Aerosol in WRF/Chem

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Part I - Introduction

- Overview of ...
  - Aerosol types
  - How aerosols are treated in atmospheric models
  - Aerosol processes
  - WRF/Chem aerosol schemes

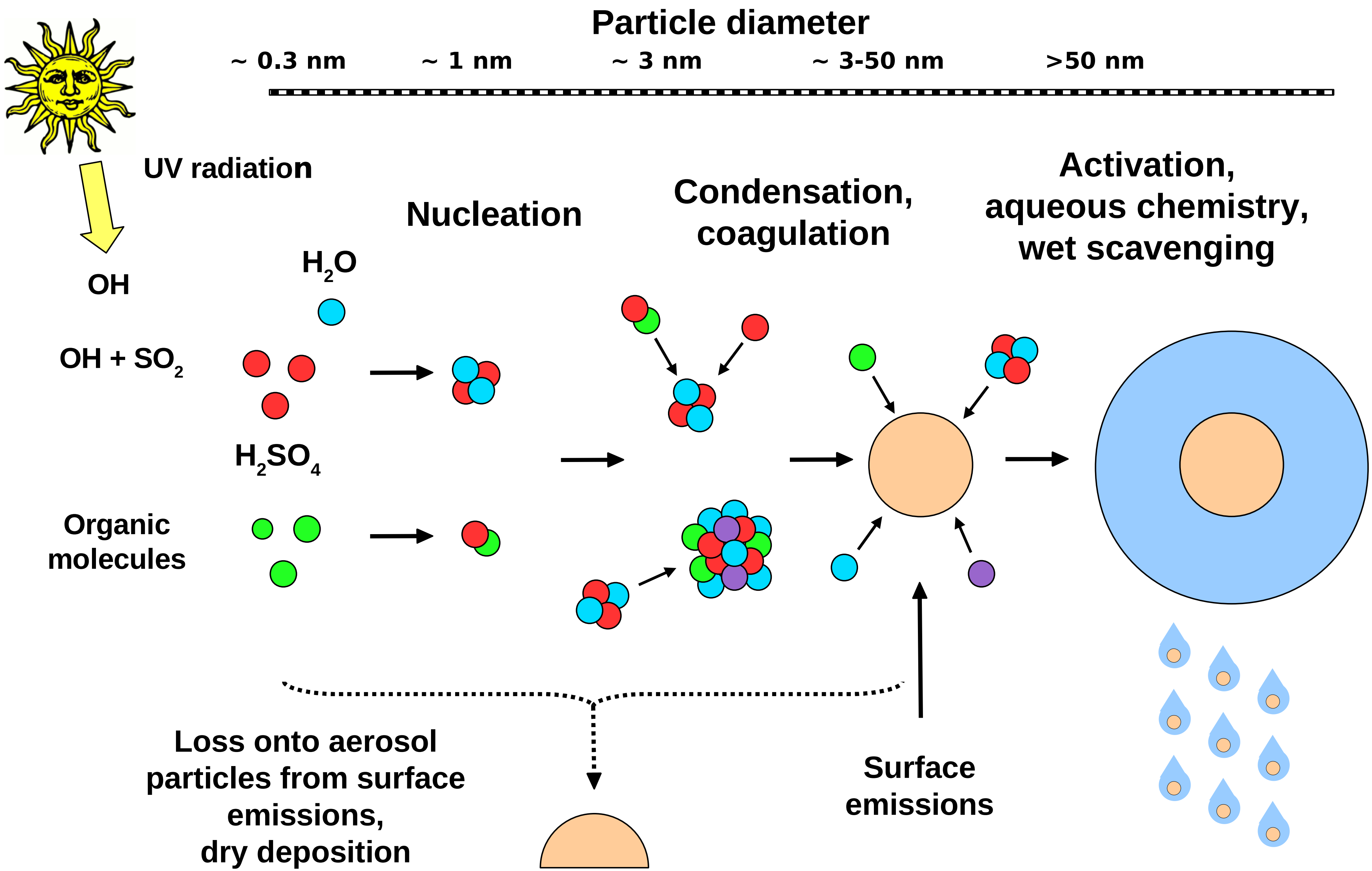
Part II – Details

- Representing the aerosol size distribution
- WRF/Chem aerosol schemes
  - How they work and what they do
  - Coupling to other processes
    - Gas phase chemistry
    - Clouds and aqueous chemistry
    - Wet deposition
- How to tell WRF/Chem what to do
- Resources

Part I – Introduction

Aerosol

Aerosol processes



How aerosols are treated in atmospheric models

Aerosol microphysics schemes describe:

- The aerosol size distribution
- Microphysical processes between aerosol particles

Aerosol chemistry schemes describe:

- Chemical processes in and on the aerosol
- Gas/partical partitioning

Coupled to:

- Gas phase chemistry: gas phase molecules can condense onto aerosol (depends on the aerosol surface area)
- Aerosol nucleation: Gas phase molecules can stick together and form new aerosol particles (depends on concentrations of gas phase species)
- Radiation: Aerosol particles scatter radiation (depends on number and size of aerosol particles)
- Cloud microphysics: Cloud drop number (depends on the number and size of aerosol particles)

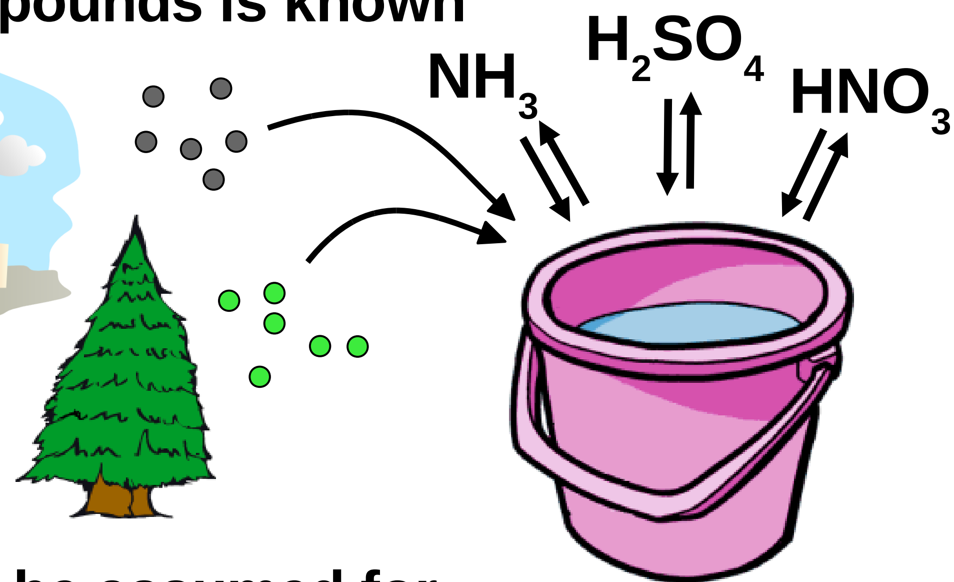
WRF/Chem aerosol schemes

- An efficient aerosol scheme from the GOCART model
  - No size information for sulfate, BC, OC
  - Size information for dust and sea salt
  - No secondary organic aerosol (SOA)
- The Modal Aerosol Dynamics Model for Europe – MADE
  - 3 log-normal modes
  - Inorganic, organic aerosol, SOA
- The Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)
  - Sectional model, 4 or 8 bins
  - Inorganic, organic aerosol, SOA
- Simple scheme for volcanic ash aerosol

Part II – The details

Bulk aerosol schemes

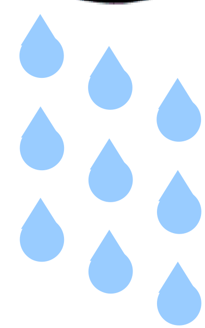
- Only total mass of aerosol compounds is known



- 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

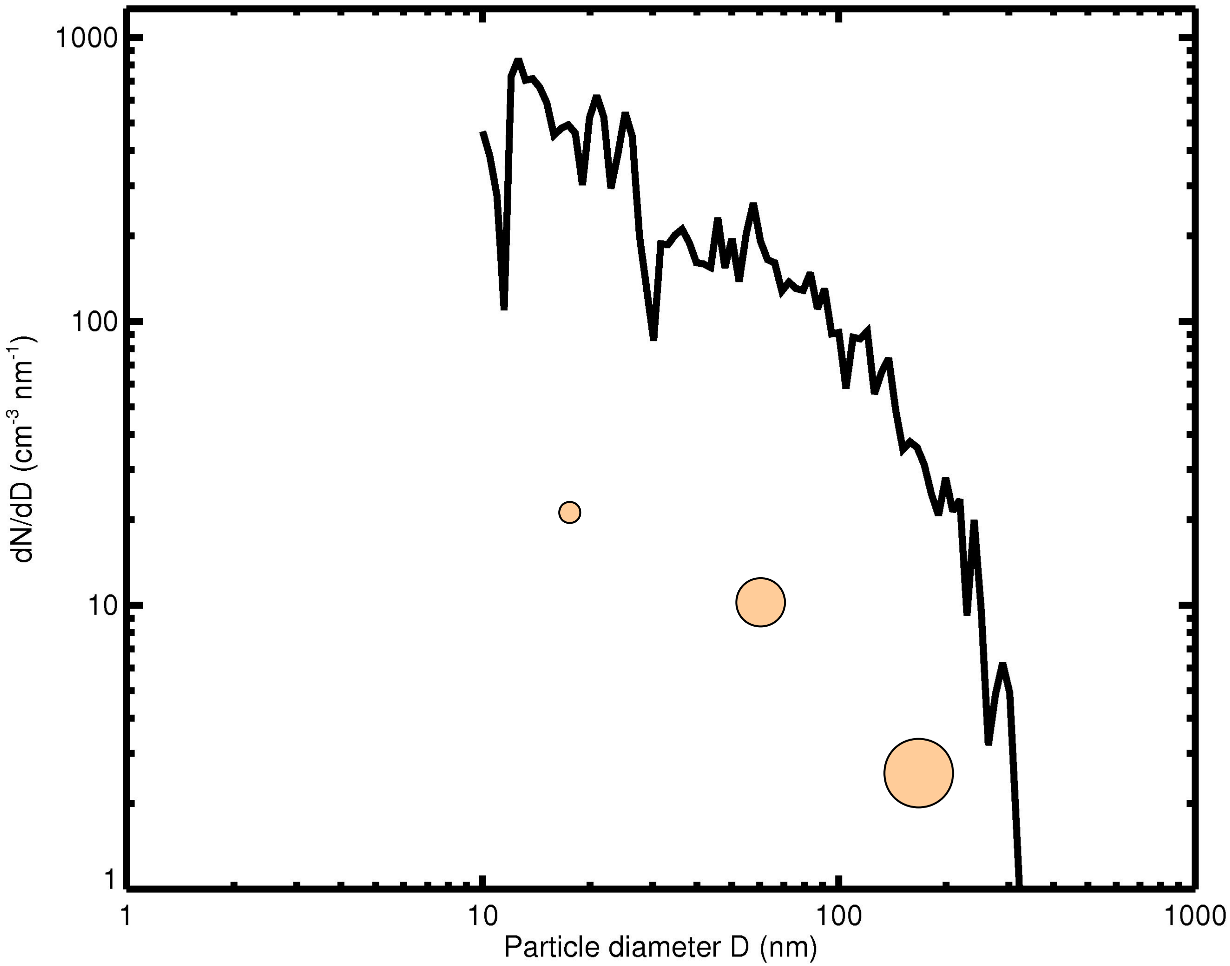


- Numerically efficient
- Useful when focus is on complex gas phase chemistry

→ GOCART (+ size resolved dust and sea salt)

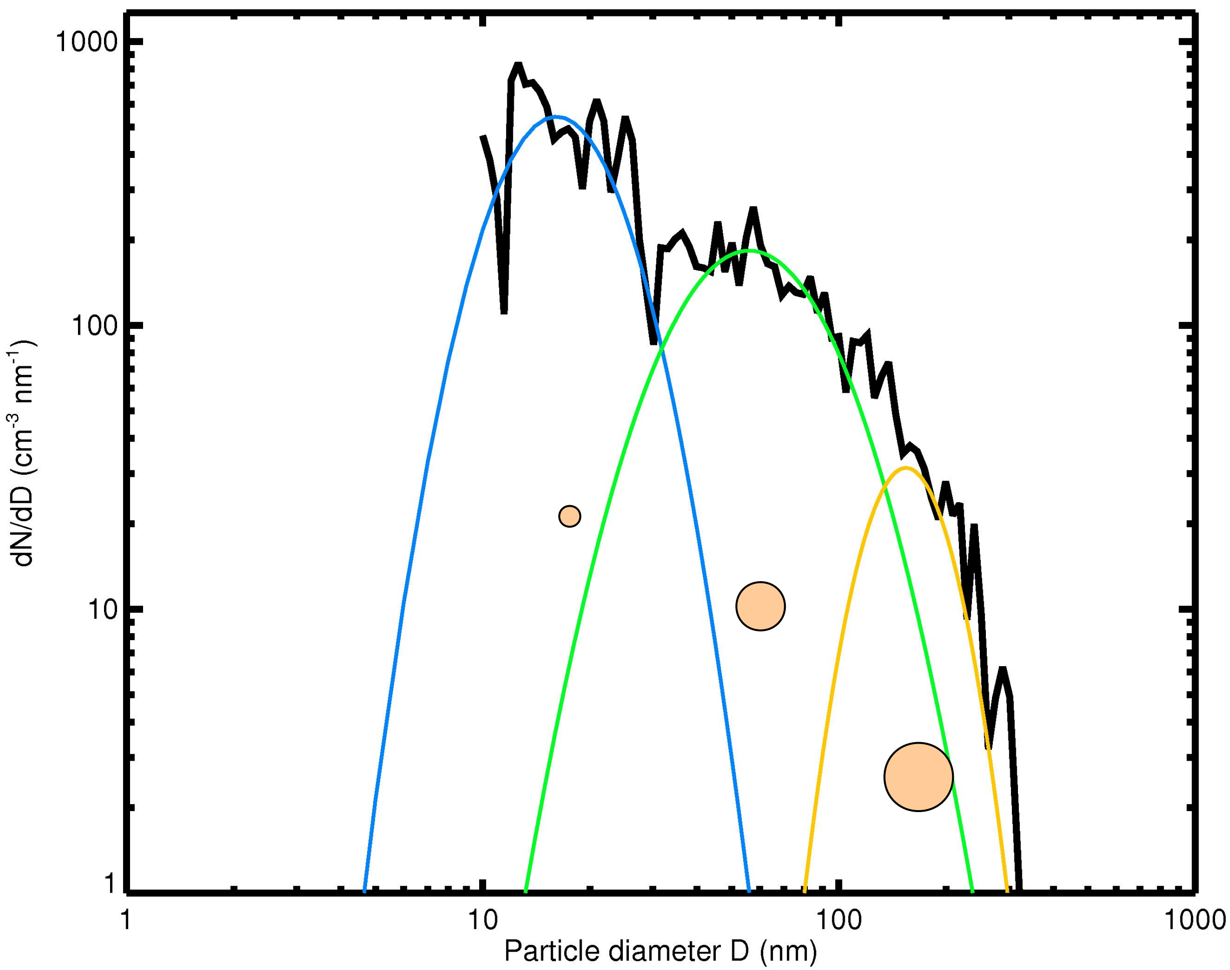
Modal aerosol schemes

Twin Otter data (black)



Modal aerosol schemes

Twin Otter data (black)



$$\frac{dN}{dD} = \frac{N}{\sqrt{2\pi}\ln(\sigma)D} e^{-\frac{1}{2}\left[\frac{\ln(D/\mu)}{\ln(\sigma)}\right]^2}$$

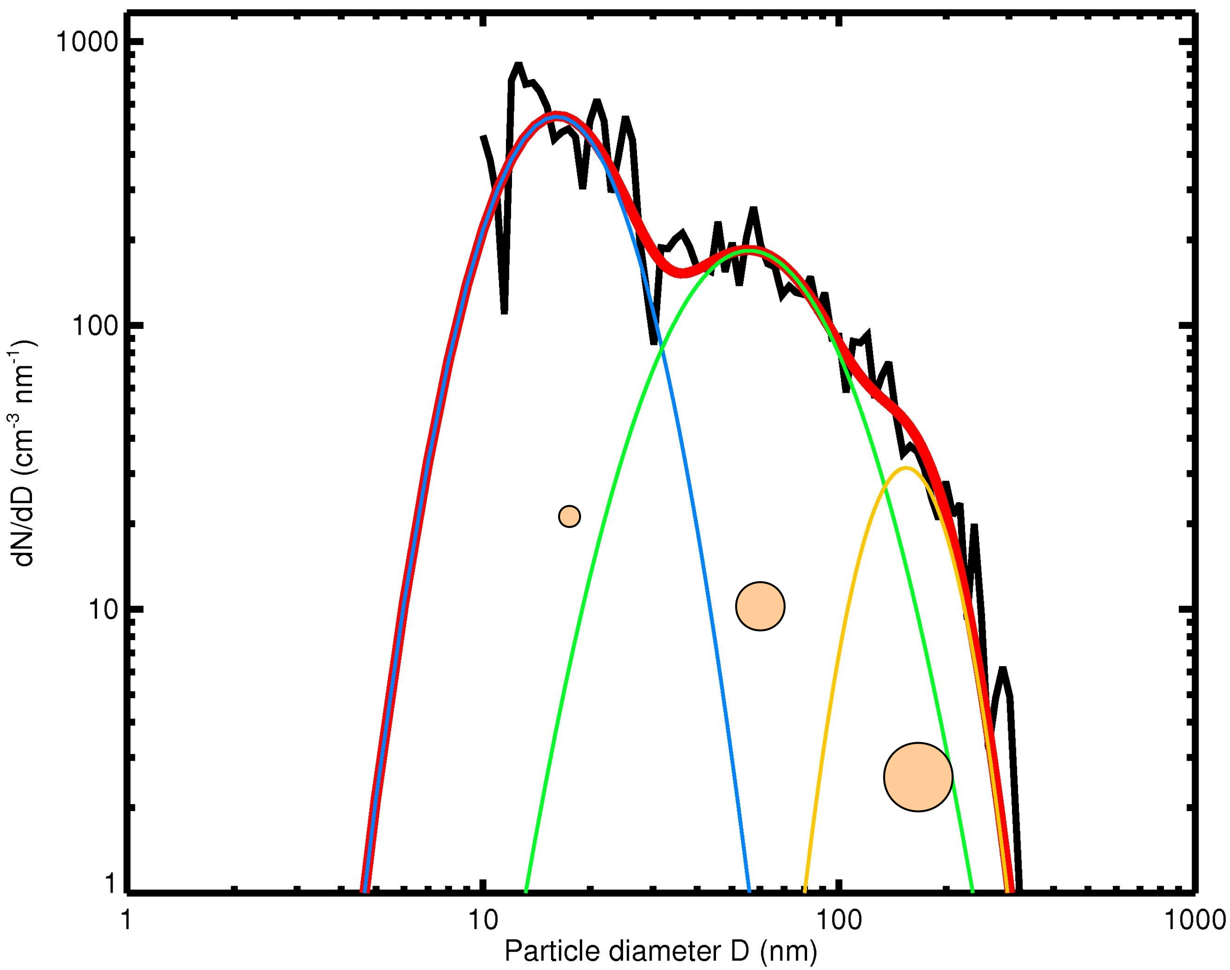
$$\frac{dN}{dD} \rightarrow N = 8195\ cm^{-3},\quad \mu = 18.22\ nm,\quad \sigma = 1.42$$

$$\frac{dN}{dD} \rightarrow N = 12732\ cm^{-3},\quad \mu = 68.44\ nm,\quad \sigma = 1.57$$

$$\frac{dN}{dD} \rightarrow N = 3140\ cm^{-3},\quad \mu = 164.41\ nm,\quad \sigma = 1.28$$

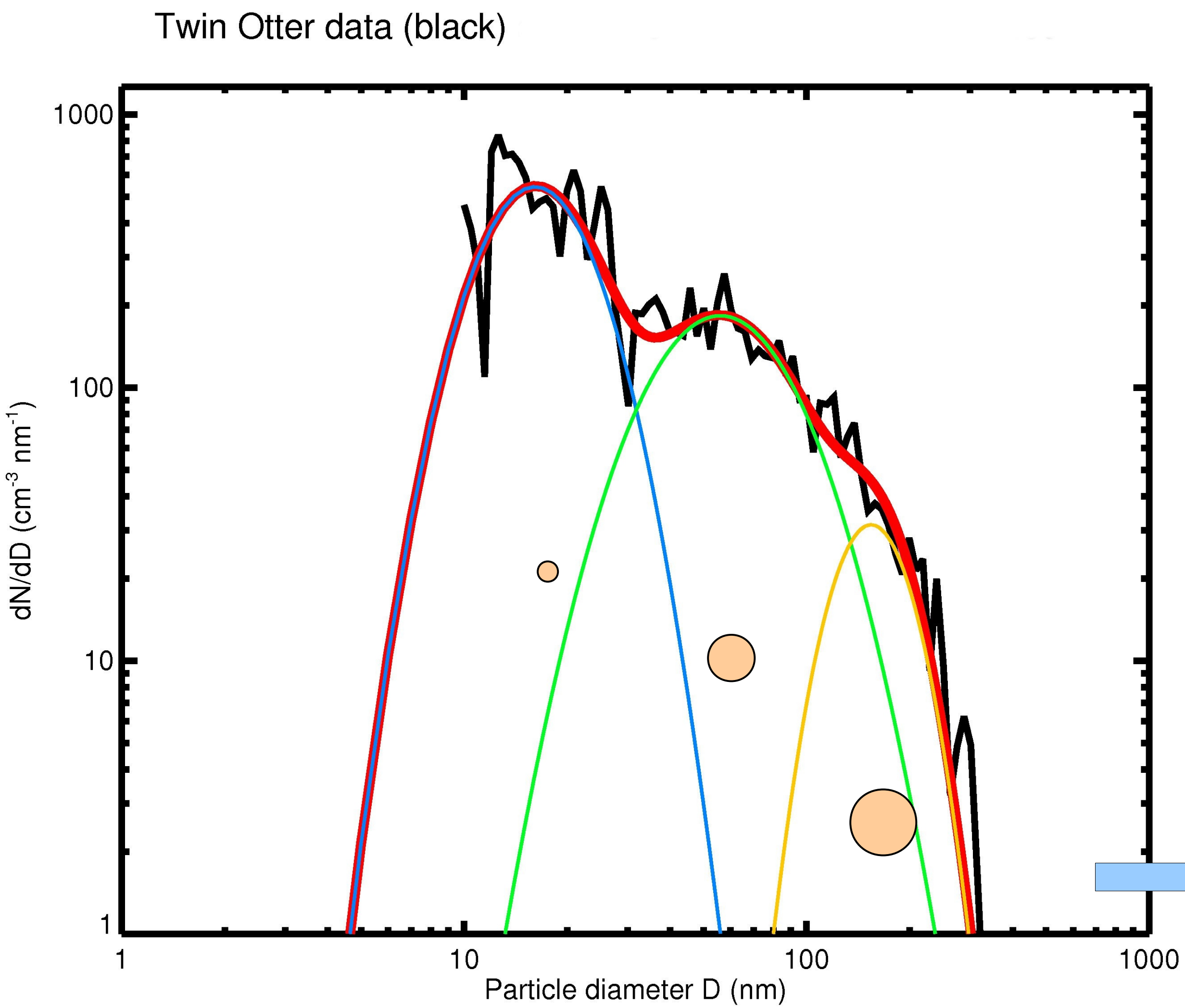
Modal aerosol schemes

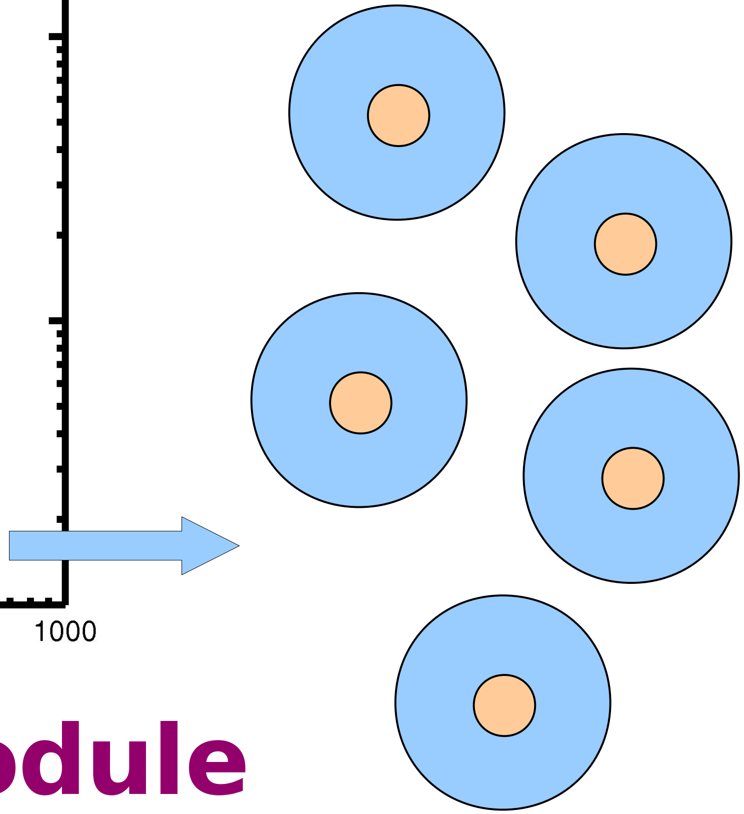
Twin Otter data (black)



$$\frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD}$$

Modal aerosol schemes

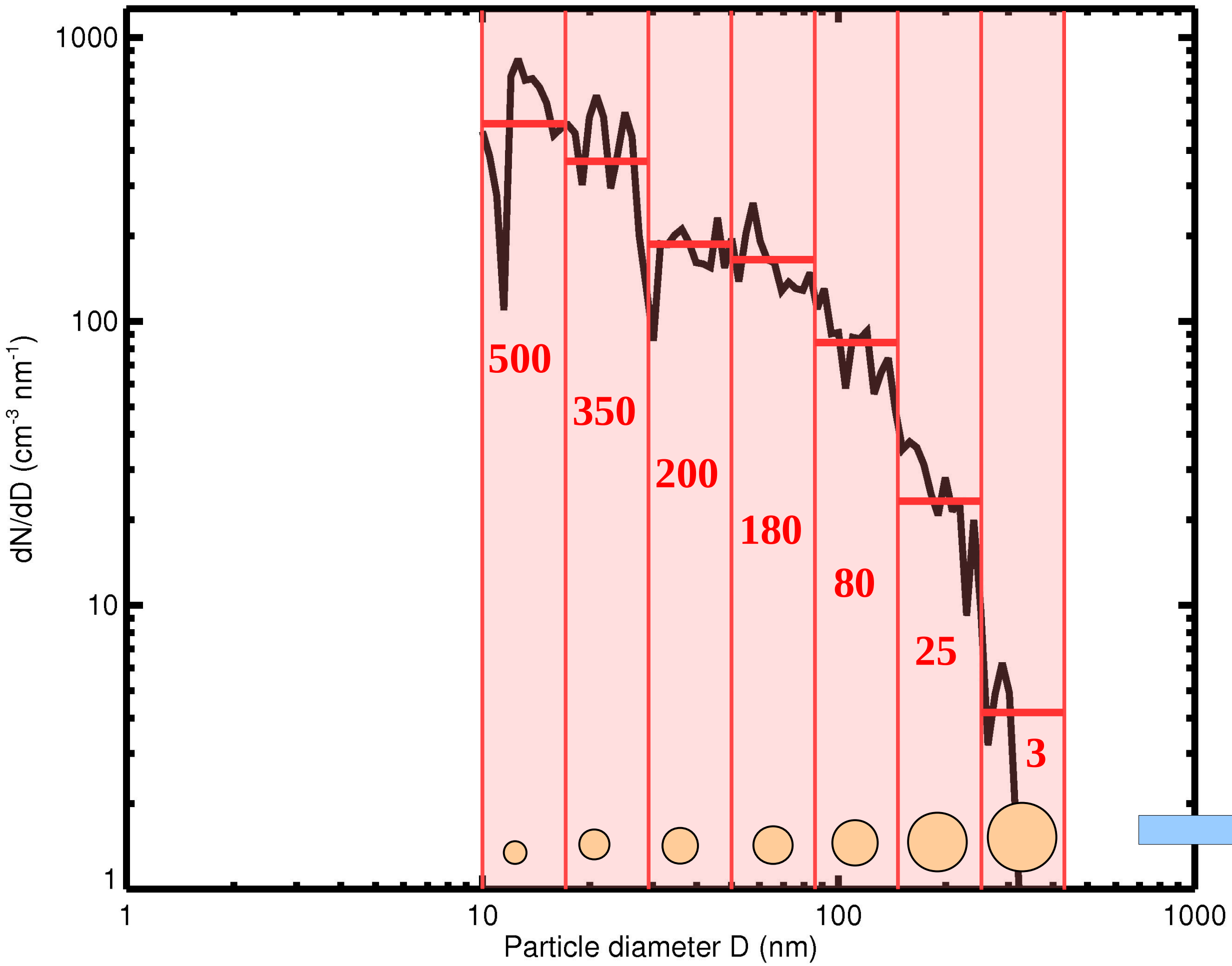


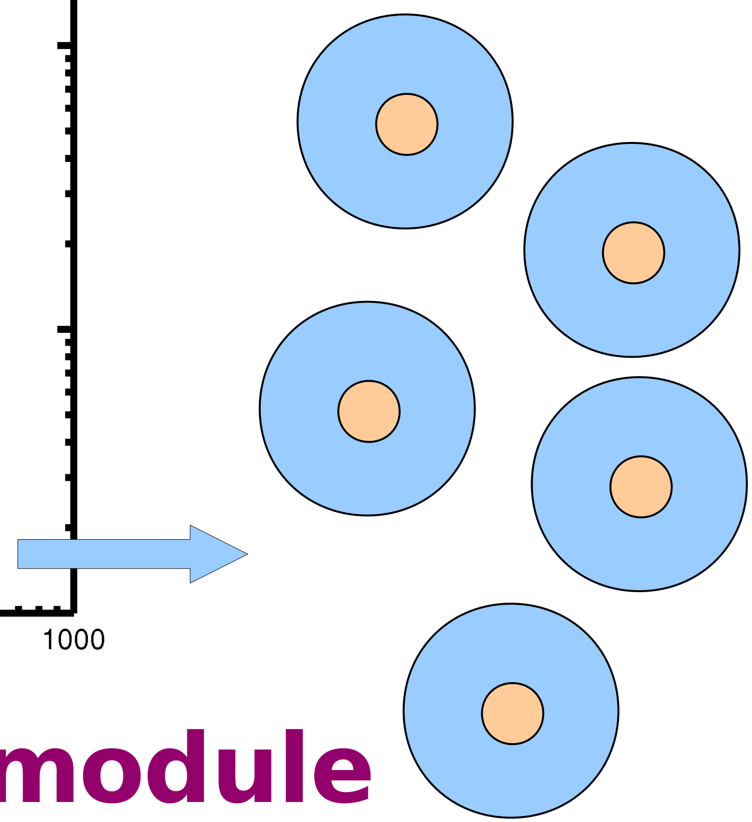


→ MADE aerosol module

Sectional aerosol schemes

Twin Otter data (black)





→ MOSAIC aerosol module

GOCART aerosol module

- Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport model (Chin et al., JGR, 2000)
  - Bulk aerosol:
    - Hydrophobic black carbon (fresh soot)
    - Hydrophilic black carbon (aged/coated soot)
    - Hydrophobic organic carbon (fresh burnt biomass)
    - Hydrophilic organic carbon (aged/coated burnt biomass)
      - Fresh → aged conversion time 2.5 days
    - Other GOCART primary PM2.5
    - Other GOCART primary PM10
    - Sulfate (only secondary aerosol species)
  - Sectional scheme for dust and sea salt:
    - Dust: 0.5, 1.4, 2.4, 4.5, 8.0 µm effective radius
    - Sea salt: 0.3, 1.0, 3.2, 7.5 µm effective radius

GOCART aerosol module

GOCART comes with sulfur gas phase chemistry:

- **DMS + OH → SO_2 + ...**
- **DMS + OH → MSA + ...**
- **DMS + NO_3 → SO_2 + ...**
- **SO_2 + OH → $SO_4^{=}$ + ...**

Extended gas phase chemistry can be used:

- **MOZART (with KPP)**
- **RACM (with KPP)**
- **RADM (with and without KPP)**

GOCART aerosol module

- **Interaction with radiation:**
  - **Direct effect for some model setups**
  - **Effect on photochemistry**
- **Interaction with clouds:**
  - **Aqueous chemistry**
    - $SO_2 + H_2O_2 \rightarrow SO_4^{=}$
    - $SO_2 + O_3 \rightarrow SO_4^{=}$
  - **No indirect effect**
  - **No wet scavenging/deposition**
- **No secondary organic aerosol (SOA)**

MADE aerosol module

Modal Aerosol Dynamics Model for Europe (Ackermann et al., Atm. Env., 1998)

- **3 log-normal aerosol modes: Aitken, accumulation, coarse**
- **Mode width σ is fixed**
- **Aerosol number and mass variable**
- **(Currently no nucleation mode)**
- **Interaction with radiation:**
  - **Direct aerosol effect**
  - **Effect on photolysis**
- **Interaction with clouds:**
  - **Aerosol number determines cloud drop number and size**
  - **Radiative response → 1st indirect effect**
    - **only for grid-scale (“dynamically resolved”) clouds**
  - **Aqueous chemistry**
  - **Wet removal (scavenging)**

MADE aerosol module

Aerosol composition in the Aitken and accumulation modes

- $SO_4^{=}$, NH_4^{+}, NO_3^{-}, H_2O
- NaCl (sea salt)
- Anthropogenic SOA from oxidation of ...
  - Alkanes
  - Alkenes
  - Aromatics
- Biogenic SOA from oxidation of ...
  - Alpha-pinene
  - Limonene
  - Isoprene
- Anthropogenic POA
- Elemental carbon (soot)
- Primary PM2.5

MADE aerosol module

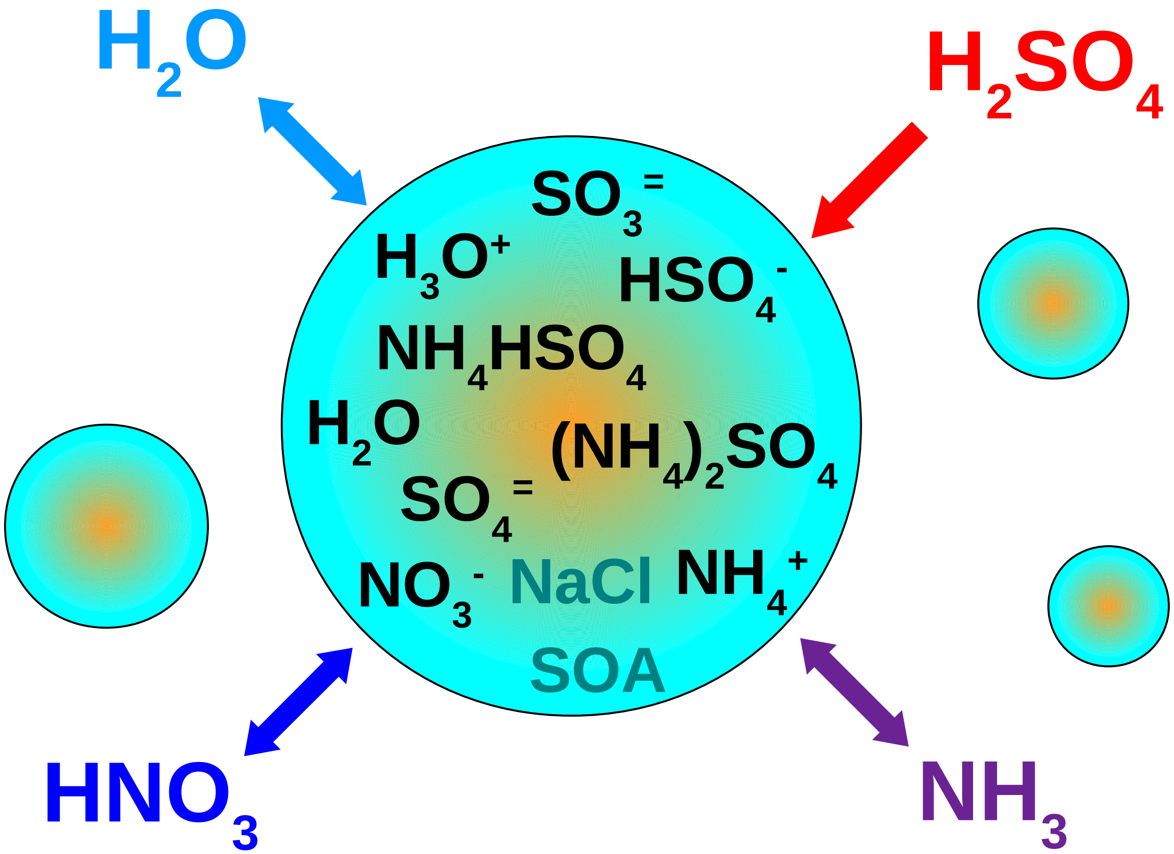
Aerosol composition in the coarse mode

- Anthropogenic primary aerosol – e.g. from
  - Coal combustion
  - Cement manufacturing
  - Metallurgy
  - Waste incineration
- Sea salt
- Soil derived particles (mineral dust)

MADE aerosol coupling with chemistry

- **Gas phase chemistry:**
  - **RADM2 (Regional Acid Deposition Model version 2)**
  - **RACM (Regional Atmospheric Chemistry Mechanism)**
  - **CBMZ (Carbon-Bond Mechanism version Z)**
    - **Hard-wired version, no indirect effect**
- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MARS (Model for an Aerosol Reacting System)**
  - **SORGAM (Secondary Organic Aerosol Model)**
  - **VBS (Volatility Basis Set)**
- **Aqueous chemistry:**
  - **CMU aqueous chemistry**
  - **CMAQ (EPA) aqueous chemistry**
  - **Only for Aitken and accumulation mode**
  - **Only for selected gas phase chemistry options**

MADE and MARS: Inorganic aerosol chemistry

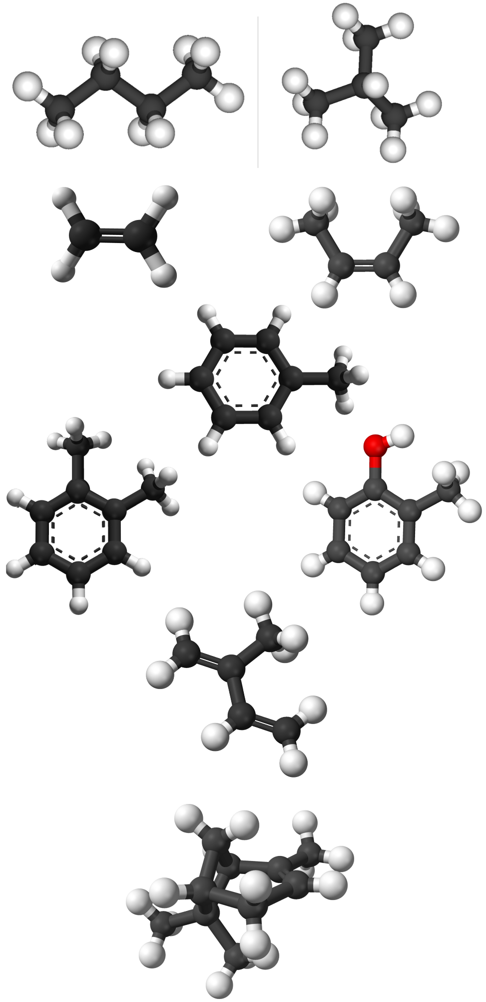


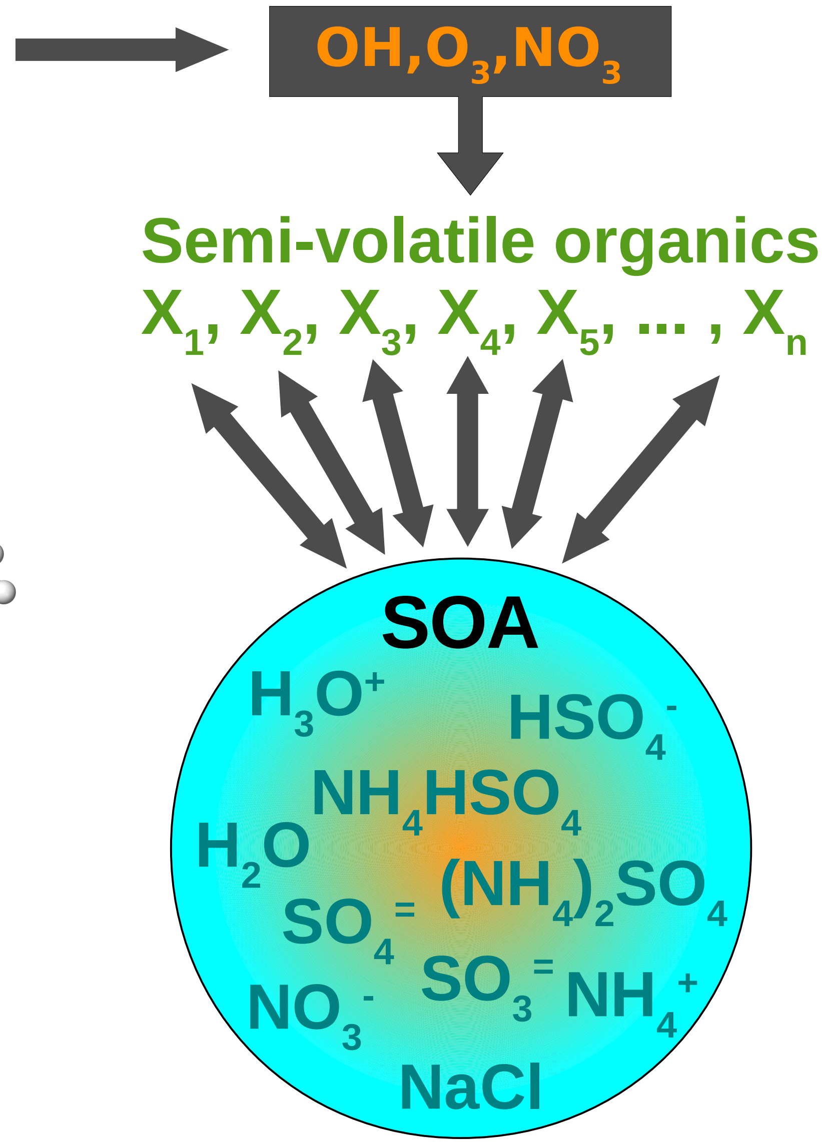
MARS (Model for an Aerosol Reacting System), Saxena et al., Atm. Env., 1986

MADE/SORGAM

Gas phase scheme (RADM2, RACM)

- Alkanes
- Alkenes
- Toluene
- Xylene, cresole, ...
- Isoprene
- Sesquiterpene
- Alpha-pinene, limonene



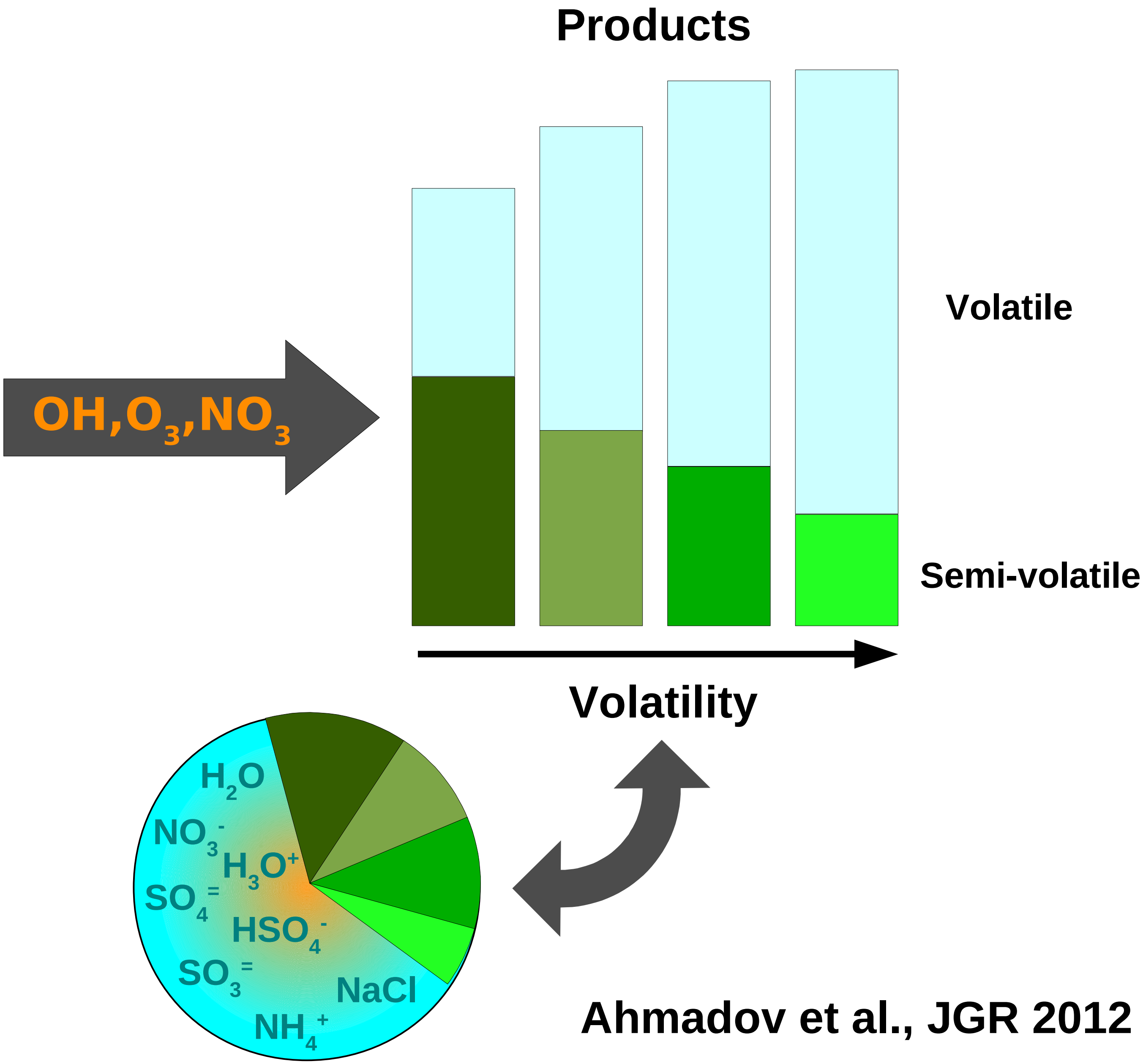


SORGAM (Secondary Organic Aerosol Model), Schell et al., JGR, 2001

MADE/VBS (Volatility Basis Set)

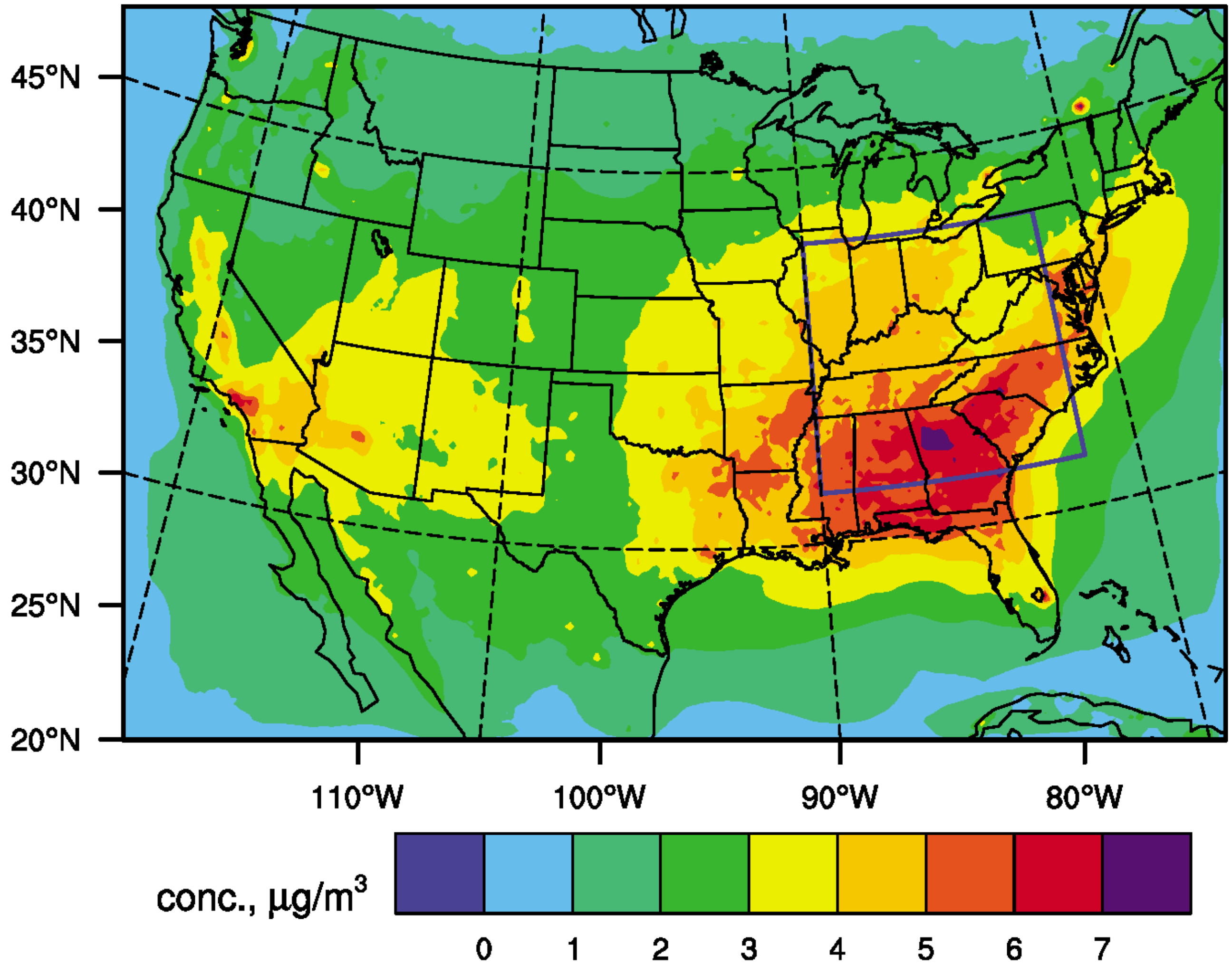
Gas phase scheme (RACM)

- Alkanes
- Alkenes
- Toluene
- Xylene, cresole, ...
- Isoprene
- Sesquiterpene
- Alpha-pinene, limonene



Ahmadov et al., JGR 2012

MADE/VBS (Volatility Basis Set)



Organic aerosol mass in the surface layer
(August - September 2006)

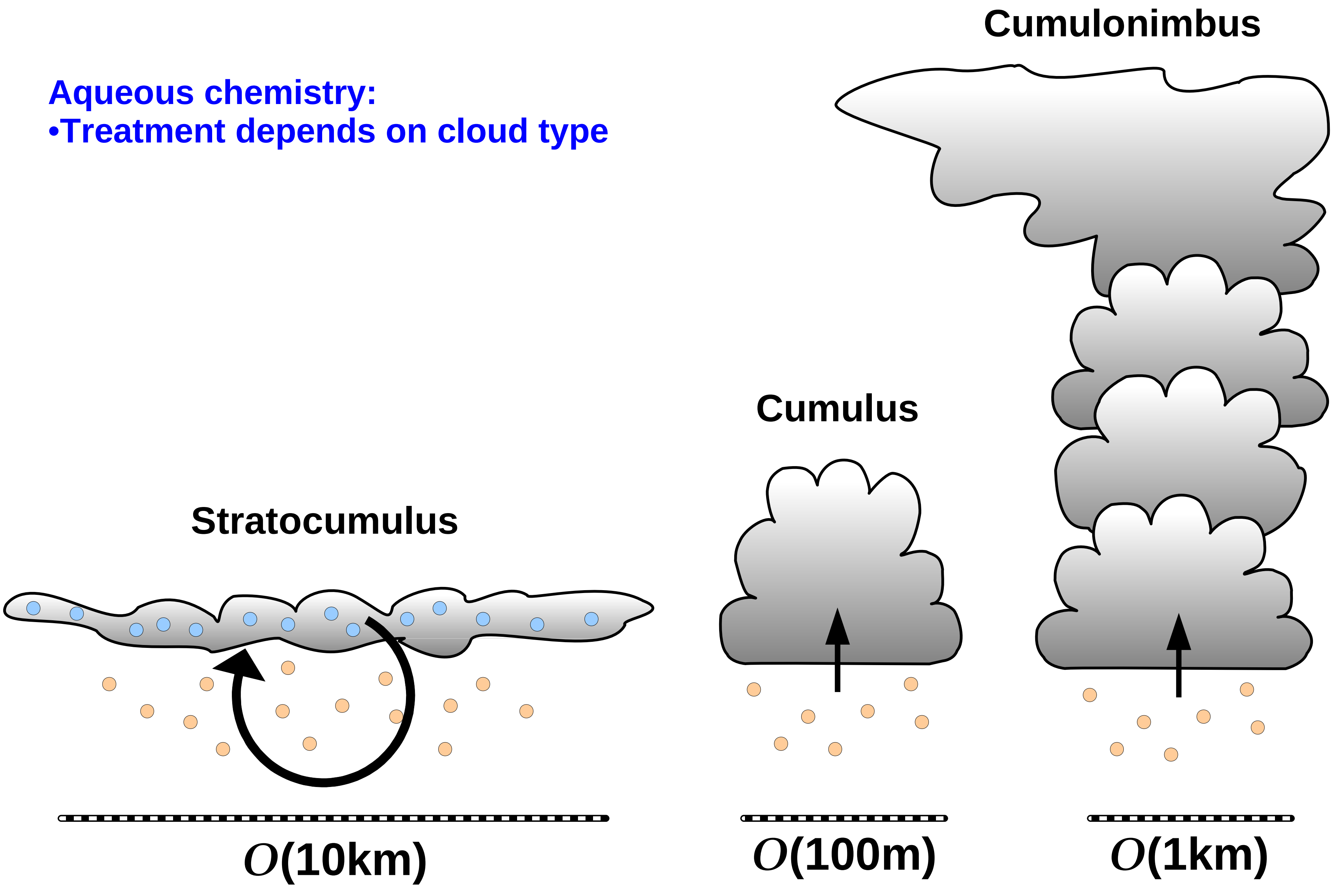
Ahmadov et al., JGR 2012

MADE and aqueous chemistry

- CMU aqueous chemistry (Fahey & Pandis, Atm. Env., 2001)
  - Only for Sc clouds
  - Slow
  - Does not conserve mass
- CMAQ (EPA) aqueous chemistry (Walcek & Taylor, JAS, 1986)
  - For both Sc and Cu clouds
  - Relatively fast
  - Conserves mass very well
  - Can be enabled for Cu together with the CMU scheme for Sc
- MADE and aqueous chemistry for selected gas phase chemistry options
- KPP versions of gas phase chemistry schemes: watch for bug fixes on WRF/Chem web site

MADE and CMAQ aqueous chemistry

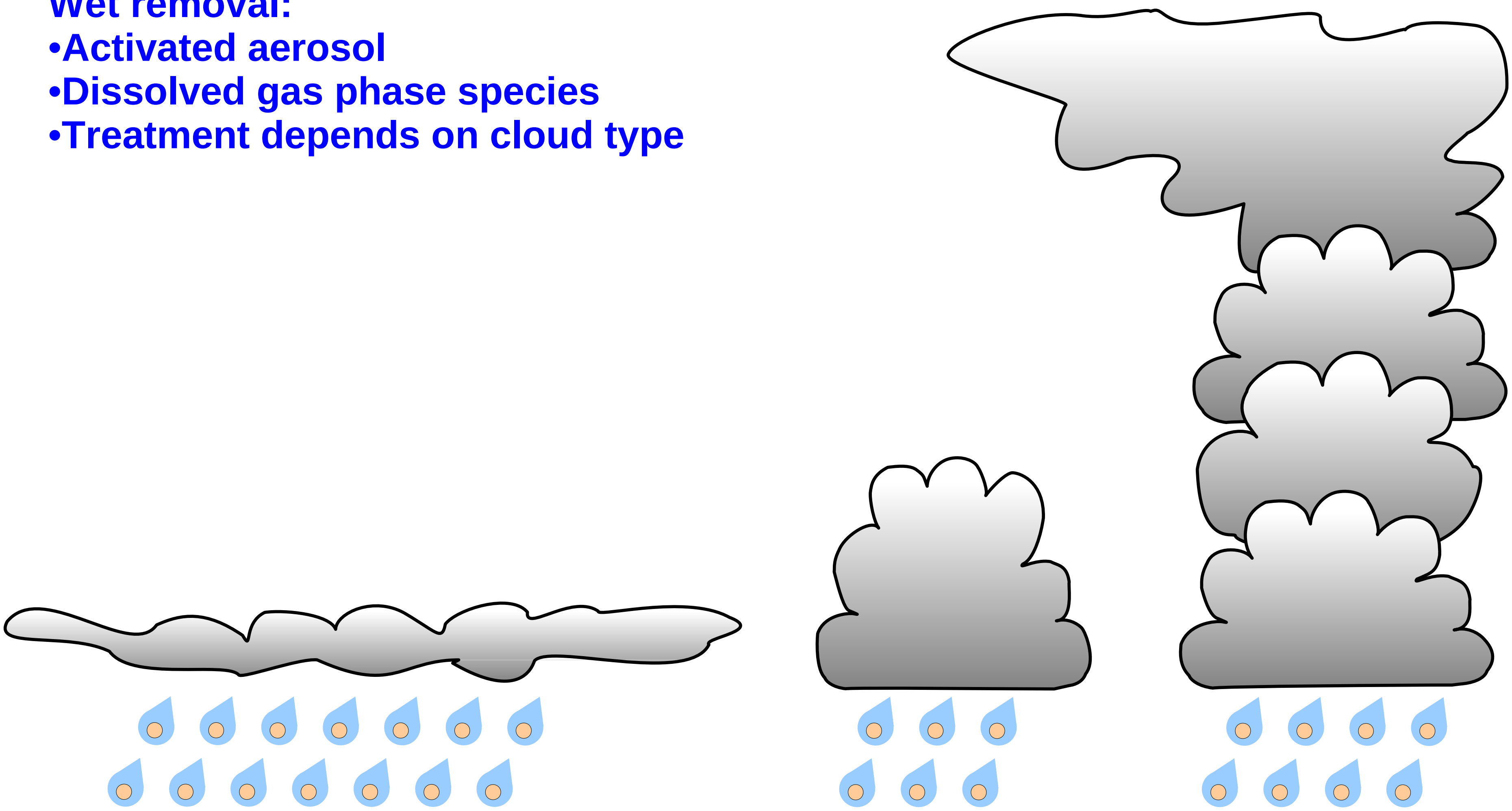
Aqueous chemistry:
•Treatment depends on cloud type



MADE aerosol and wet deposition

CIRES

Wet removal:
- Activated aerosol
- Dissolved gas phase species
- Treatment depends on cloud type

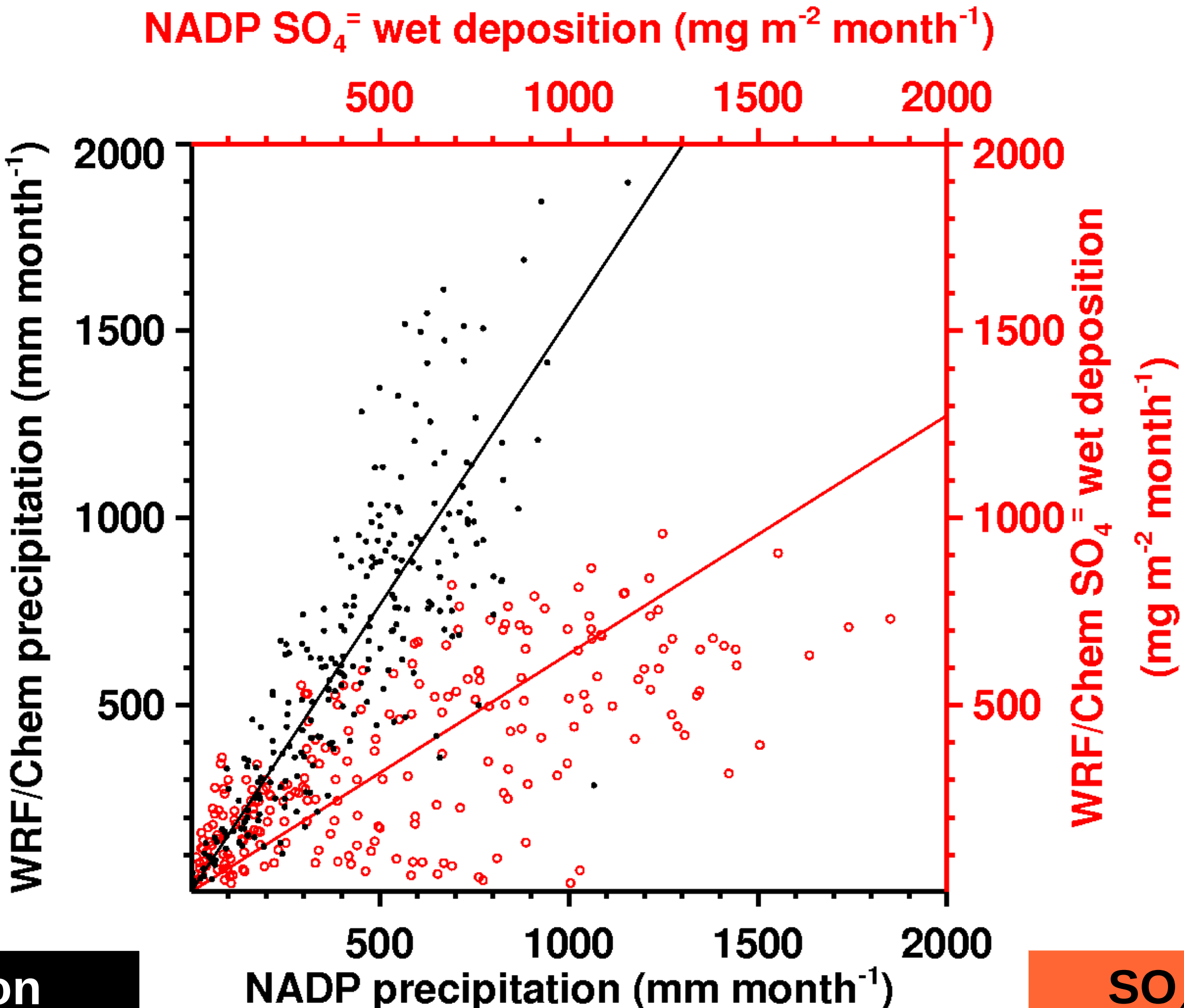


No regeneration, but uptake of H_2SO_4, H_2O_2, SO_2

Regeneration, but no uptake from gas phase

$SO_4^{=}$, NO_3^{-}

MADE aerosol and wet deposition



Precipitation	
r	model/obs.
0.81	1.25

$SO_4^{=}$ wet dep.	
r	model/obs.
0.86	0.53

May-September 2006
(National Atmospheric Deposition Program)

MOSAIC aerosol module

Model for Simulating Aerosol Interactions and Chemistry (Zaveri et al., JGR, 2008)

- **Most modern aerosol scheme in WRF/Chem**
- **4 or 8 aerosol size sections (bins) 39 nm – 10 µm**
- **(Lower bin boundary of 39 nm too large for nucleation)**
- **Interaction with radiation:**
  - **Direct aerosol effect**
  - **Effect on photolysis**
- **Interaction with clouds:**
  - **Aerosol number determines cloud drop number and size**
  - **Radiative response → 1st indirect effect**
  - **Aqueous chemistry**
  - **Wet removal (scavenging)**
  - **only for grid-scale (“dynamically resolved”) clouds**

MOSAIC aerosol module

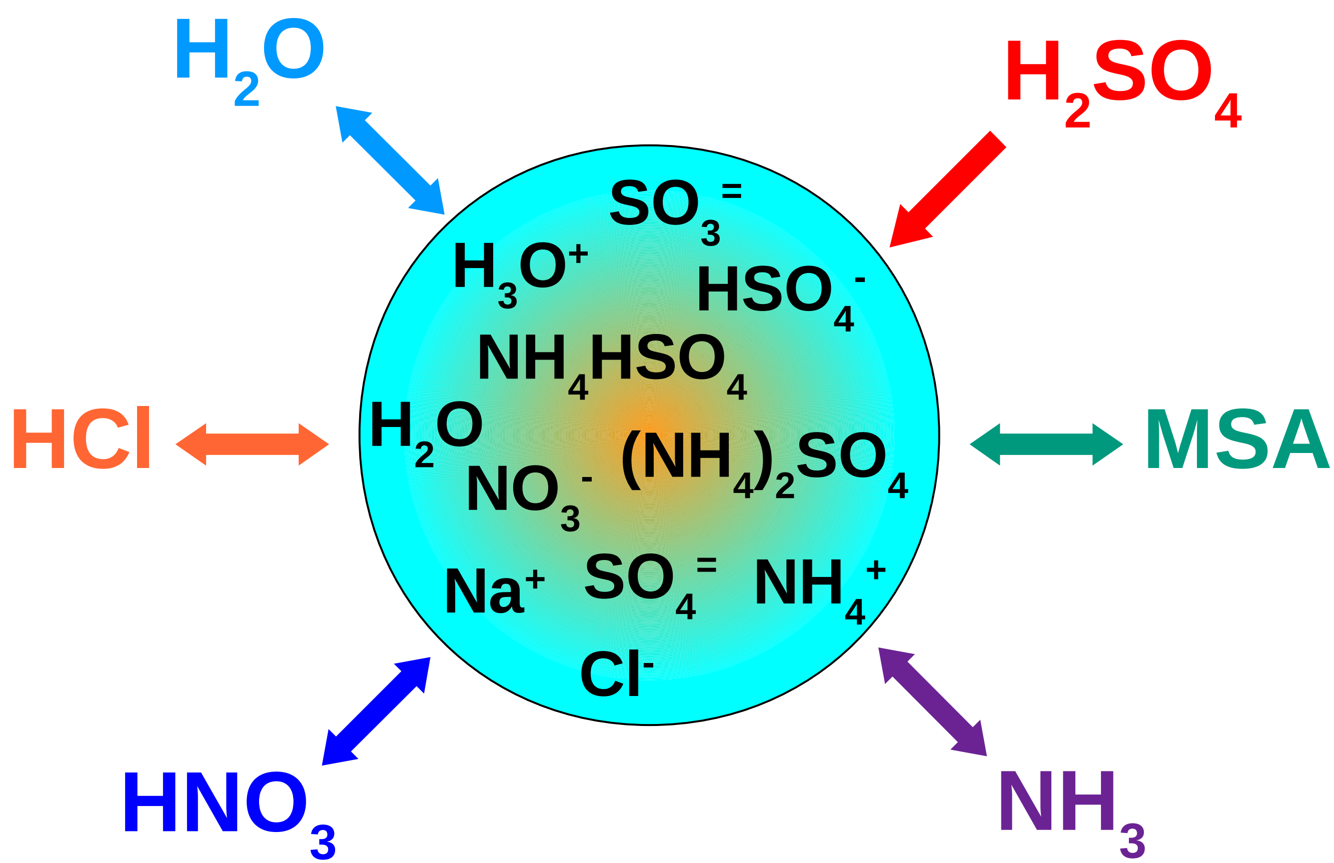
Aerosol composition

- $SO_4^{=}$, NH_4^{+}, NO_3^{-}, H_2O
- NaCl (sea salt)
- CH_3SO_3 (methanesulfonate)
- carbonate (CO_3)
- calcium (Ca)
- black carbon (BC)
- primary organic mass (OC)
- other inorganic mass (minerals, trace metals)

MOSAIC aerosol coupling with chemistry

- **Gas phase chemistry:**
  - **CBMZ (Carbon-Bond Mechanism version Z)**
    - **“Standard” gas phase chemical scheme for MOSAIC**
  - **SAPRC99 (extensive VOC chemistry)**
    - **Works with the VBS SOA scheme**
  - **MOZART (Model for Ozone and Related chem. Tracers)**
    - **Works with the VBS SOA scheme**
- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MTEM (Multicomponent Taylor Expansion Method)**
  - **MESA (Multicomponent Equilibrium Solver for Aerosols)**
  - **VBS (Volatility Basis Set)**
- **Aqueous chemistry:**
  - **CMU aqueous chemistry, only for grid-scale (dynamically resolved) clouds**
  - **Not with KPP versions of gas phase chemistry schemes**

MOSAIC, MTEM, and MESA



MTEM calculates activity coefficients
MESA solves ion-equilibria in the liquid phase
For SOA: VBS (Volatility Basis Set) scheme

MTEM (Multicomponent Taylor Expansion Method), Zaveri et al., JGR 2005a
MESA (Multicomponent Equilibrium Solver for Aerosols), Zaveri et al., JGR 2005b

Volcanic ash/SO_2

- 10 bins for volcanic ash aerosol
- Transport, settling, dry deposition
- Currently no other aerosol
- Single active volcano
- 1535 volcanoes (latitude, longitude, height)
- SO_2 degassing from the volcano on/off

How to tell WRF/Chem what to do

../WRFV3/test/em_real/real.exe

../WRFV3/test/em_real/namelist.input

../WRFV3/test/em_real/...

../WRFV3/test/em_real/...

```
  ...
  ...
 &chem
 chem_opt         = 42
 photdt           = 0.25
 chemdt           = 0
  ...
aerchem_onoff     = 1
  ...
conv_tr_aqchem    = 1
```

MADE/SORGAM CMAQ (EPA) aq. chemistry

Switches all aerosol processes on/off

CMAQ (EPA) aq. chemistry in Cu

Resources

- WRF/Chem User's Guide
  - Model options (namelist parameters)
  - Combinations of physical/chemical schemes
  - ...
- Papers referenced in the WRF/Chem User's Guide
- WRF/Chem source code

- WRF/Chem Help (wrfchemhelp.gsd@noaa.gov)
- Yours truly (jan.kazil@noaa.gov)