Aerosol in WRF-Chem

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Based on Jan Kazil's slides

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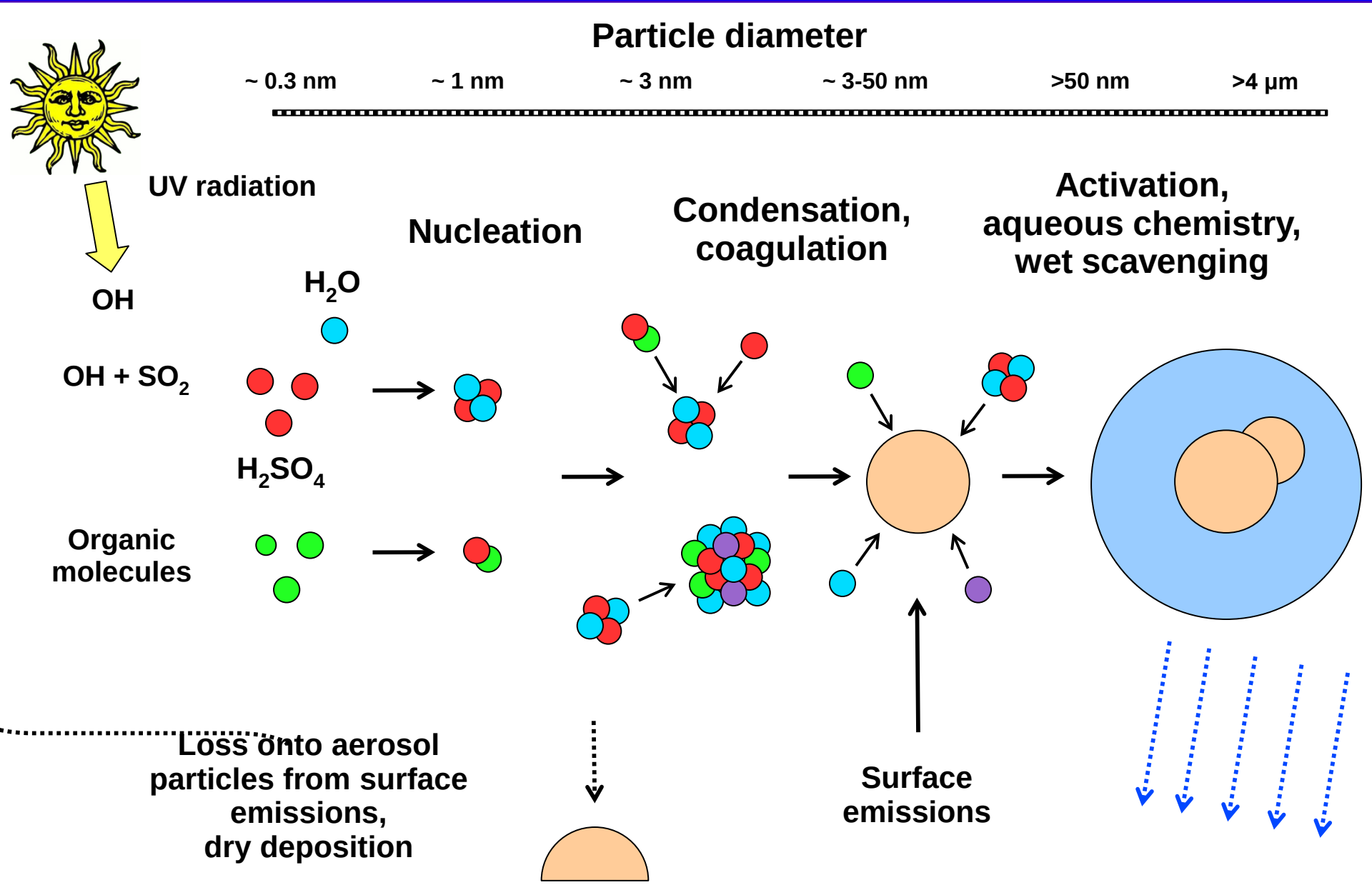
Outline

- Aerosol in the atmosphere
- Know your problem
- Representation of the aerosol size distribution
- Aerosol schemes in WRF/Chem:
  - What they do (and what not)
- Coupling to gas phase chemistry
- WRF/Chem registry
- WRF/Chem namelists
- Initialization

Examples

Aerosol processes



Know your problem

You want to run WRF/Chem with aerosol ...

What does it take?

- Know your problem
- Get to know WRF/Chem:
  - WRF/Chem has different aerosol schemes
  - Which one to use?

Know your problem

Two examples:

1.You investigate tropospheric ozone:

- You will need a detailed gas phase chemistry
- You may not need
  - a detailed aerosol scheme
  - aerosol indirect effects
  - aqueous chemistry
- GOCART aerosols, MOZART gas phase chemistry

2.You investigate SOA and PM2.5:

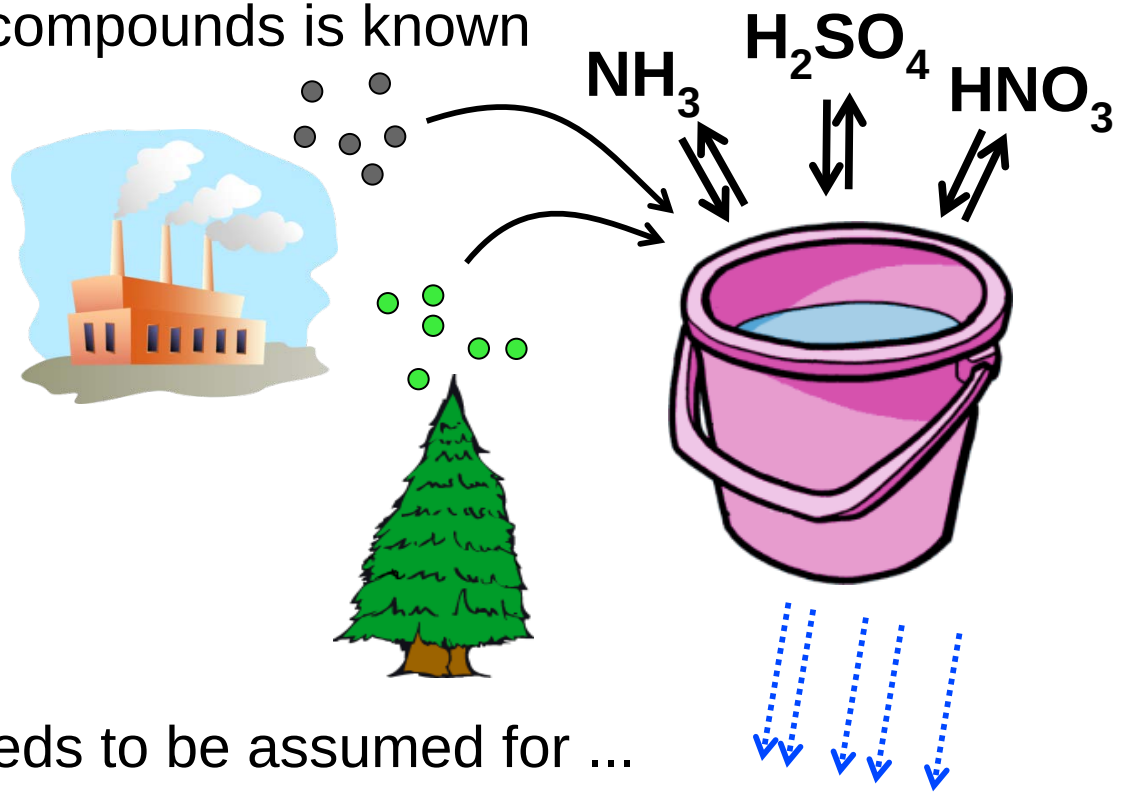
- You will need a detailed gas phase chemistry with VOCs
- You will need an aerosol scheme with SOA mass formation
- MADE/SORGAM aerosols, RADM2/RACM gas phase chemistry

Aerosol schemes in WRF/Chem

- The WRF/Chem aerosol schemes differ in their approach to describe the aerosol:
  - Size distribution
  - Composition
  - Interaction with ...
    - gas and aqueous phase chemistry
    - clouds
    - radiation
  - Number and complexity of processes
  - Execution speed
- The user needs to identify the aerosol scheme that:
  - provides features needed for the given research task
  - Is numerically affordable
- You may be have to implement missing features yourself

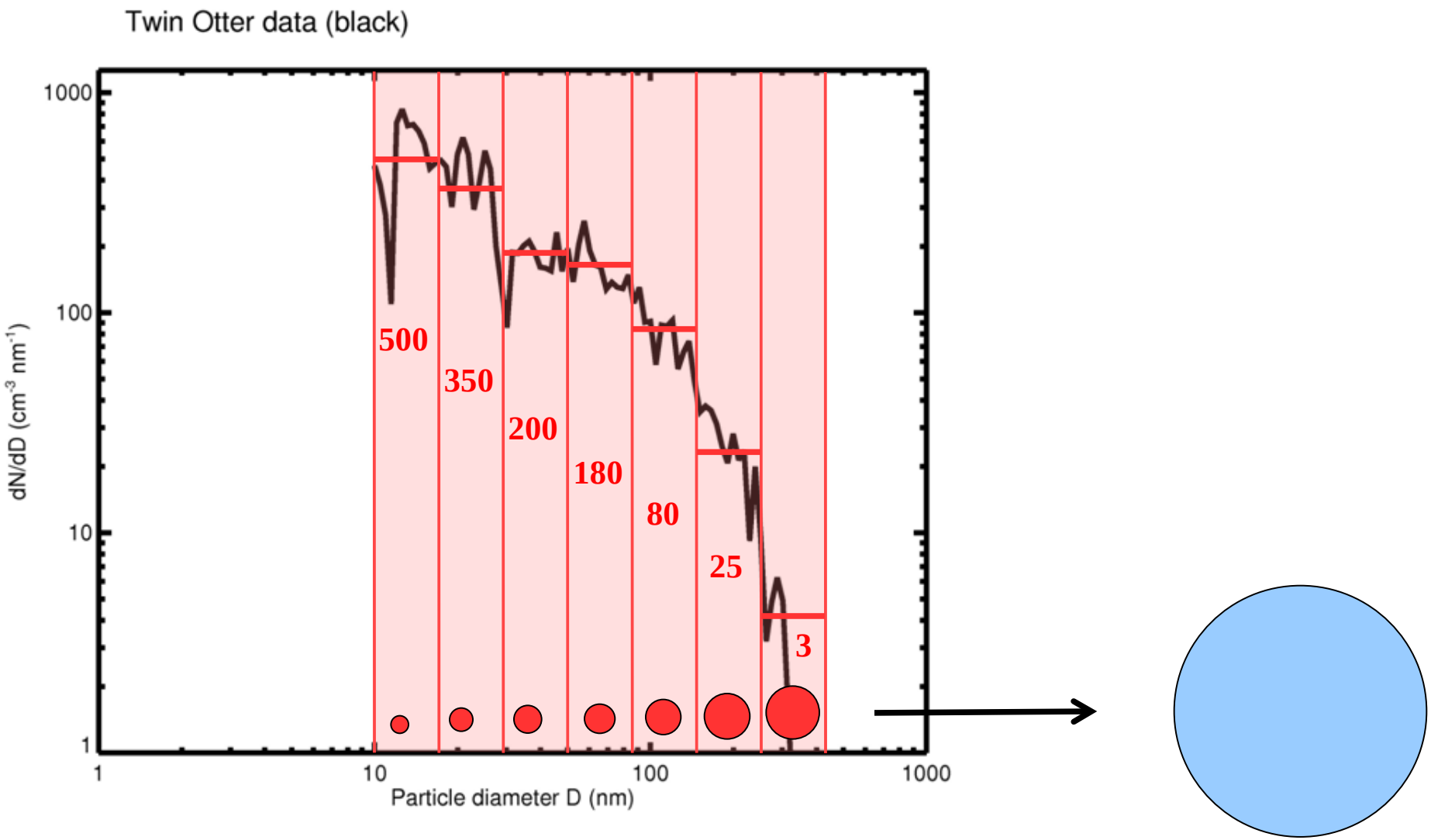
Bulk aerosol scheme

- Only total mass of aerosol compounds is known

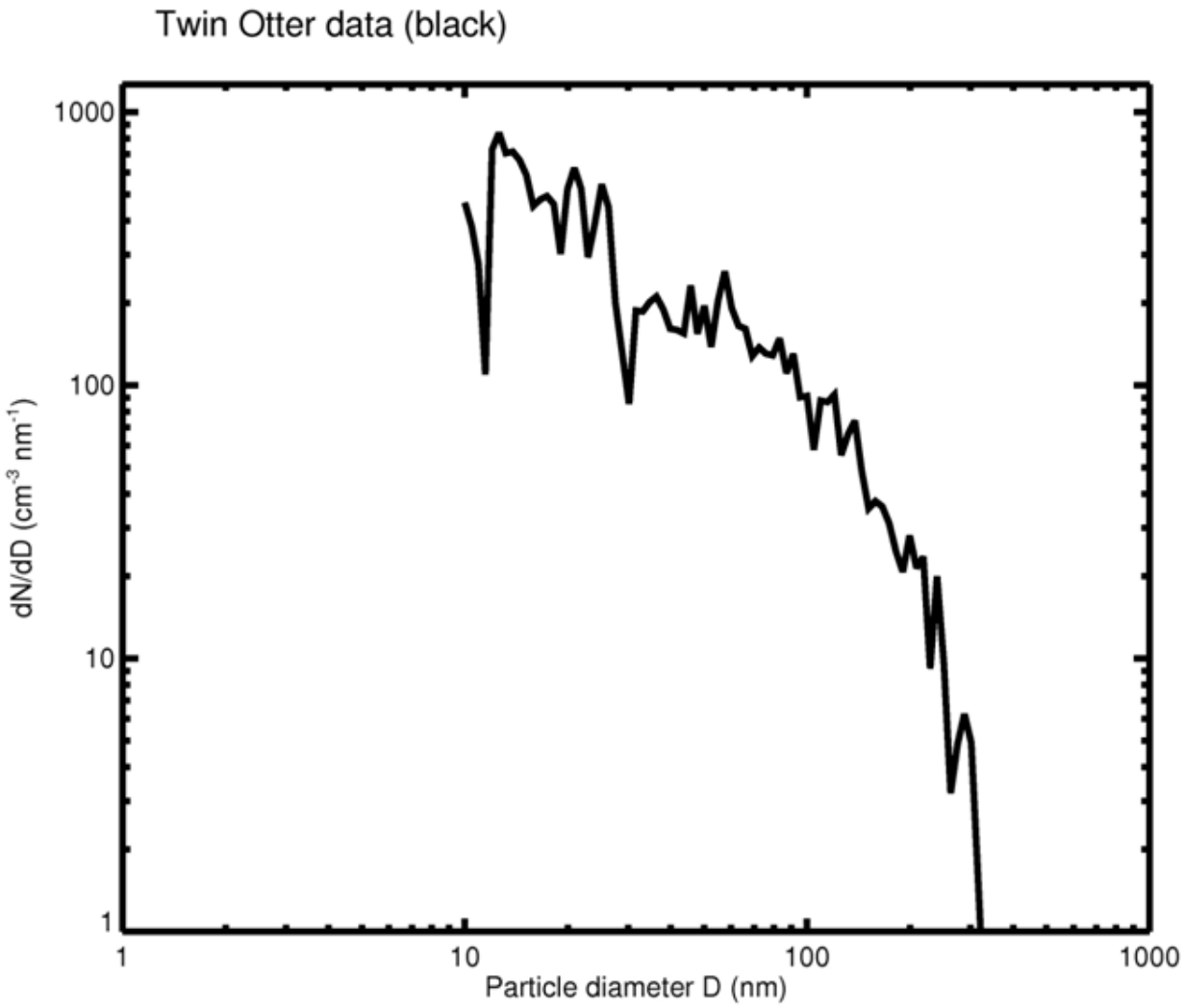


- No information on
  - Particle number
  - Aerosol size distribution
- Aerosol size distribution needs to be assumed for ...
  - radiative transfer
  - response of cloud properties to aerosol number
- Can't do aerosol nucleation
- **Numerically efficient**
- **Useful when focus is on complex gas phase / aerosol chemistry**

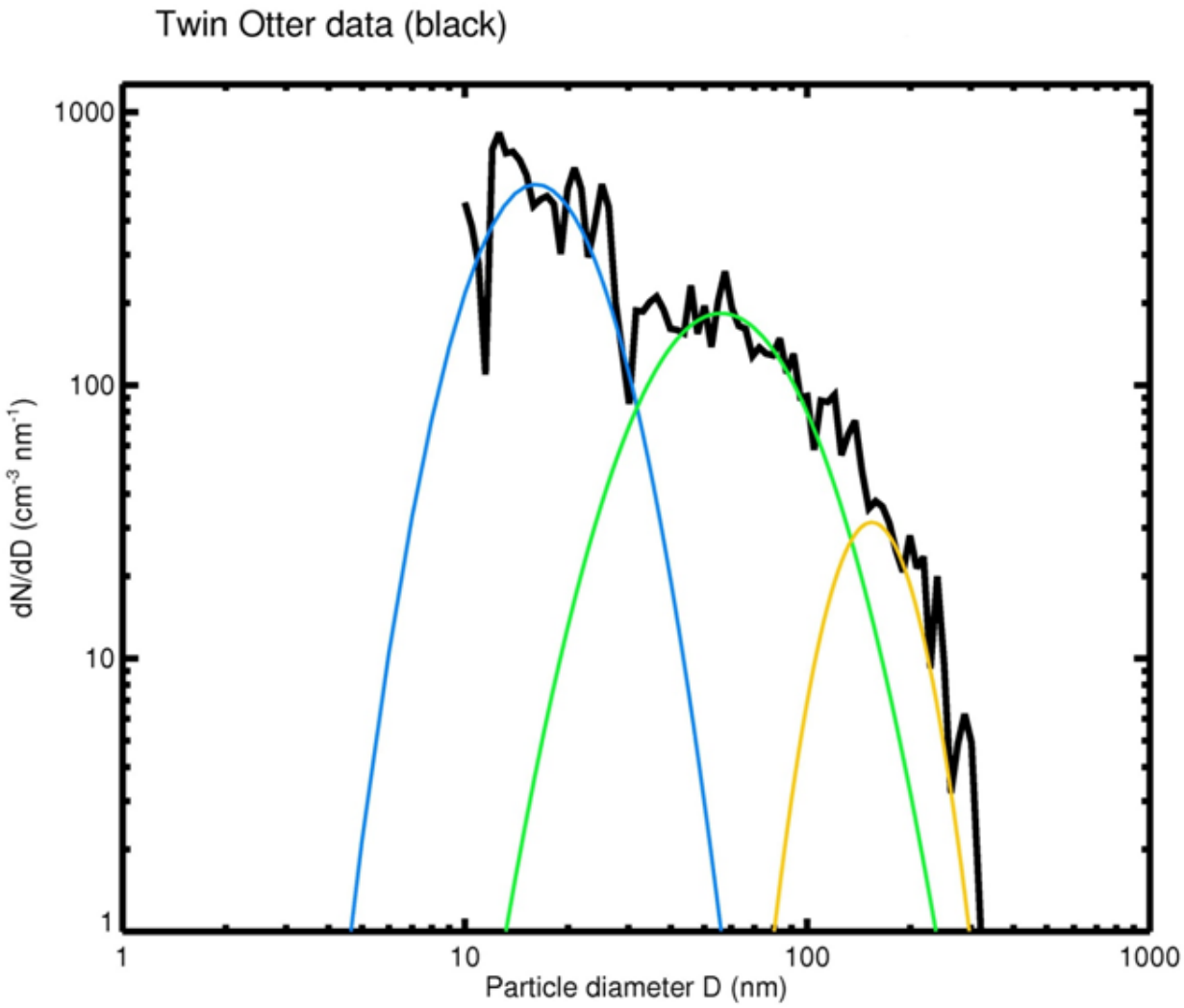
Sectional (bin) aerosol scheme



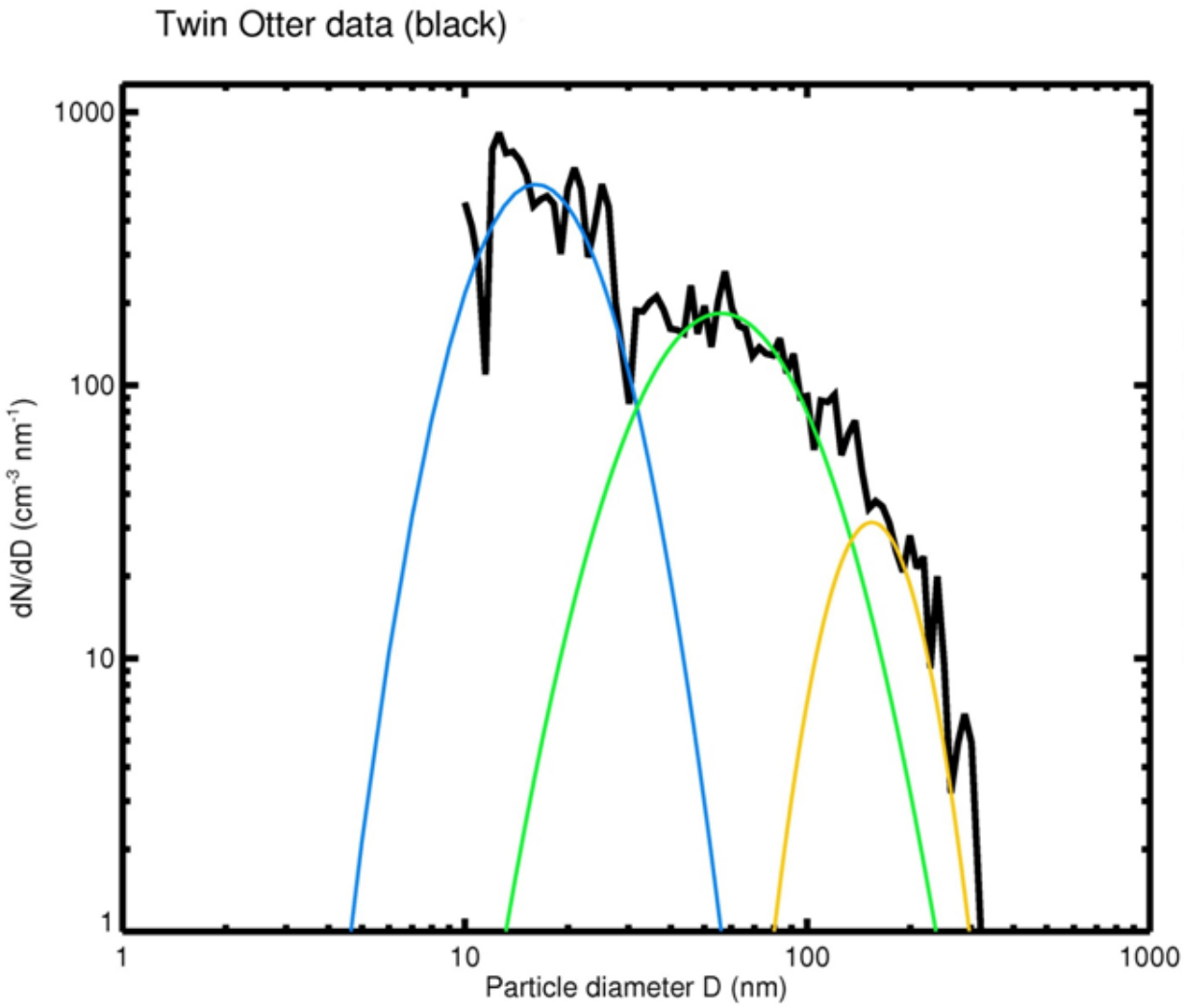
Modal aerosol scheme



Modal aerosol scheme



Modal aerosol scheme



$dN/dD = c \cdot \exp\{-0.5 \cdot [\ln(D/\mu)/\ln(\sigma)]^2\}/[(2\pi)^{0.5}\ln(\sigma)D]$:

$c = 8194.98\ cm^{-3}$

$\mu = 18.22$ nm

$\sigma = 1.42$

$dN/dD = c \cdot \exp\{-0.5 \cdot [\ln(D/\mu)/\ln(\sigma)]^2\}/[(2\pi)^{0.5}\ln(\sigma)D]$:

$c = 12732.53\ cm^{-3}$

$\mu = 68.44$ nm

$\sigma = 1.57$

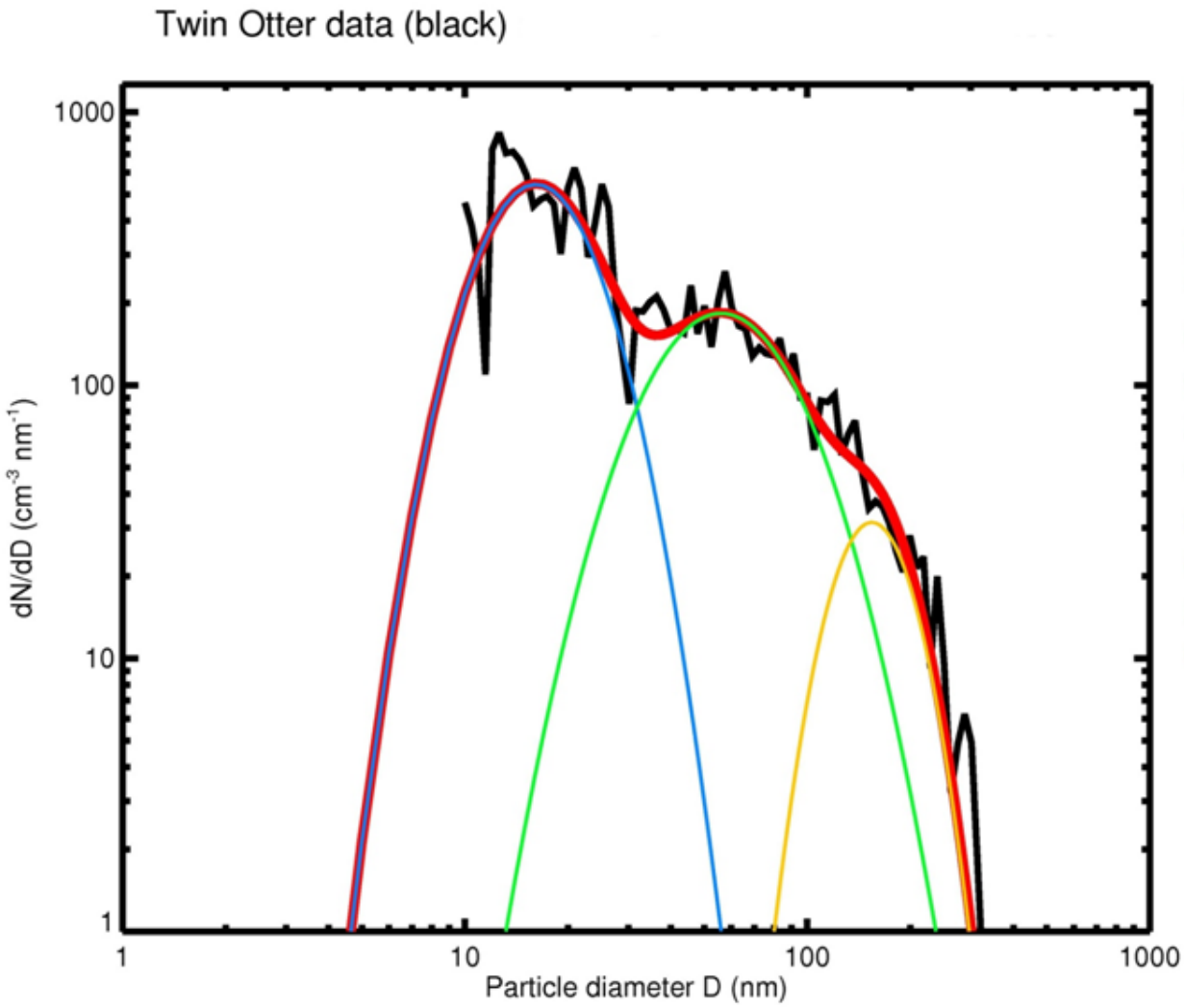
$dN/dD = c \cdot \exp\{-0.5 \cdot [\ln(D/\mu)/\ln(\sigma)]^2\}/[(2\pi)^{0.5}\ln(\sigma)D]$:

$c = 3139.90\ cm^{-3}$

$\mu = 164.41$ nm

$\sigma = 1.28$

Modal aerosol scheme



dN/dD = dN/dD + dN/dD + dN/dD

dN/dD = c·exp{-0.5·[ln(D/μ)/ln(σ)]²}/[(2π)^0.5 ln(σ)D] :

c = 8194.98 cm^{-3}

μ = 18.22 nm

σ = 1.42

dN/dD = c·exp{-0.5·[ln(D/μ)/ln(σ)]²}/[(2π)^0.5 ln(σ)D] :

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c = 3139.90 cm^{-3}

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σ = 1.28

Aerosol schemes in WRF/Chem

- **GOCART** aerosol scheme
  - Simple and efficient bulk/sectional scheme
  - **Chin, M.**, et al., Atmospheric sulfur cycle simulated in the global model GOCART: Model description and global properties, JGR, 105, 24671-24687, 2000
- **MADE/SORGAM**
  - Modal aerosol scheme with SOA
  - **Ackermann, I. J.**, et al., Modal Aerosol Dynamics Model for Europe: Development and first applications, Atmos. Env., 32, 17, 2981-2999, 1998
  - **Schell B.**, et al., Modeling the formation of secondary organic aerosol within a comprehensive air quality model system, JGR, 106, D22, 28275-28293, 2001
- **MOSAIC**
  - Sectional scheme, the most actively developed scheme in WRF/Chem
  - **Zaveri, R. A.**, et al., Model for simulating aerosol interactions and chemistry (MOSAIC), JGR, 113, D13204, doi:10.1029/2007JD008782, 2008

GOCART

- **GOCART** aerosol scheme:
  - Aerosol module from the ***Go***ddard ***C***hemistry ***A***erosol ***R***adiation and ***T***ransport model
  - Sulfate, ammonium, organic carbon, black carbon
    - Internally mixed
    - Bulk scheme: Only aerosol mass known, but not particle number/size distribution
  - No aerosol nitrate (NO_3^-)
  - Dust, sea salt:
    - Sectional (bin) scheme
  - No aerosol nucleation (bulk scheme!)

MADE/SORGAM

- **MADE**: ***M***odal ***A***erosol ***D***ynamics Model for ***E***urope
  - Modal aerosol scheme:
    - Aitken/nucleation, accumulation, coarse mode
  - Sulfate, nitrate, ammonium, sea salt, dust
  - Aerosol internally mixed (in each mode)
  - Calculates aerosol microphysical properties and processes:
    - mode diameters, mass, moments ...
    - Gas/particle partitioning of
      - HNO_3, NH_3, H_2O
    - Condensation of H_2SO_4 onto aerosol
    - Coagulation rates
    - Mode transfer rates
    - H_2SO_4/H_2O nucleation (Kulmala et al., JGR 1998)

MADE/SORGAM

- **SORGAM: *S*econdary *Org*anic *A*erosol *M*odel**
  - Calculates the gas/particle partitioning of semi-volatile organic vapors
  - Treats oxidation products of VOCs:
    - Higher alkenes/alkanes (anthropogenic)
    - Toluene, xylene, cresols (anthropogenic)
    - α-pinene and limonene (biogenic)
  - (with the appropriate gas phase chemical scheme)

Predicts very little SOA!

MOSAIC

- **MOSAIC** aerosol scheme:
  - ***Mo***del for ***S***imulating ***A***erosol ***I***nteractions and ***C***hemistry
  - Sectional scheme: 4 or 8 size bins
  - Sulfate, nitrate, ammonium, organic carbon, black carbon, sodium, chlorine, dust
  - Gas-phase species that partition to the particle-phase:
    - H_2SO_4, HNO_3, HCl, NH_3, MSA, H_2O
  - Aerosol compounds internally mixed (in each bin)
  - H_2SO_4/H_2O nucleation (Wexler et al., Atm. Env. 1994)
  - ($H_2SO_4/NH_3/H_2O$ nucleation Napari et al., JGR 2002))
  - SOA – VBS approach (Shrivastava et al., ACP 2011)

chem_opt settings

File namelist.input (parameters for the WRF/Chem run)

Namelist "chem"

```
&chem
 chem_opt            = 112
 photdt              = 0.5
 chemdt              = 0.05
 emiss_opt           = 3
 seas_opt            = 2
 dust_opt            = 2
 aer_drydep_opt      = 1
 wetscav_onoff       = 1
 gaschem_onoff       = 1
 aerchem_onoff       = 1
 cldchem_onoff       = 1
 vertmix_onoff       = 1
    .
    .
    .
 /
```

How to find the aerosol quantities in the model ?

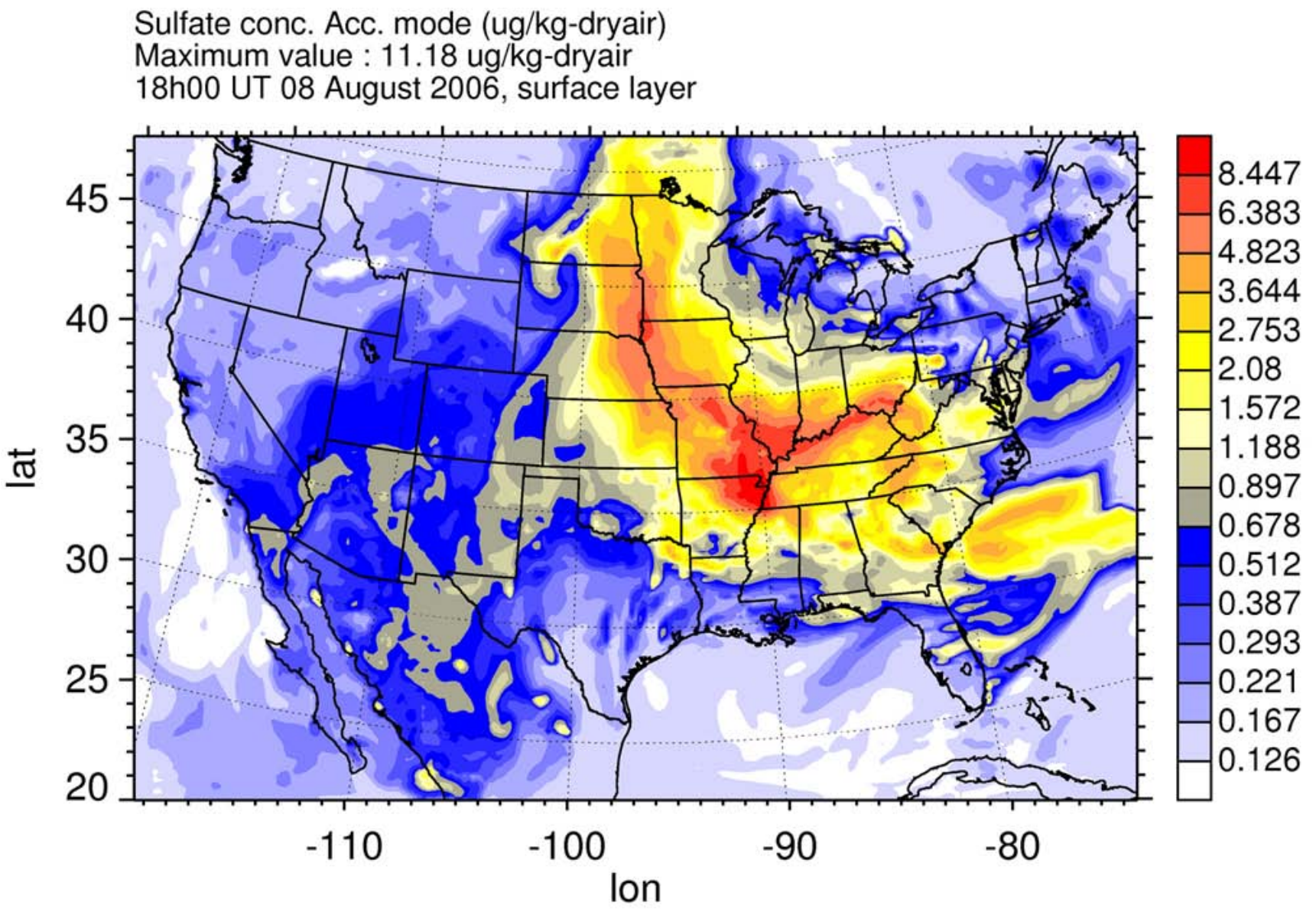
- File ../WRFV3/Registry/registry.chem
- Declares the internal structure of the WRF/Chem model
- Towards the end, entries such as:

package **radm2sorg_aq chem_opt==11** – **chem**:so2,sulf,no2,no,o3,hno3,h2o2, ...
... ald,hcho,op1,op2,paa,ora1,ora2,nh3,n2o5,no3,pan,hc3,hc5,hc8,eth,co, ...
... ol2,olt,oli,tol,xyl,aco3,tpan,hono,hno4,ket,gly,mgly,dcb,onit,csl, ...
... iso,hcl,ho,ho2,...
... so4ak,**so4aj**,so4ai,nh4ak,nh4aj,nh4ai,no3ak,no3aj,no3ai, ...
... orgaro1j,orgaro1i,orgaro2j,orgaro2i,orgalk1j,orgalk1i,orgole1j, ...
... orgole1i,orgba1j,orgba1i,orgba2j,orgba2i,orgba3j,orgba3i,orgba4j, ...
... orgba4i,orgpaj,orgpai,ecj,eci,p25j,p25i,antha,seas,soila,**nu0,ac0,corn**, ...
...

...
... so4cwk,**so4cwj**,so4cwi,nh4cwk,nh4cwj,nh4cwi,no3cwk,no3cwj,no3cwi, ...
... orgaro1cwj,orgaro1cwi,orgaro2cwj,orgaro2cwi,orgalk1cwj,orgalk1cwi, ...
... orgole1cwj,orgole1cwi,orgba1cwj,orgba1cwi,orgba2cwj,orgba2cwi, ...
... orgba3cwj,orgba3cwi,orgba4cwj,orgba4cwi,orgpacwj,orgpacwi,eccwj, ...
... eccwi,p25cwj,p25cwi,anthcw,seascw,soilcw,**nu0cw,ac0cw,corncw**

- This helps you find a given quantity in the code:
- chem(i,k,j,p_so4aj) = Accumulation mode sulfate

Example


Sulfate conc. Acc. mode (ug/kg-dryair)
Maximum value : 11.18 ug/kg-dryair
18h00 UT 08 August 2006, surface layer
lat
45
40
35
30
25
20
-110
-100
-90
-80
lon
8.447
6.383
4.823
3.644
2.753
2.08
1.572
1.188
0.897
0.678
0.512
0.387
0.293
0.221
0.167
0.126

A few words on emissions

```
&chem
 chem_opt            = 112
 photdt              = 0.5
 chemdt              = 0.05
 emiss_opt           = 3
 seas_opt            = 2
 dust_opt            = 2
 aer_drydep_opt      = 1
 wetscav_onoff       = 1
 gaschem_onoff       = 1
 aerchem_onoff       = 1
 cldchem_onoff       = 1
 vertmix_onoff       = 1
     .
     .
     .
 /
```

emiss_opt = 0 no anthropogenic emissions
= 2 use radm2 anthropogenic emissions
= 3 use radm2/MADE/SORGAM anthropogenic emissions
= 4 use CBMZ/MOSAIC anthropogenic emissions
= 5 GOCART RACM_KPP emissions
= 6 GOCART simple emissions
= 7 MOZART emissions
= 8 MOZCART (MOZART + GOCART aerosols) emissions
= 13 SAPRC99 emissions

This doesn't switch on/specify emissions !

Only declares an emissions array in the WRF/Chem code:

package eradmsorg **emiss_opt==3** - **emis_ant**:e_iso,e_so2,e_no,e_co,e_eth, ...
... e_hc3,e_hc5,e_hc8,e_xyl,e_ol2,e_olt,e_oli,e_tol,e_csl,e_hcho,e_ald, ...
... e_ket,e_ora2,e_nh3,e_pm25i,e_pm25j,e_pm_10,e_eci,e_ecj,e_orgi,e_orgj, ...
... e_so4i,e_so4j,e_no3i,e_no3j

SOA mechanisms in WRF-CHEM

Currently available: SORGAM and VBS approach couple to the MOSAIC scheme

Another SOA scheme based on VBS approach couples to RACM-KPP gas chemistry, MADE aerosol scheme, will be available in the next release

Check the SOA mechanisms, you may need to modify the parameters, different SOA formation mechanisms, the SOA precursors, emissions of VOCs/SVOCs/IVOCs for specific applications!