Introduction to aerosol modeling with WRF/Chem

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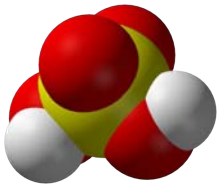
Outline

1. Aerosols in the atmosphere:
    - Sources
    - Processes
    - Interaction with radiation
    - Interaction with clouds
2. Representation of aerosols in atmospheric models:
    - Sectional (bin) scheme
    - Modal scheme
    - Bulk scheme
3. Aerosol modeling with WRF/Chem:
    - Available aerosol schemes
    - Settings in the file namelist.input (name lists)
    - Initial values
    - Quick look at some output

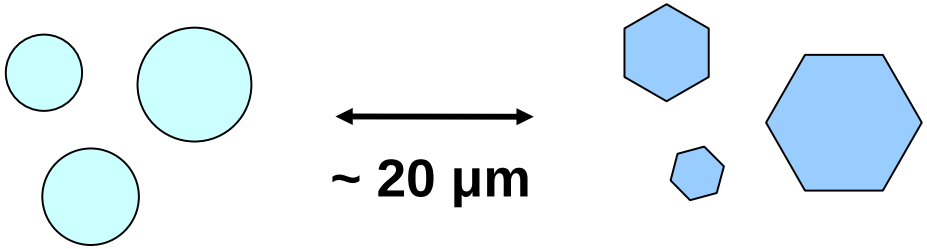
Aerosol particles - size considerations

~ 0.3 nm



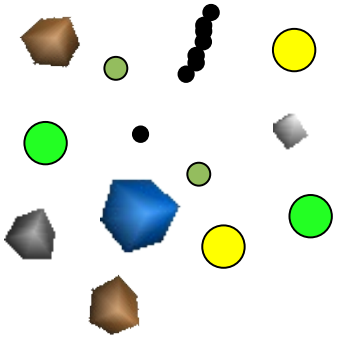
H_2SO_4

Cloud droplets and ice crystals

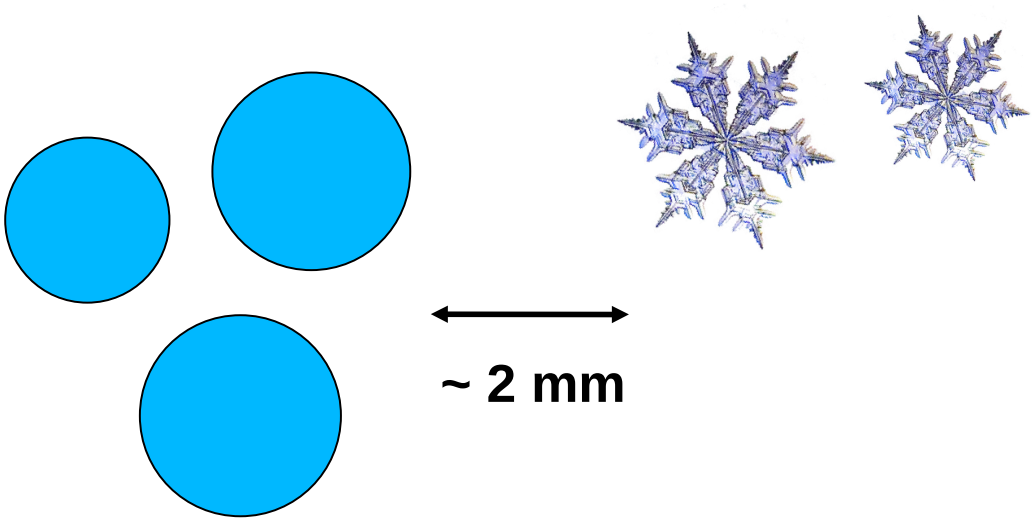


Aerosol particles

3 nm - 2 µm



Rain and snow

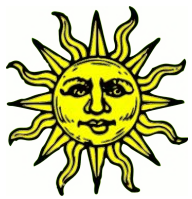


Atmospheric dynamics: 100 m – 1000 km

Typical WRF resolution: 300 m – 30 km

Aerosol sources

Aerosol processes



Particle diameter

~ 0.3 nm | ~ 1 nm | ~ 3 nm | ~ 3-50 nm | >50 nm | >4 µm

UV radiation

OH

$OH + SO_2 \rightarrow H_2SO_4$

Ions (Radon, galactic cosmic rays)

OH + BVOC → oxidation prodcts

H_2O

H_2SO_4

Nucleation

Growth by coagulation and vapor condensation

Aitken mode aerosol: Growth by vapor condensation

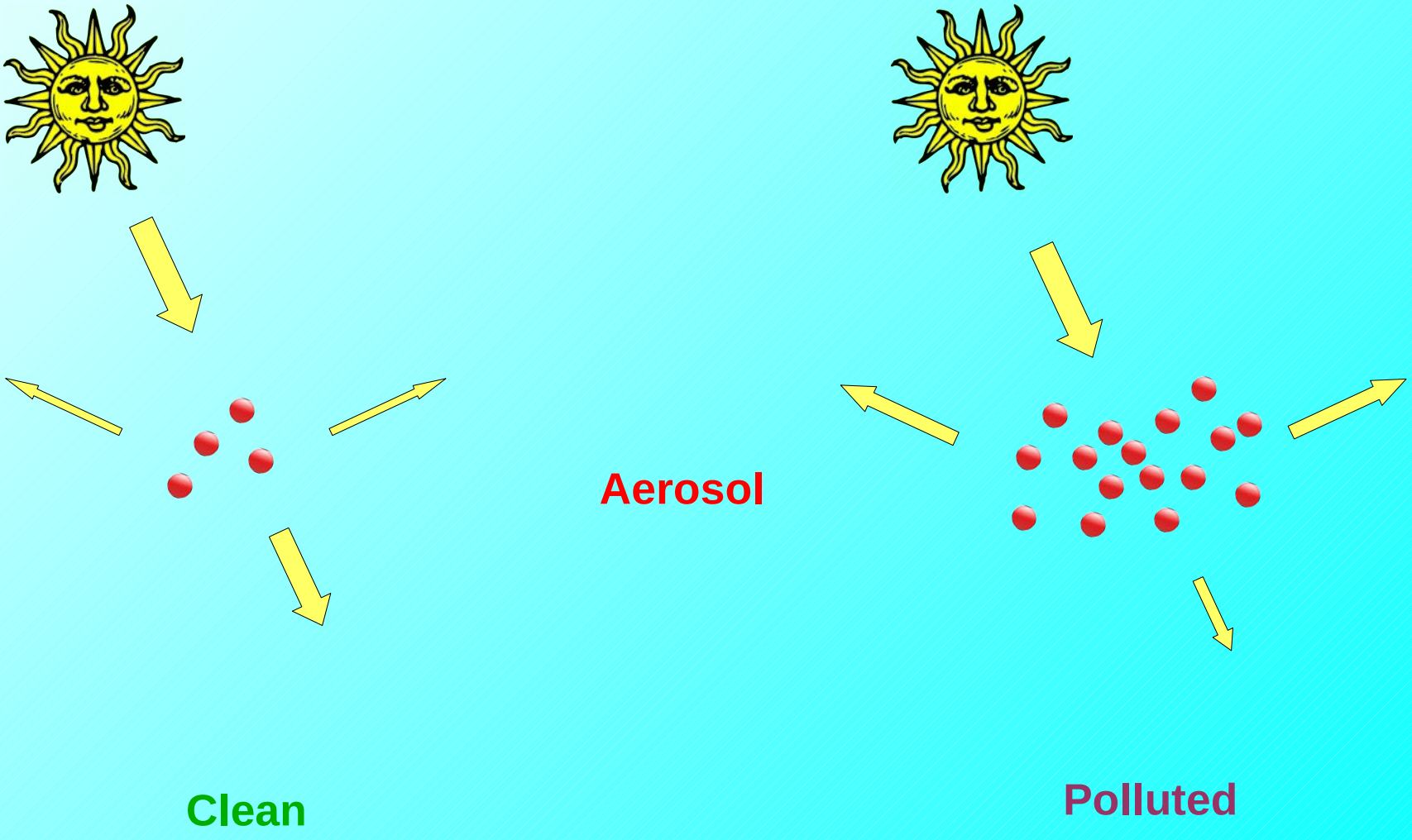
Accumulation mode aerosol: Growth by cloud processing

Cloud droplets

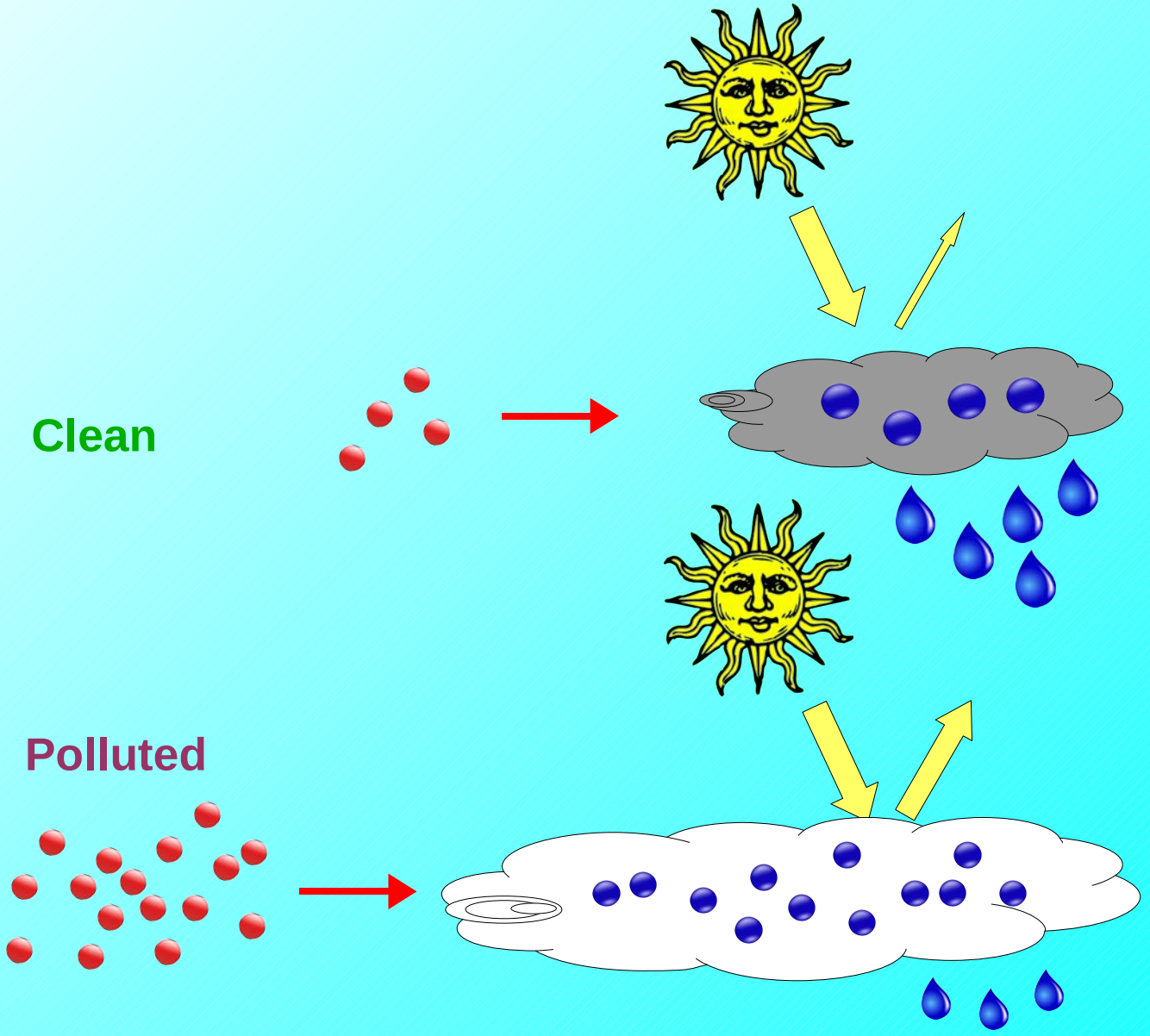
Surface emissions

Loss onto preexisting aerosol particles

Aerosols direct effect: Scattering/absorption



Aerosols indirect effects: Coupling to clouds



Aerosol indirect effect: Satellite view

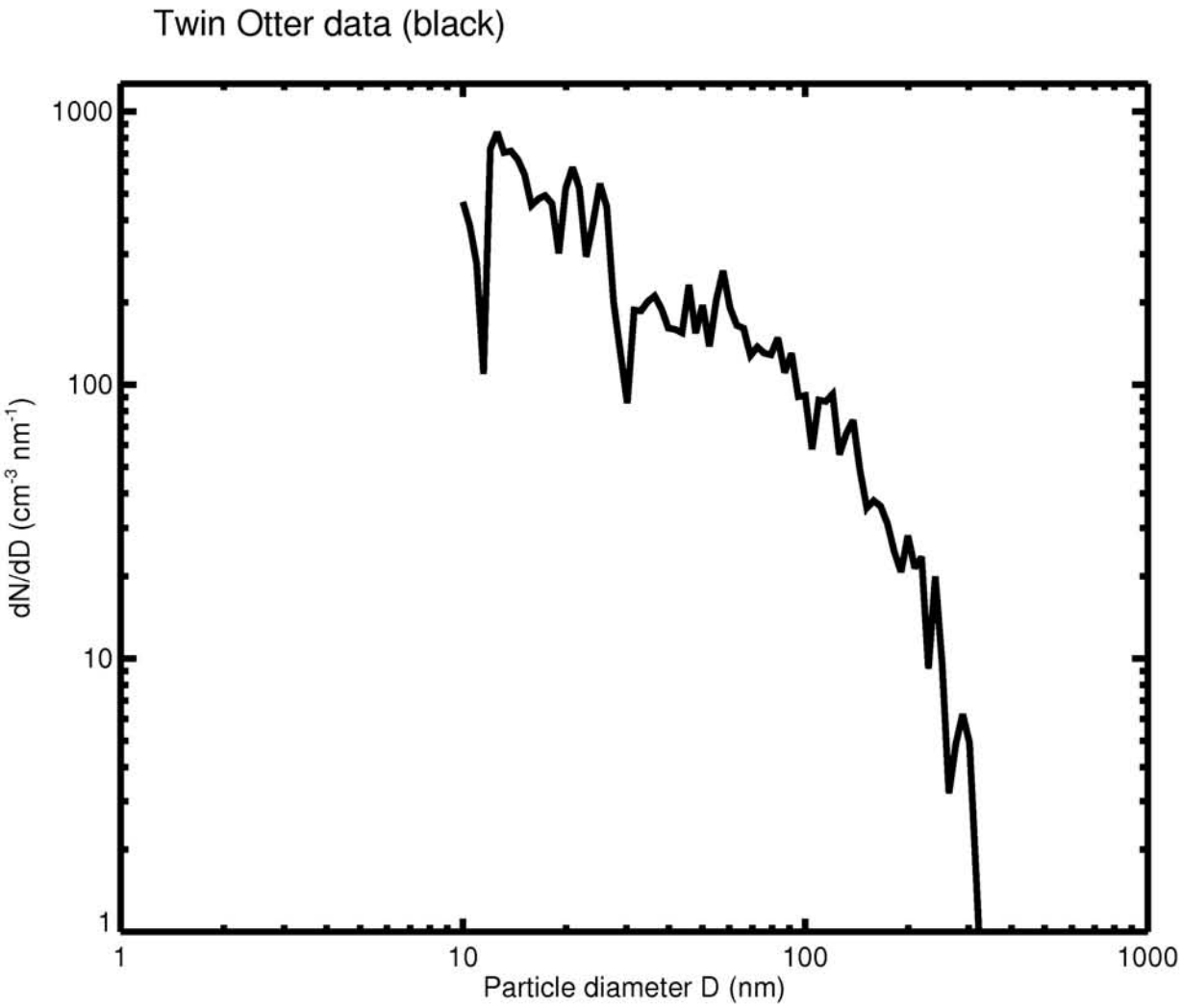
Satellite image courtesy of NASA

How do we represent aerosols in atmospheric modeling?

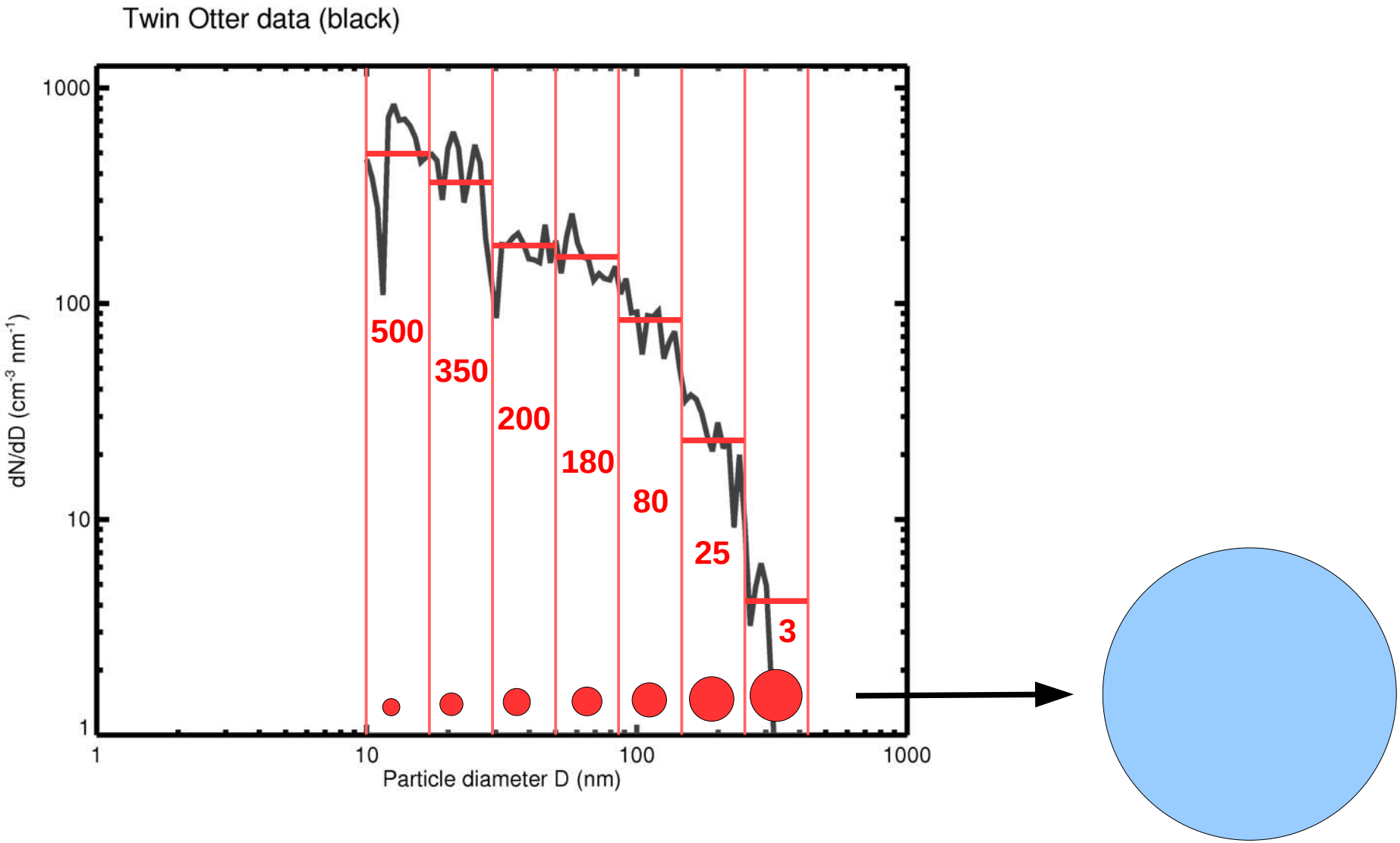
What we want:

- A mathematical method to calculate “how much aerosol there is” after a given time Δt, depending on:
  - How much aerosol there was at the start of the time step
  - Surface emissions
  - Formation from the gas phase (nucleation)
  - Condensation of gas phase molecules
  - Coagulation
  - Formation of cloud droplets and their evaporation
  - Loss due to wash-out by precipitation
  - Dry deposition
  - ...
- Most widely used approaches:
  - represent the size and composition of the aerosol particles
  - do the math with this information

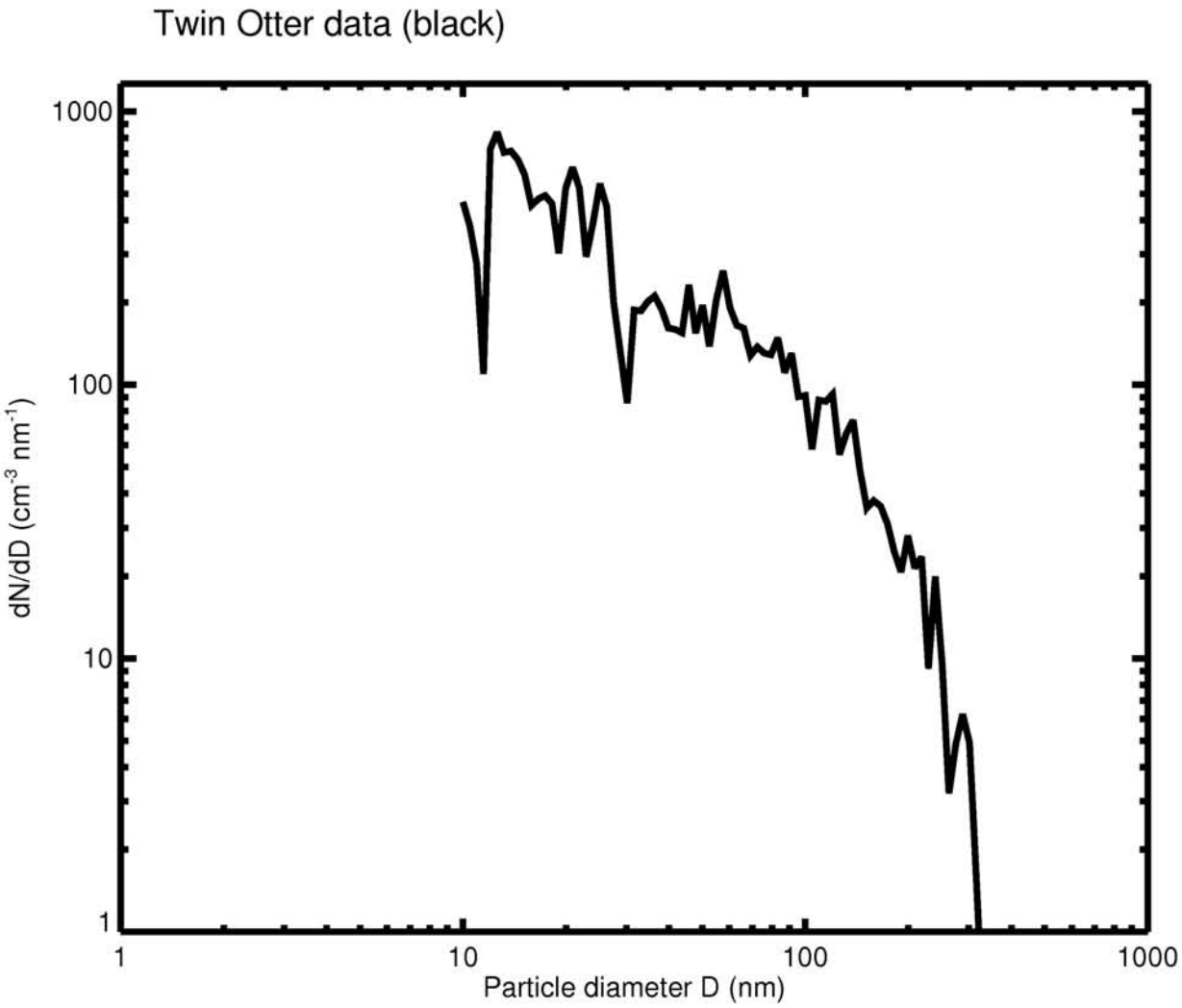
How do we represent aerosols in an atmospheric model?



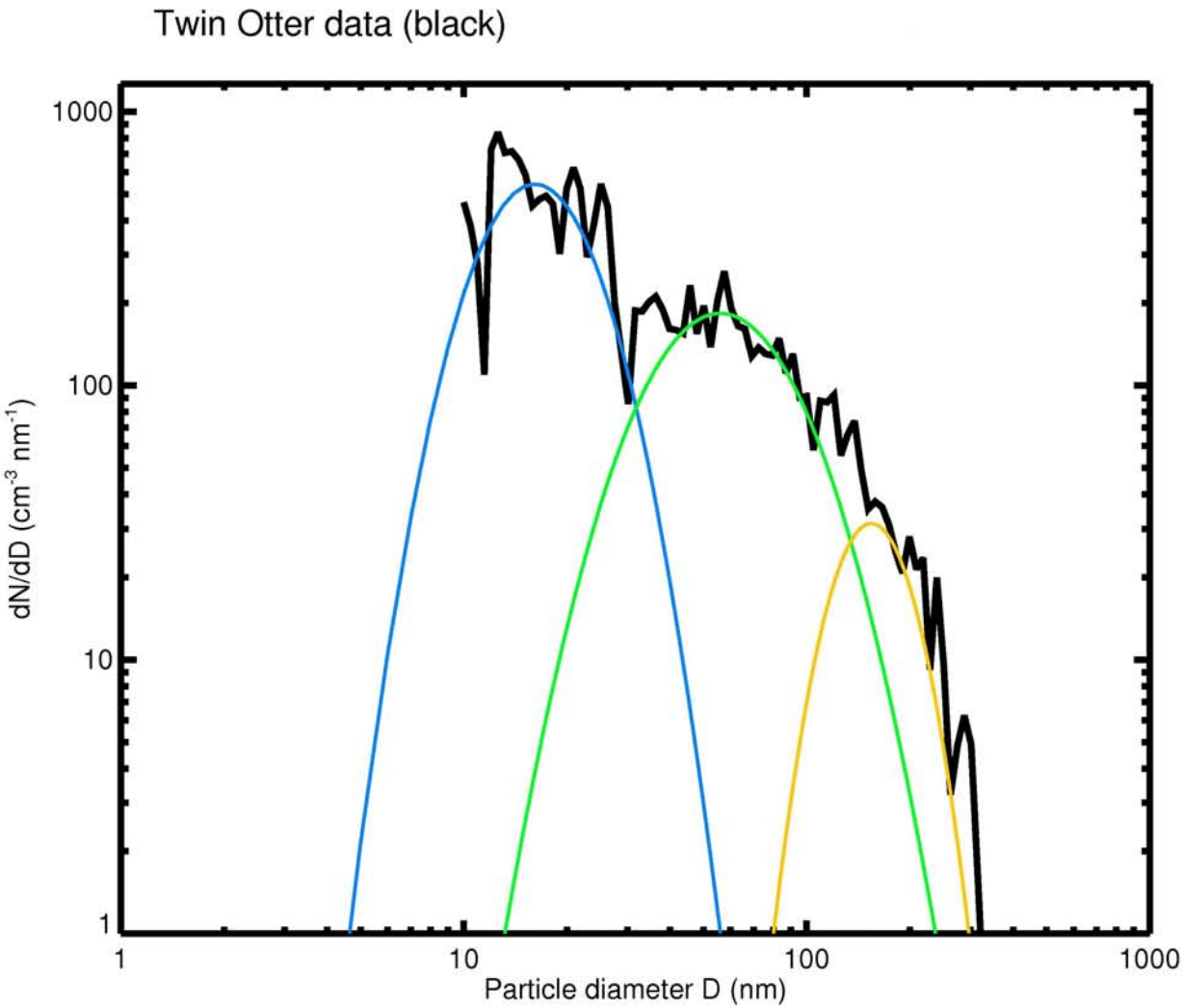
Sectional (bin) aerosol scheme



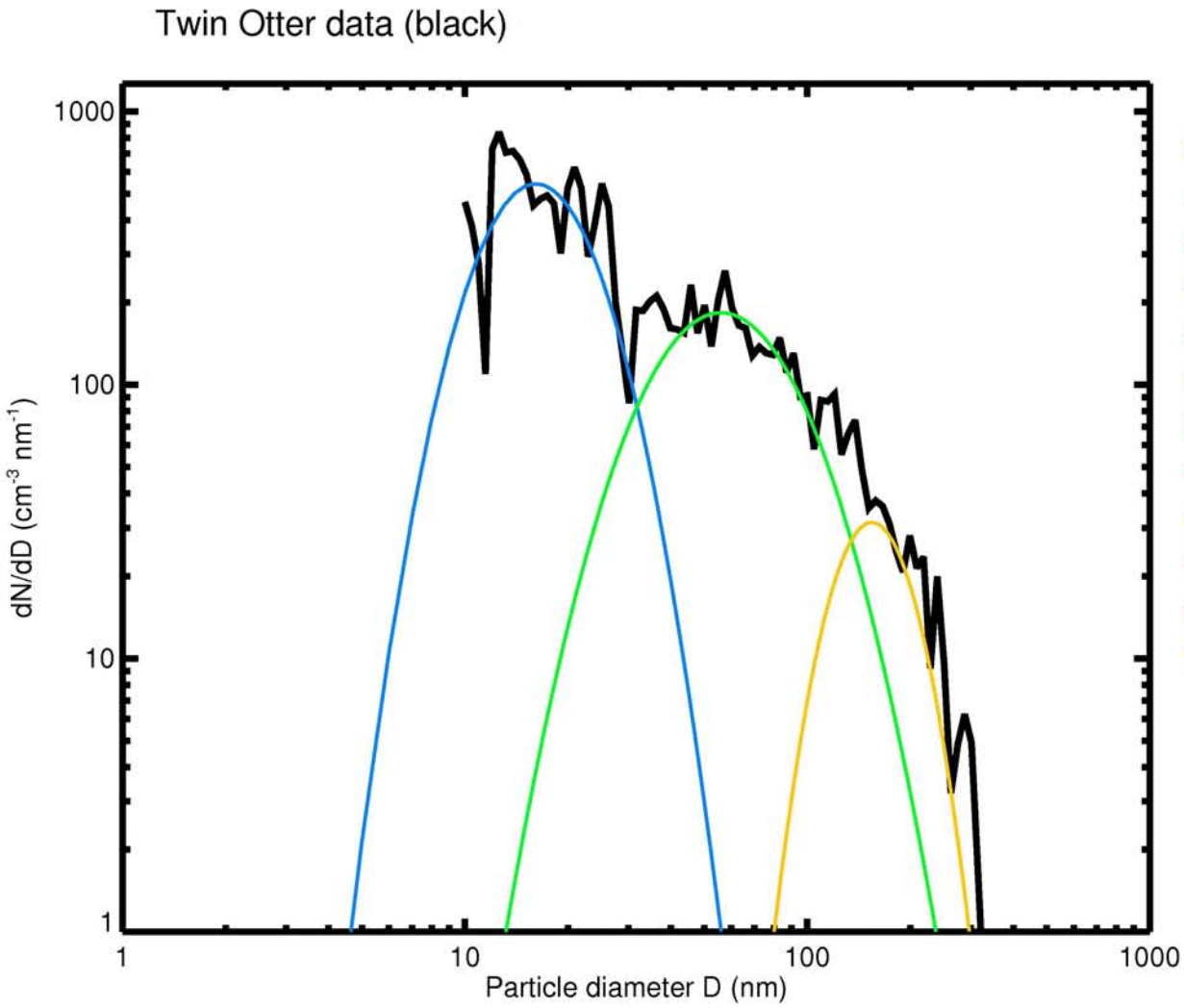
Modal aerosol scheme



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

$\sigma = 1.57$

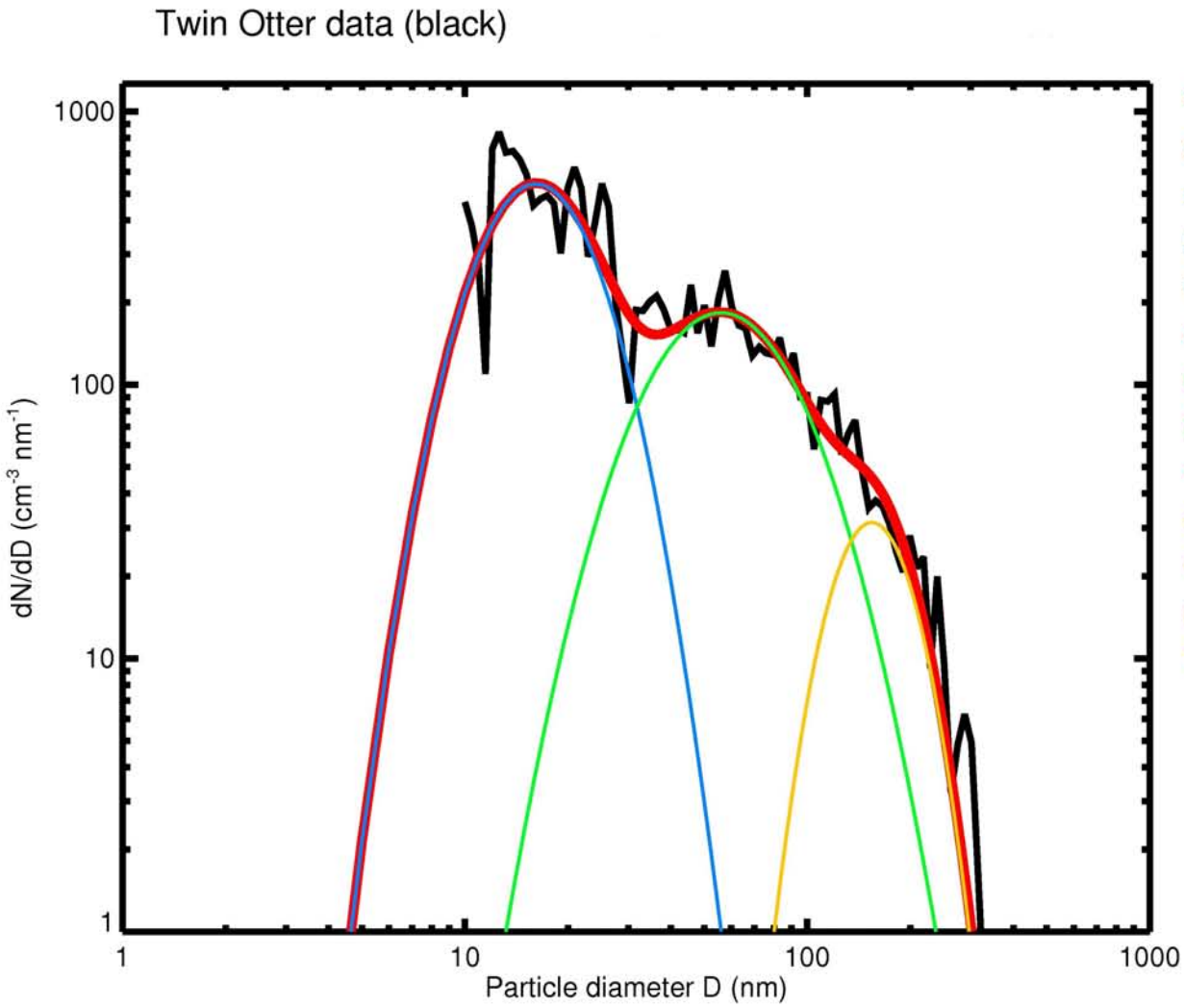
$dN/dD = c \cdot \exp\{-0.5 \cdot [\ln(D/\mu)/\ln(\sigma)]^2\}/[(2\pi)^{0.5}\ln(\sigma)D]$:

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

$\mu = 164.41$ 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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dN/dD = c·exp{-0.5·[ln(D/μ)/ln(σ)]²}/[(2π)^0.5 ln(σ)D] :

c = 3139.90 cm^{-3}

μ = 164.41 nm

σ = 1.28

Bulk scheme

- Much simpler than the sectional and model schemes
  - Calculates only with the total mass of the aerosol components
  - Provides no information on
    - Particle size
    - Particle concentration
  - E.g., when particles grow, the aerosol mass increases but we don't know how their size/number changes
- Numerically very efficient
- Allows complex gas/aqueous phase chemistry
- Difficult to couple with radiation/cloud processes

Aerosol (and chemistry) schemes in WRF/Chem

WRF/Chem aerosol schemes:

- GOCART: From the Goddard Chemistry Aerosol Radiation and Transport model
  - Bulk aerosol scheme
- MOSAIC: Model for Simulating Aerosol Interactions and Chemistry
  - Bin aerosol scheme
- MADE/SORGAM: The Modal Aerosol Dynamics Model for Europe
  - Modal aerosol scheme

WRF/Chem gas phase chemistry schemes:

- CBM-Z: Carbon bond mechanism v. Z
- RACM: Regional Atmospheric Chemistry Mechanism
- RADM2: Regional Acid Deposition Model v. 2

Aerosol schemes in WRF/Chem

GOCART

- Works with the RACM-KPP gas phase chemical scheme
  - Using the KPP means that chemical reactions can be added/modified easily
- Predicts mass of aerosol components:
  - Sulfate, dust, sea salt, organic carbon, black carbon
- Numerically very efficient
- Complex gas phase chemistry possible
- But:
  - No aerosol size information
  - No secondary organic aerosol
  - No interaction with radiation (direct effect)
  - No coupling with cloud processes (aqueous chemistry, indirect effects)

Aerosol schemes in WRF/Chem

MOSAIC

- Works with the CBM-Z gas phase chemistry scheme
- Includes some aqueous reactions
- Predicts mass of aerosol components:
  - Sulfate, nitrate, ammonium, sea salt, organic carbon, black carbon, dust (= other inorganic mass)
  - In preparation: secondary organic aerosol
- Predicts size of aerosol particles:
  - 4 or 8 size bins
- Can be coupled with atmospheric radiation (direct effect)
- Can be coupled with cloud microphysics (indirect effects)
- Still, numerically efficient
- This is the most actively developed aerosol module in WRF/Chem

MADE/SORGAM

- Predicts mass of aerosol components:
  - sulfate, nitrate, ammonium, sea salt, organic carbon, black carbon, dust
  - secondary organic aerosol:
    - SORGAM = Secondary Organic Aerosol Model
- Predicts size of aerosol particles:
  - Three log-normal aerosol modes (Aitken, accumulation, coarse)
  - Mean diameter of the modes varies (particle growth)
  - Mode width is fixed

MADE/SORGAM

- Several gas phase chemistry schemes available:
  - RADM2 (hard wired)
  - RADM2 (hard wired) + some aqueous reactions
  - RADM2-KPP gas phase chemistry (flexible)
  - In preparation: RADM2-KPP gas phase chemistry (flexible) + some aqueous reactions
- Can be coupled with atmospheric radiation (direct effect)
- Can be coupled with cloud microphysics (indirect effects)
- Has SOA
- But:
  - Numerically more expensive
  - Less actively developed in recent years than MOSAIC

Model setup

File **namelist.input**:

- Resides in the same directory as wrf.exe
- Contains “namelists”:
  - Lists of keywords and their values
  - These determine the model behavior
  - Namelists for aerosols (examples follow):
    - “chem”
    - “phys”
  - Not all possible settings can be combined: The aerosol schemes work only
    - with specific gas phase chemistry schemes
    - with specific radiation/cloud couplings
    - with specific cloud schemes
  - Details: WRF/Chem User's Guide 3.1

“chem” namelist

```
&chem
 chem_opt                = 106
 photdt                  = 0.5
 chemdt                  = 0.05
 drydep_opt              = 0
 aer_ra_feedback         = 0
 emiss_inpt_opt          = 1
 emiss_opt               = 0
 chem_in_opt             = 0
 phot_opt                = 1
 bio_emiss_opt           = 0
 dust_opt                = 0
 dmsemis_opt             = 0
 seas_opt                = 0
 gas_bc_opt              = 1
 gas_ic_opt              = 1
 aer_bc_opt              = 1
 aer_ic_opt              = 1
 gaschem_onoff           = 1
 aerchem_onoff           = 1
 cldchem_onoff           = 1
 wetscav_onoff           = 1
 vertmix_onoff           = 0
 chem_conv_tr            = 1
 /
```

- **If an option is not set/used in the namelist, then its default value is used.**
- **The default values are defined in the file**

WRFV3/Registry/registry.chem

Option “chem_opt”

```
chem_opt =   0   no chemistry
         =   1   RADM2 - no aerosols
         =   2   RADM2 + MADE/SORGAM aerosols

         =   5   CBMZ with DMS (Dimethylsulfide)
         =   6   CBMZ without DMS

         =   7   CBMZ (chem_opt=6) and MOSAIC, 4 bins
         =   8   CBMZ (chem_opt=6) and MOSAIC, 8 bins
         =   9   CBMZ (chem_opt=6) and MOSAIC, 4 bins, some aqueous reactions
         =  10   CBMZ (chem_opt=6) and MOSAIC, 8 bins, some aqueous reactions

         =  11   RADM2 + MADE/SORGAM aerosols, some aqueous reactions
         =  12   RACM  + MADE/SORGAM aerosols, some aqueous reactions
         = 106   RADM2 KPP + MADE/SORGAM aerosols

         =       ...

         = 301   RACM (KPP) + GOCART
```

Emission options

- Anthropogenic emissions (similar for biogenic emissions):

```
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
emis_inpt_opt      = 0 no emissions data read
                   = 1 Emissions speciation for RADM2/SORGAM
                   = 101 Emission speciation follows the CBMZ/MOSAIC framework
                   = 102 Emission speciation follows the RADM2/SORGAM framework
```

- Dust:

```
dust_opt           = 0 No dust emissions
                   = 1 include GOCART dust emissions - need to provide fractional
                     erosion map data
                   = 2 MOSAIC and MADE/SORGAM dust emissions option (does not
                     requires extra input data)
```

- Sea salt:

```
seas_opt           = 0 no sea salt emissions
                   = 1 GOCART sea salt emissions
                   = 2 MOSAIC or MADE/SORGAM sea salt emissions
```

Other options in the “chem” namelist

```
gaschem_onoff      = 0/1 (Default is 1)
aerchem_onoff      = 0/1 (Default is 1)
cldchem_onoff      = 0/1 (Default is 0)
```

```
cldchem_onoff      = 0/1 (Default is 0)
wetscav_onoff      = 0/1 (Default is 0)
aer_ra_feedback    = 0   No aerosol-radiation feedback (default)
                   = 1   Aerosol radiation feedback
```

Initialization option in the “chem” name list

```
chem_in_opt        = 0 Idealized vertical distribution (profile) to initialize
                       chemistry/aerosols
                       hardwired in WRFV3/chem/chemics_init.F
                   = 1 Use results from previous simulation for initialization
```

```
do j=jts,jte                                ! Tile south-north
  do k=kts,kte                              ! Tile bottom-top
    do i=its,ite                            ! Tile west-east
      chem(i,k,j,p_co)    =    40.0e-3 ! ppmv
      chem(i,k,j,p_o3)    =    35.0e-3 ! ppmv
      chem(i,k,j,p_so2)   =    75.0e-6 ! ppmv
      ! Initialization of H2SO4(g) + aerosol SO4--, the partitioning
      ! is treated in aerosols_sorgam_init:
      chem(i,k,j,p_sulf) =  150.0e-6 ! ppmv
    enddo
  enddo
enddo
```

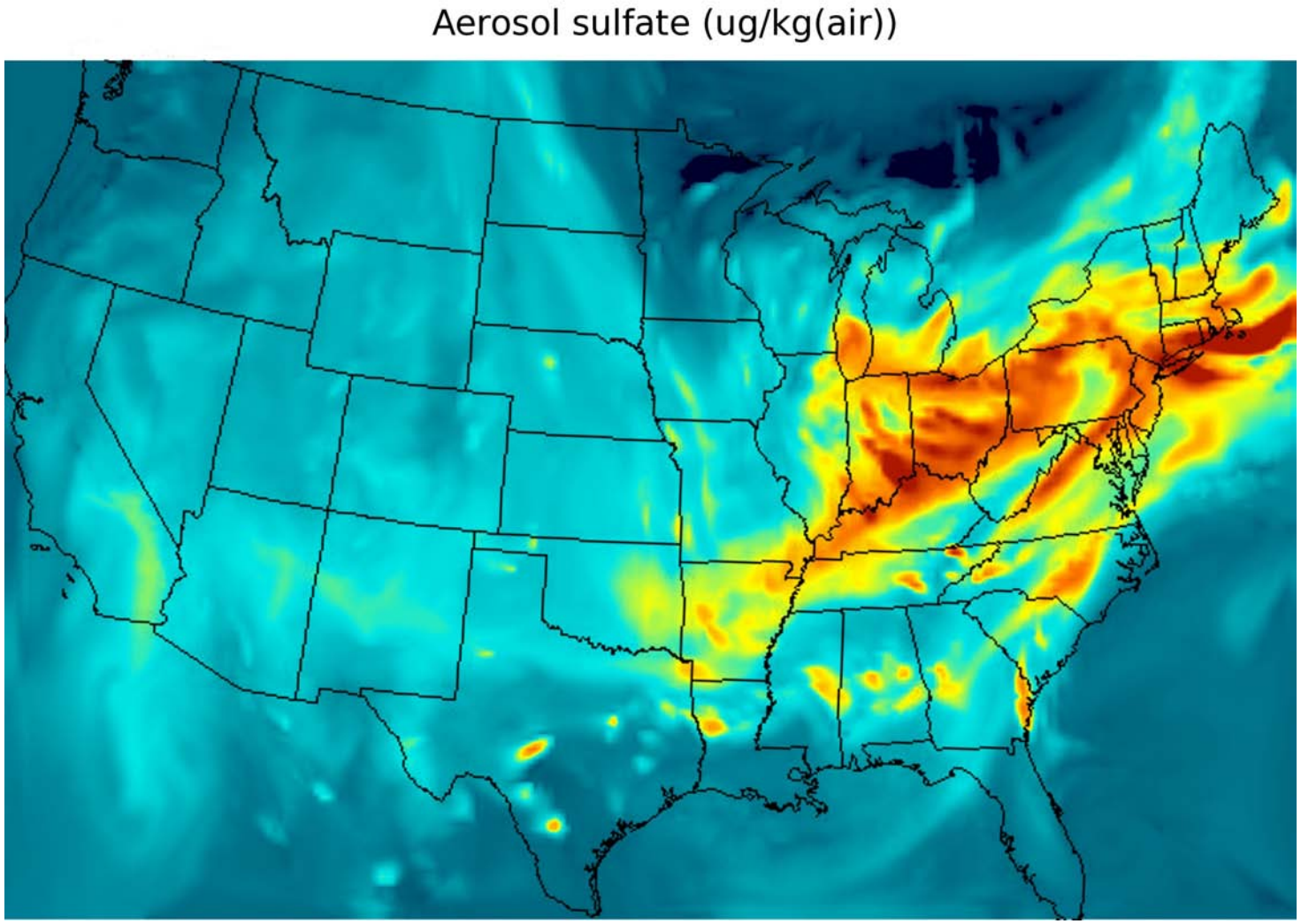
Options in the “phys” namelist

- The “**phys**” namelist controls physical processess in WRF:
  - Radiation
  - Cloud microphysics (cloud water condensation, evaporation, ...)
  - ...
- “**phys**” namelist options related to aerosols:
  - **mp_physics** (cloud microphysics option):
    - Determines how cloud properties are calculated
    - Cloud drop mass/number
    - Snow mass/number
    - ...
  - **progn** (prognostic cloud droplet number option):
    - Switches on prognostic cloud droplet number calculation
  - **ra_sw_physics** (shortwave radiation scheme):
    - Determines how shortwave radiative transfer in the atmosphere is calculated

Settings in the “phys” namelist

- Indirect aerosol effect:
  - `mp_physics = 2` (Lin et al. cloud microphysics scheme)
  - `progn = 1` (prognostic cloud droplet calculation)
- Aerosol-radiation feedback:
  - `ra_sw_physics = 2` (Goddard shortwave scheme)

Example results



Light blue: 1 µg/kg(air)

Red: 3.5 µg/kg(air)

Plot courtesy of Si-Wan Kim, NOAA CSD