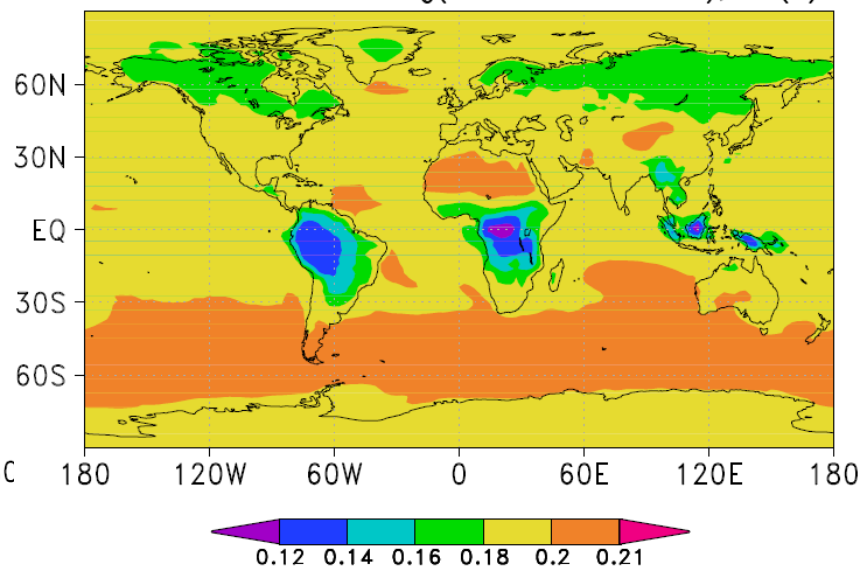


Example output from a 1 year PD simulation, CAM4-Oslo

Near surface modal median radius (μm), DU(a)



Near surface modal log(standard deviation), DU(a)



Example
from
old
version
without
SOA

Before growth: $r=0.22$

$\log(\sigma)=0.2014$

(Growth in this case also includes hygroscopic swelling)

Extra output (LUT), e.g. for use in AeroCom / RFMIP / AerChemMIP

used by CAM6-Nor only when set up with «#define AEROCOM»

aerodryk*.out	Parameters for calculation of effective radii in CAM-Nor, and dry mass concentrations for $r < 0.5 \mu\text{m}$ and $r > 1.25 \mu\text{m}$
aerocomk*.out	Total and component specific optical parameters at wavelengths 440, 500, 550, 670 and 870 nm (not used for radiative transfer). And, only at 550 nm: backscattering coefficient optical parameters for size ranges $r < 0.5 \mu\text{m}$ and $r > 0.5 \mu\text{m}$.

and, not used in CAM6-Nor, but useful for control purposes:

nkcomp*.out	Modified aerosol number size distributions (sectional, 44 bins).
-------------	--

where $*$ = 0, 1, 2,...,10

In a new test version (under construction):

Added mass from

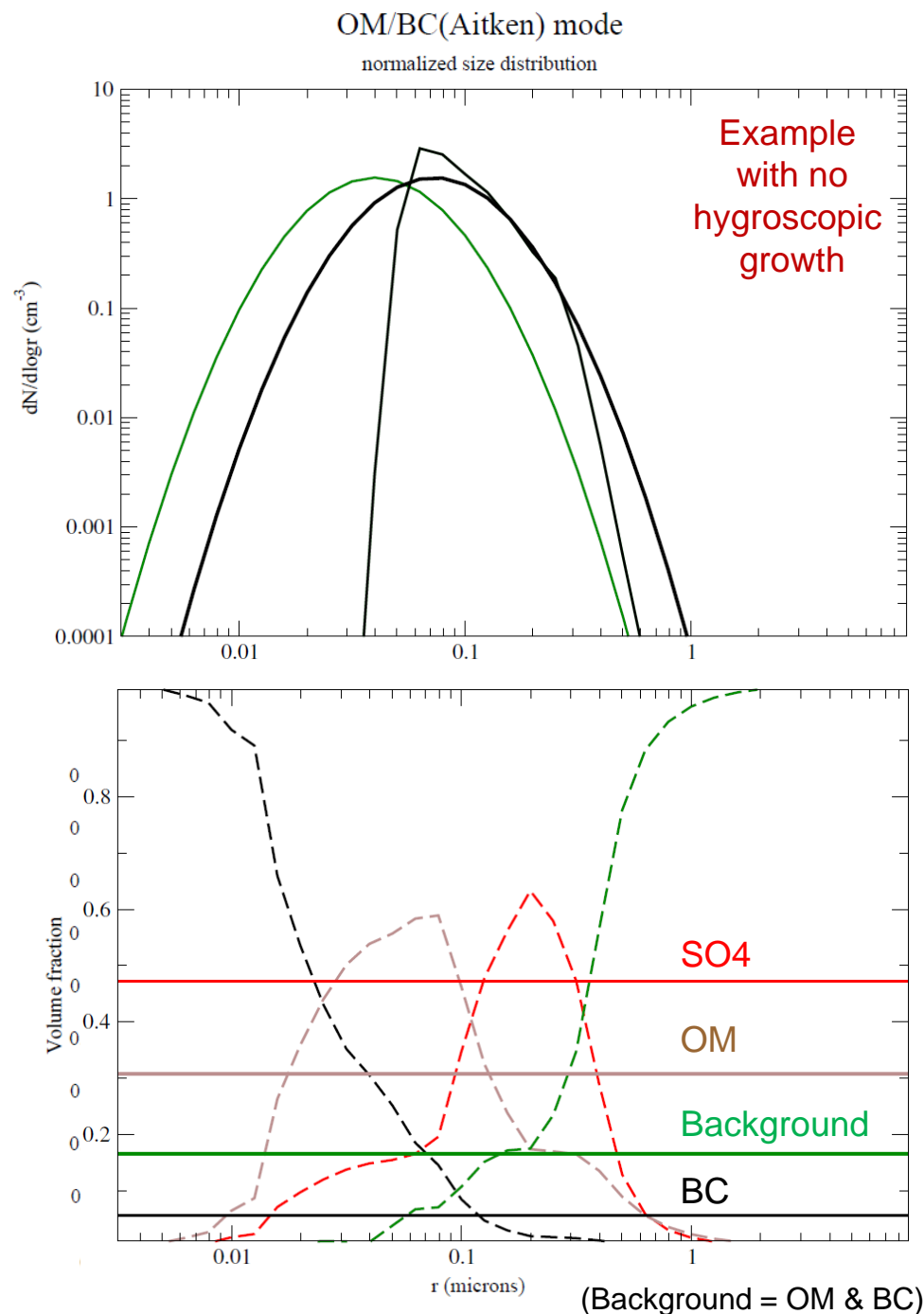
- condensation of H_2SO_4 or SOA
- coagulation of Aitken particles onto larger pre-existing particles
- cloud-processing/wet phase chemistry
- hygroscopic growth

$$\ln\left(\frac{e_r}{e_{s,w}}\right) = \frac{2M_w\sigma_{s/r}}{RT\rho_w r} - \frac{M_w}{\rho_w} \frac{1}{\left[\left(\frac{r}{r_0}\right)^3 - 1\right]} \sum_{\kappa} \nu_{\kappa} \Phi_{\kappa} \frac{\rho_{\kappa} \nu_{\kappa,k}(r_0)}{M_{\kappa}}$$

will here be mixed homogeneously,
preserving log-normal number size
distributions (similar to MAM)

→ check effects of complexity on
optics, size and CCN activation !

If results are acceptable, this can
form the basis of a light version of
AeroTab.



Extra slides

Hygroscopic growth calculations, in koehler.f :

(... inside some do loops)

```
c      mixsub calculates hygroscopic properties (given by x)
c      for an internally mixed aerosol
      call mixsub (frr0, itot, faq, Mw, rhow,
$           j, vsk, vbck, vock, x, rh, kcomp)
      rhumg=rhum
c      the Koehler equation
      rhum=e**(2e3*Mw*sigm/(Rg*T*rhow*rk(i))
$           -x/((rk(i)/rk(j))**3-1.0))
```

$x=x(r)$

$$\ln\left(\frac{e_r}{e_{s,w}}\right) = \frac{2M_w\sigma_s/r}{RT\rho_w r} - \frac{\frac{M_w}{\rho_w}}{\left[\left(\frac{r}{r_0}\right)^3 - 1\right]} \sum_{\kappa} v_{\kappa} \Phi_{\kappa} \frac{\rho_{\kappa} v_{\kappa,k}(r_0)}{M_{\kappa}}$$

and calculating x in mixsub.f,
e.g. for (NH₄)₂SO₄:

```
c ammonium sulphate:
Ms=1.3214e2
rhosl=1.769e3
if(frr0.le.1.02) then
  ai=-23.7649*frr0+24.4955
elseif(frr0.gt.1.02.and.frr0.le.1.05) then
  ai=10.6373*frr0-10.5947
elseif(frr0.gt.1.05.and.frr0.le.1.11) then
  ai=9.3474*frr0-9.2404
elseif(frr0.gt.1.11.and.frr0.le.1.22) then
  ai=6.2080*frr0-5.7556
elseif(frr0.gt.1.22.and.frr0.le.1.325) then
  ai=1.8385*frr0-0.4248
elseif(frr0.gt.1.325.and.frr0.le.1.424) then
  ai=-2.0065*frr0+4.6699
elseif(frr0.gt.1.424.and.frr0.le.1.65) then
  ai=-0.8021*frr0+2.9548
elseif(frr0.gt.1.65.and.frr0.le.1.974) then
  ai=-0.1192*frr0+1.8279
elseif(frr0.gt.1.974.and.frr0.le.2.593) then
  ai=0.1629*frr0+1.2712
elseif(frr0.gt.2.593.and.frr0.le.3.185) then
  ai=0.1734*frr0+1.2437
else
  ai=1.8
endif
xa=ai*(Mw/Ms)*(rhosl/rhow)
```

from offline parameterization:
x is a function of frr0 (=r/r₀)

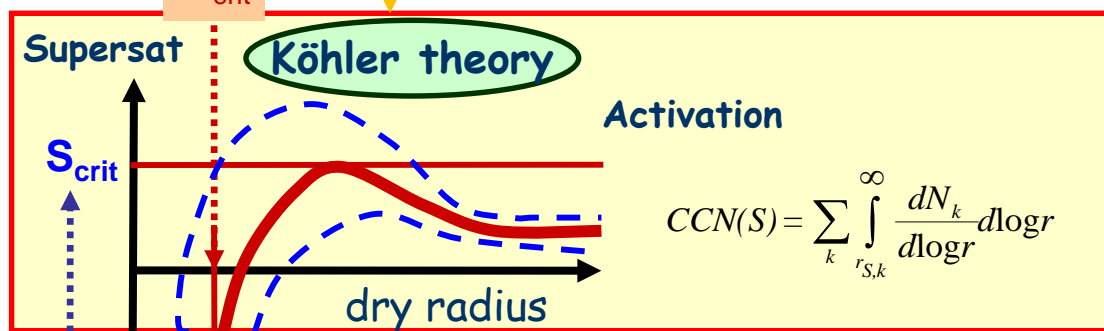
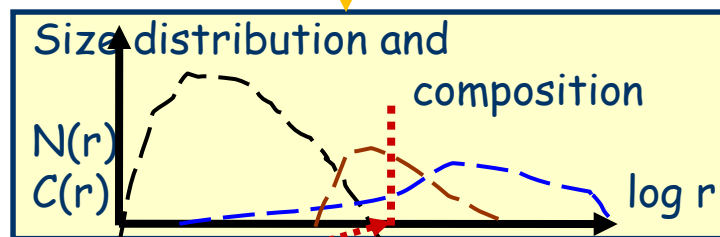
Simplify: **x = const.**

e.g. internally mixed in mode 4, OC&BC(a):

```
elseif(kcomp.eq.4) then                                ! BC or OC + H2SO4 + (NH4)2SO4
  if(itot.eq.0) then
    x=xbg
  else          ! internal mixture
    if(rh.lt.0.37) then
      x=(1.0-vsk(i)-vbck(i))*xbg+vsk(i)*(1.0-faq)*xs
    else
      x=(1.0-vsk(i)-vbck(i))*xbg+vsk(i)*(faq*xa+(1.0-faq)*xs)
    endif
  endif
end1301.2020
```

From life cycle calculations:
DU, SS and process specific SO_4 , BC, OC
+ assumed supersaturation S

Cond., coag. + cloud processing
(solve continuity eq.)



Prescribed S :

0.10% Stratiform clouds
0.15% Conv. clouds over land
0.80% Conv. clouds over ocean

Principle: Scheme
for diagnostic
cloud droplet number
concentrations (CDNC)

Seland et al. (2008)
Kirkevåg et al. (2008)

Look-up
tables

This CAM(3)-Oslo
diagnostic option
is not fully implemented
in CAM4-Oslo !

CDNC = CCN(S)

effective droplet radii,
liquid water content

Radiative
forcing, W/m^2