Aerosol modeling with WRF/Chem

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WRF/Chem Tutorial, 3 August 2015

(WRF/Chem 3.7)

Part I - Introduction

- **Overview of ...**
  - **Aerosol**
  - **Aerosol processes and life cycle**
  - **Model treatment of aerosol**
  - **WRF/Chem aerosol schemes**

Part II – The details

- **Representing the aerosol size distribution**
- **Walk through the WRF/Chem aerosol schemes**
  - **How they work and what they do**
  - **Coupling to other processes**
    - **Gas phase chemistry**
    - **Aqueous chemistry**
    - **...**
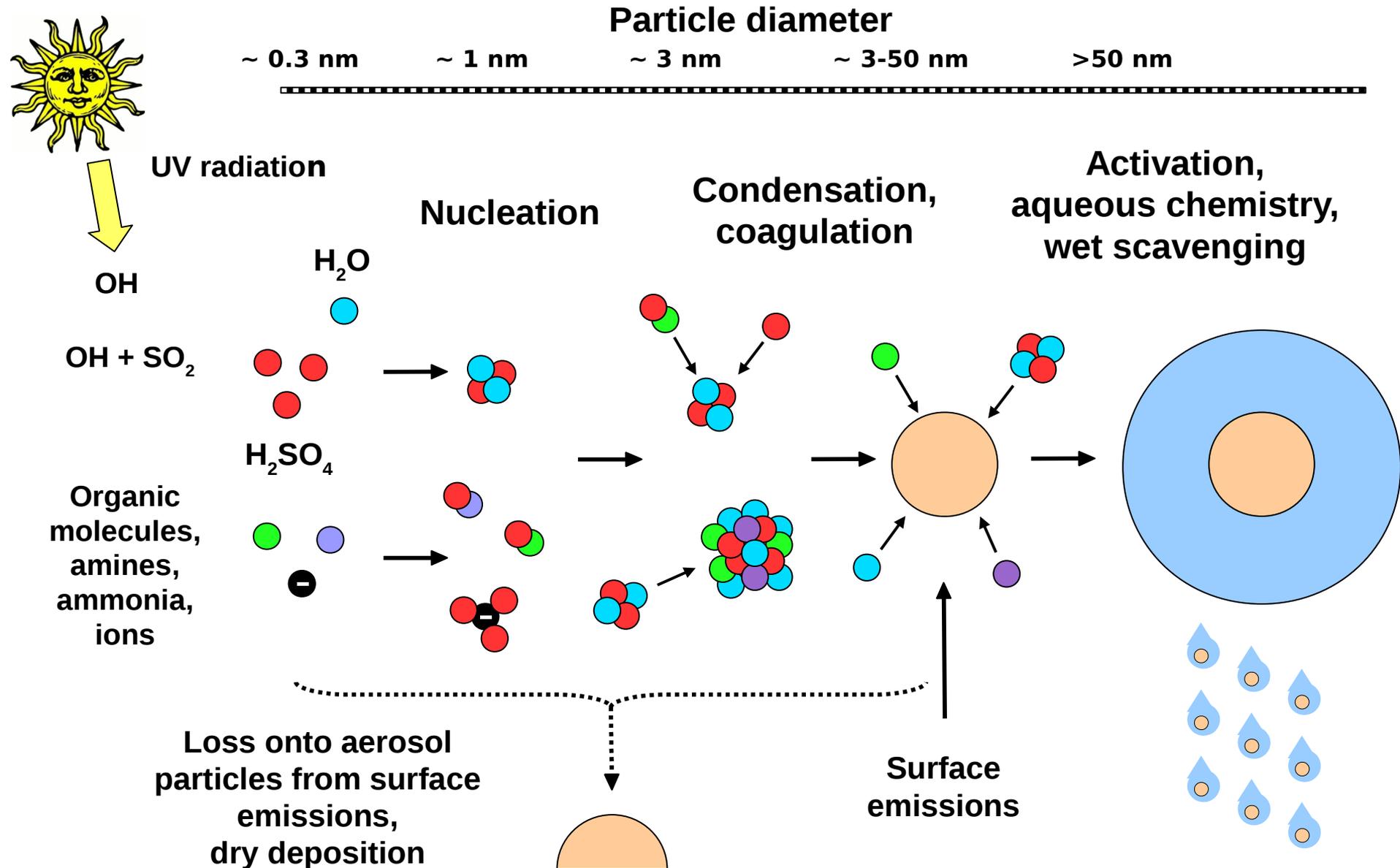- **Hint on how to tell WRF/Chem what to do**
- **Resources**
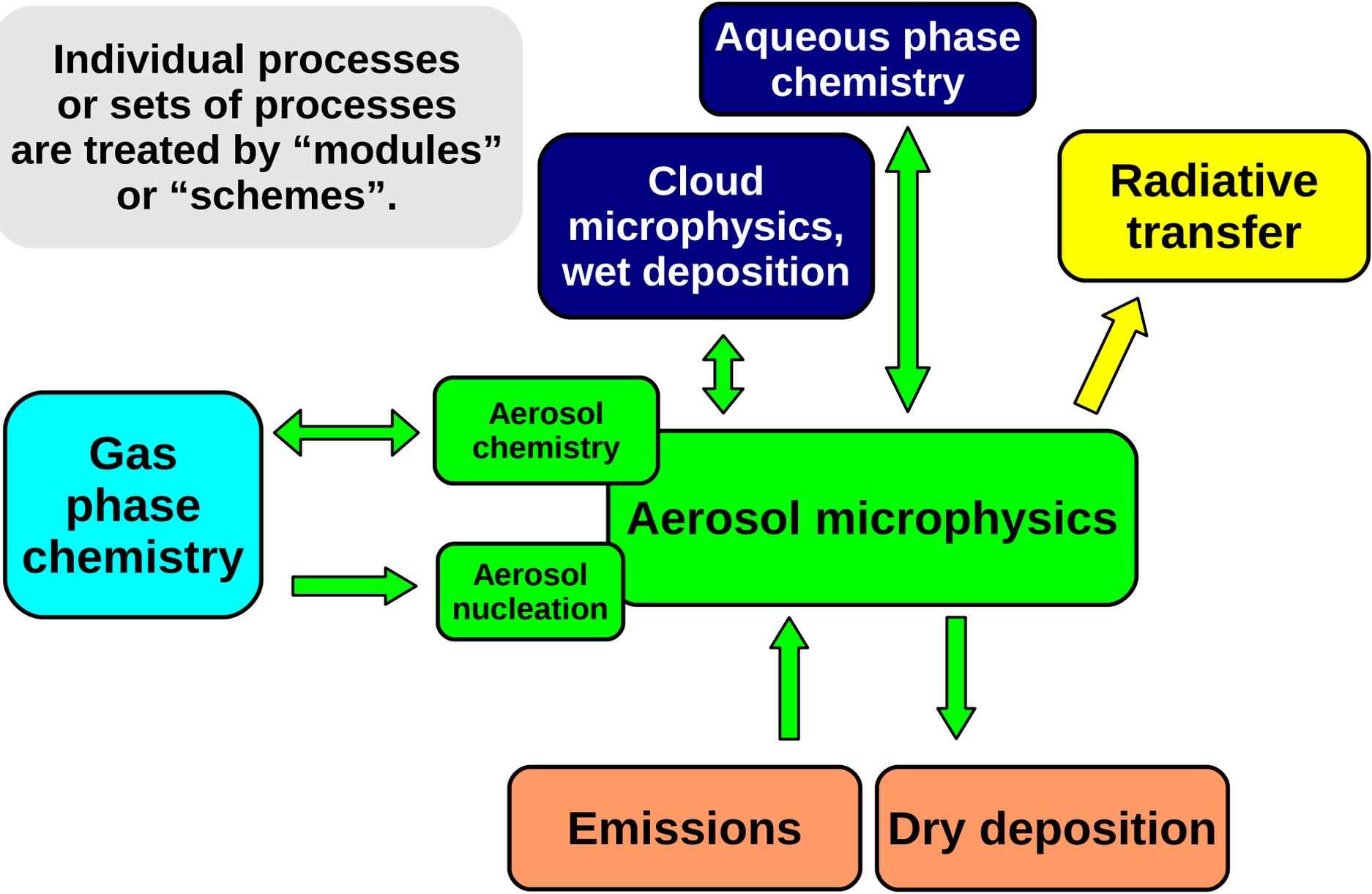
Part I – Introduction

Aerosol

Aerosol life cycle and processes

Particle diameter

~ 0.3 nm   ~ 1 nm   ~ 3 nm   ~ 3-50 nm   >50 nm

UV radiation

OH

OH + SO$_2$

H$_2$SO$_4$

Organic molecules, amines, ammonia, ions

H$_2$O

Nucleation

Condensation, coagulation

Activation, aqueous chemistry, wet scavenging

Loss onto aerosol particles from surface emissions, dry deposition

Surface emissions

Model treatment of aerosol

Individual processes or sets of processes are treated by "modules" or "schemes".

Aqueous phase chemistry

Cloud microphysics, wet deposition

Radiative transfer

Gas phase chemistry

Aerosol chemistry

Aerosol nucleation

Aerosol microphysics

Emissions

Dry deposition

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)
- **Modal Aerosol Dynamics Model for Europe – MADE**
  - 3 log-normal modes
  - Inorganic, organic aerosol, SOA
- **Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)**
  - Sectional aerosol scheme, 4 or 8 bins
  - Inorganic, organic aerosol, SOA
- **MAM – Modal Aerosol Model from CAM5**
  - 3 or 7 log-normal modes
  - Inorganic, organic aerosol, SOA, sea salt, BC, mineral dust
- **Simple sectional (bin) scheme for volcanic ash aerosol**

Part II – The details

Bulk aerosol schemes

- **Only total mass of aerosol compounds is known**

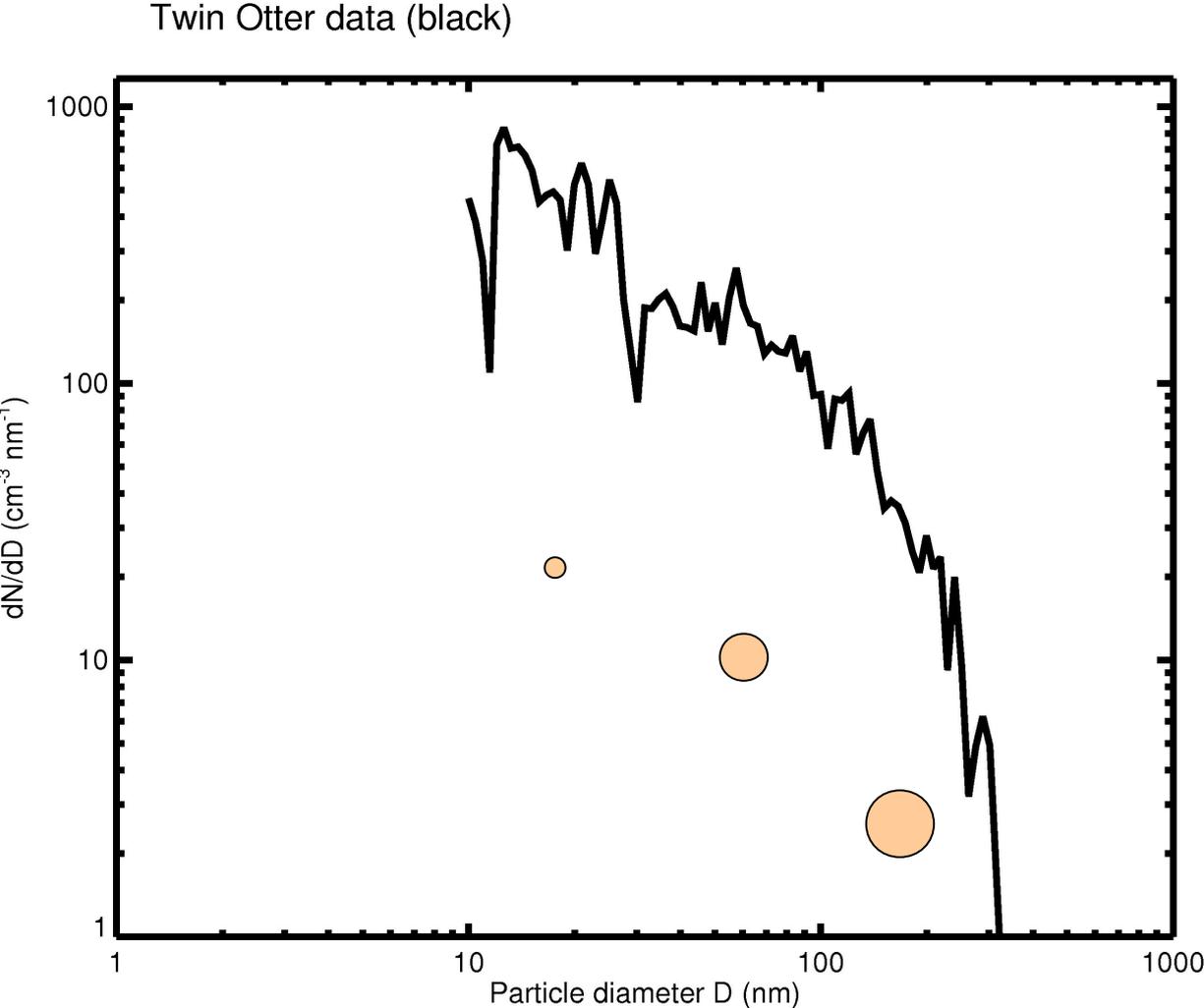NH_3 H_2SO_4 HNO_3
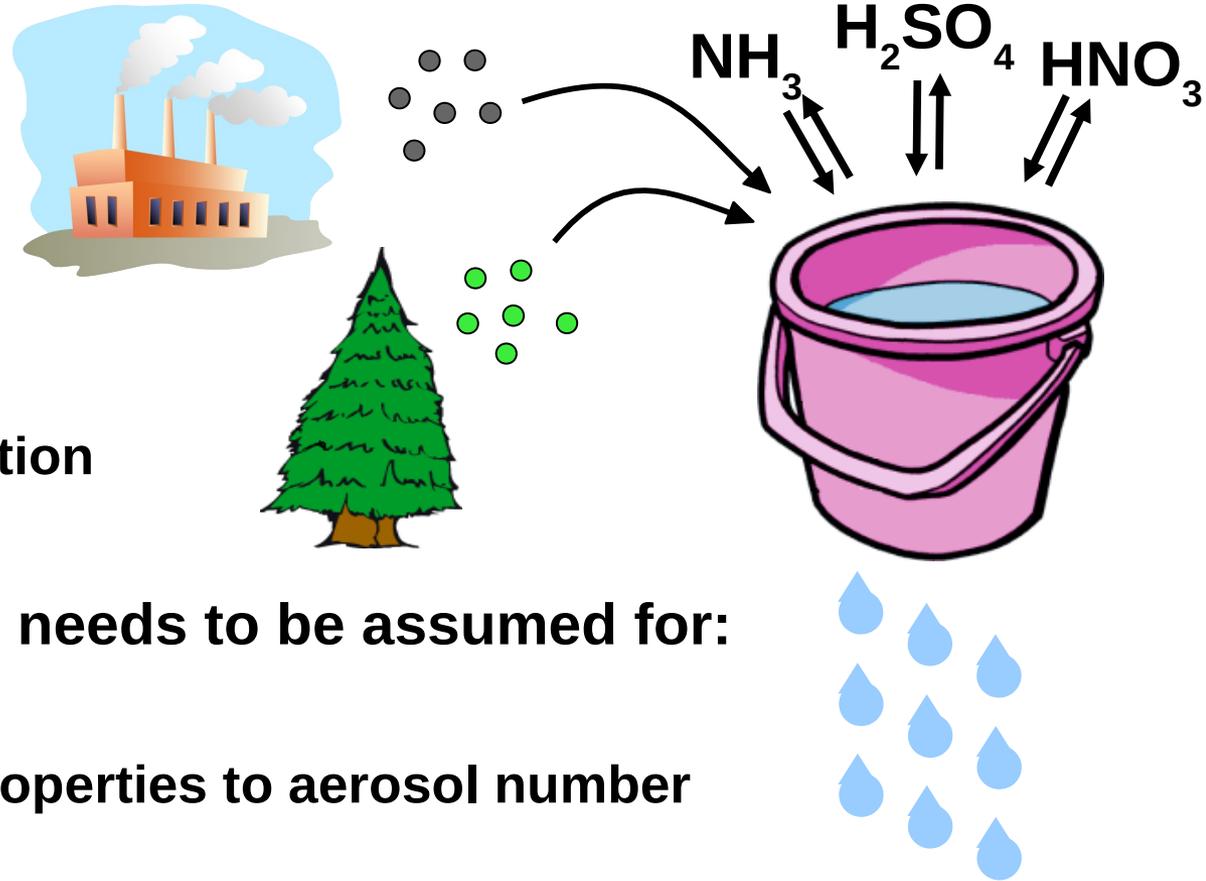
- **No information on**
  - **Particle number**
  - **Aerosol size distribution**

Aerosol size distribution needs to be assumed for:
  - **radiative transfer**
  - **response of cloud properties to aerosol number**

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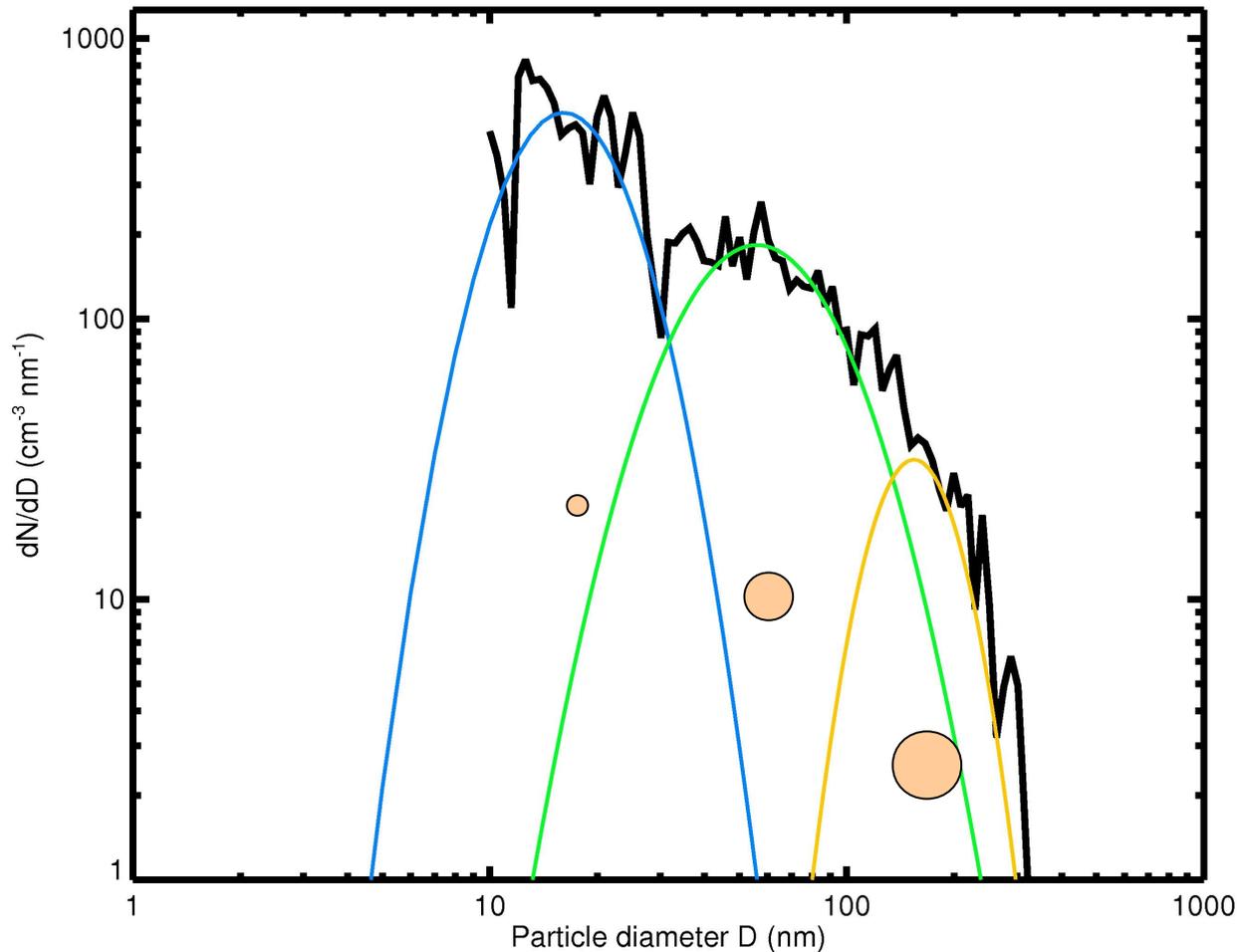- **Useful when focus is on complex gas phase chemistry**

→ **GOCART (+ size resolved dust and sea salt)**

Modal aerosol schemes

Twin Otter data (black)

Modal aerosol schemes

Twin Otter data (black)

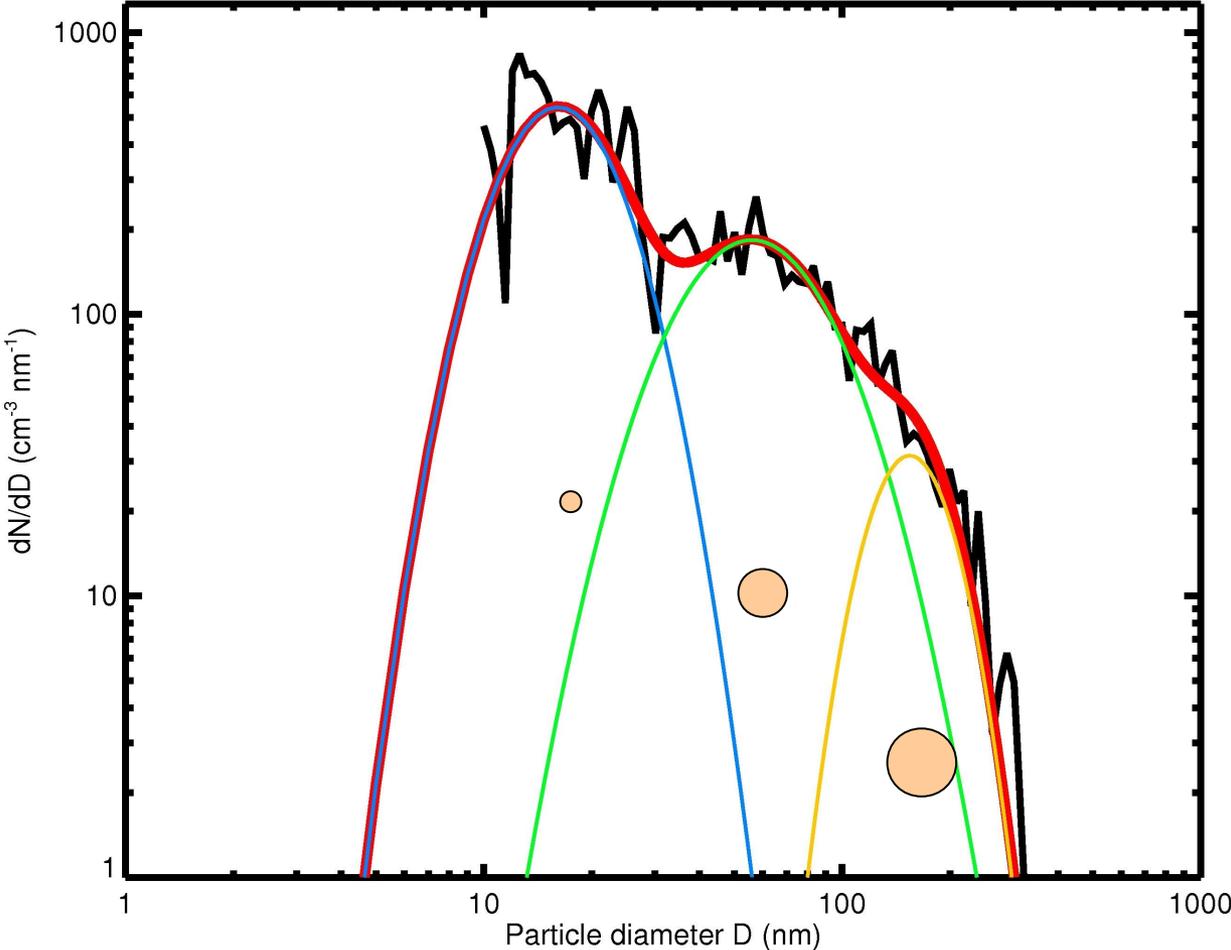$$\frac{dN}{dD} = \frac{N}{\sqrt{2\pi}\ln(\sigma)D} e^{-\frac{1}{2}\left[\frac{\ln(D/\mu)}{\ln(\sigma)}\right]^2}$$

$\dfrac{dN}{dD} \rightarrow$ *N = 8195 cm⁻³*
$\mu = 18.22$ nm
$\sigma = 1.42$

$\dfrac{dN}{dD} \rightarrow$ *N = 12732 cm⁻³*
$\mu = 68.44$ nm
$\sigma = 1.57$

$\dfrac{dN}{dD} \rightarrow$ *N = 3140 cm⁻³*
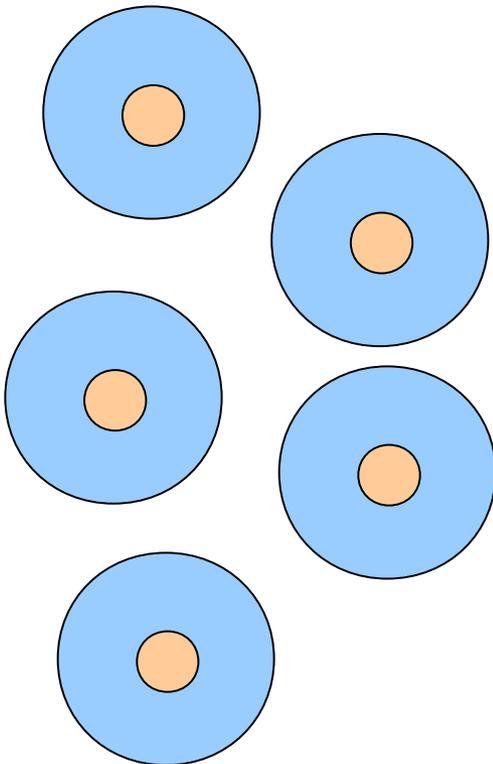$\mu = 164.41$ nm
$\sigma = 1.28$
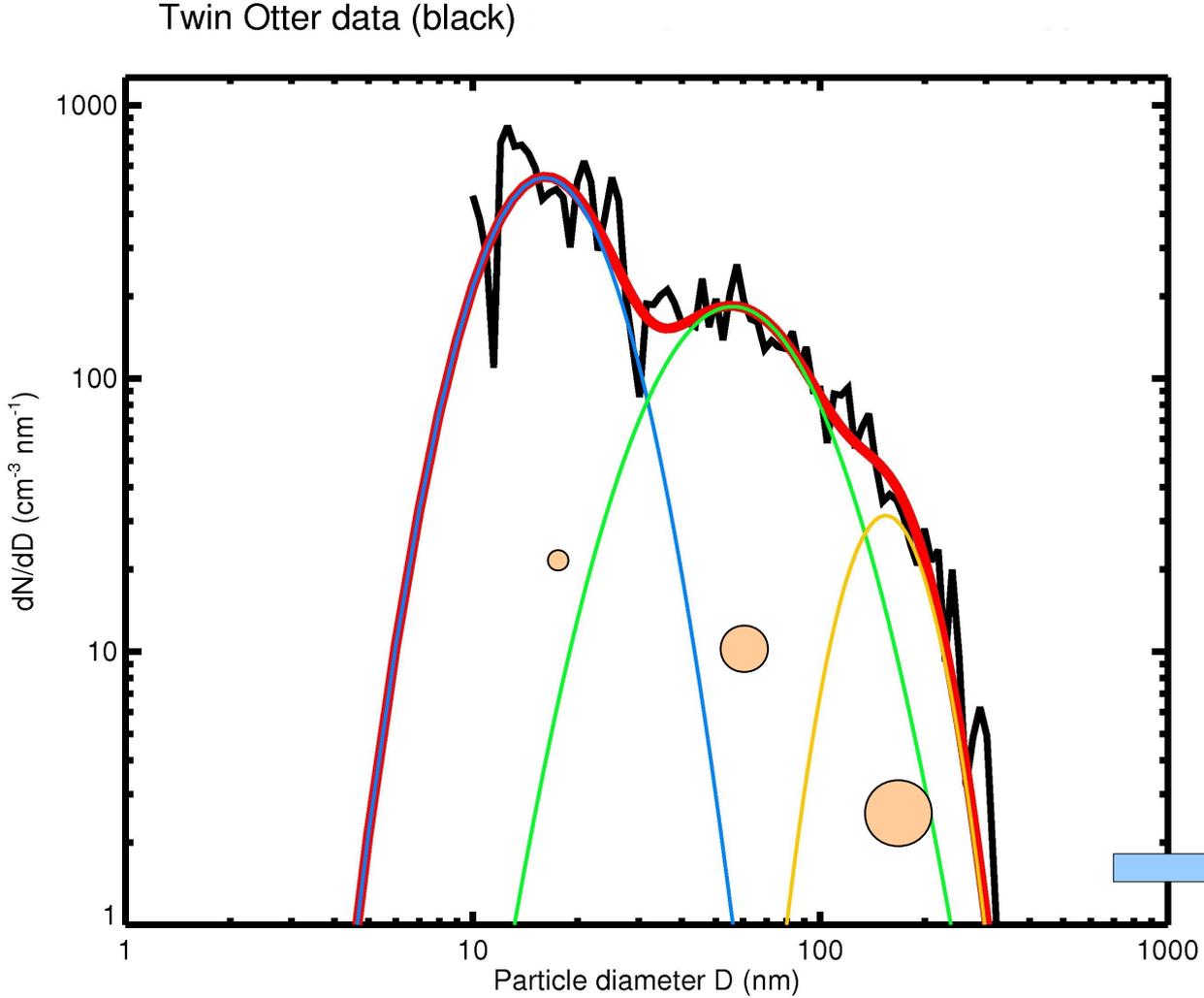
Modal aerosol schemes

Twin Otter data (black)

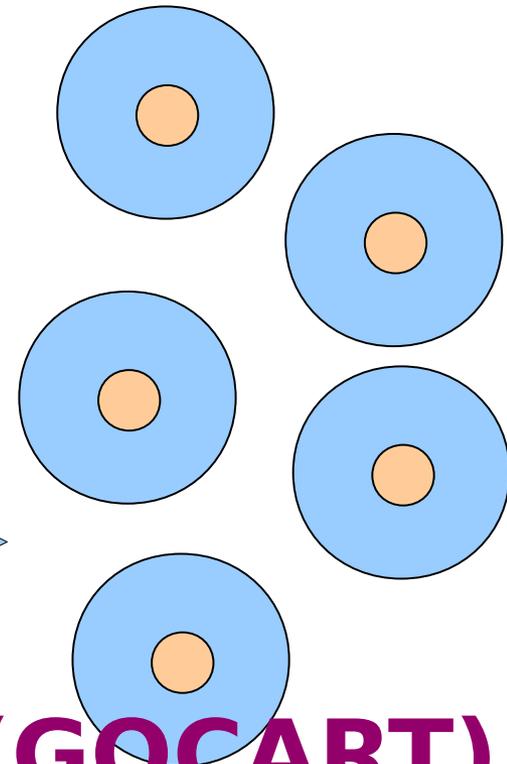$$\frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD}$$
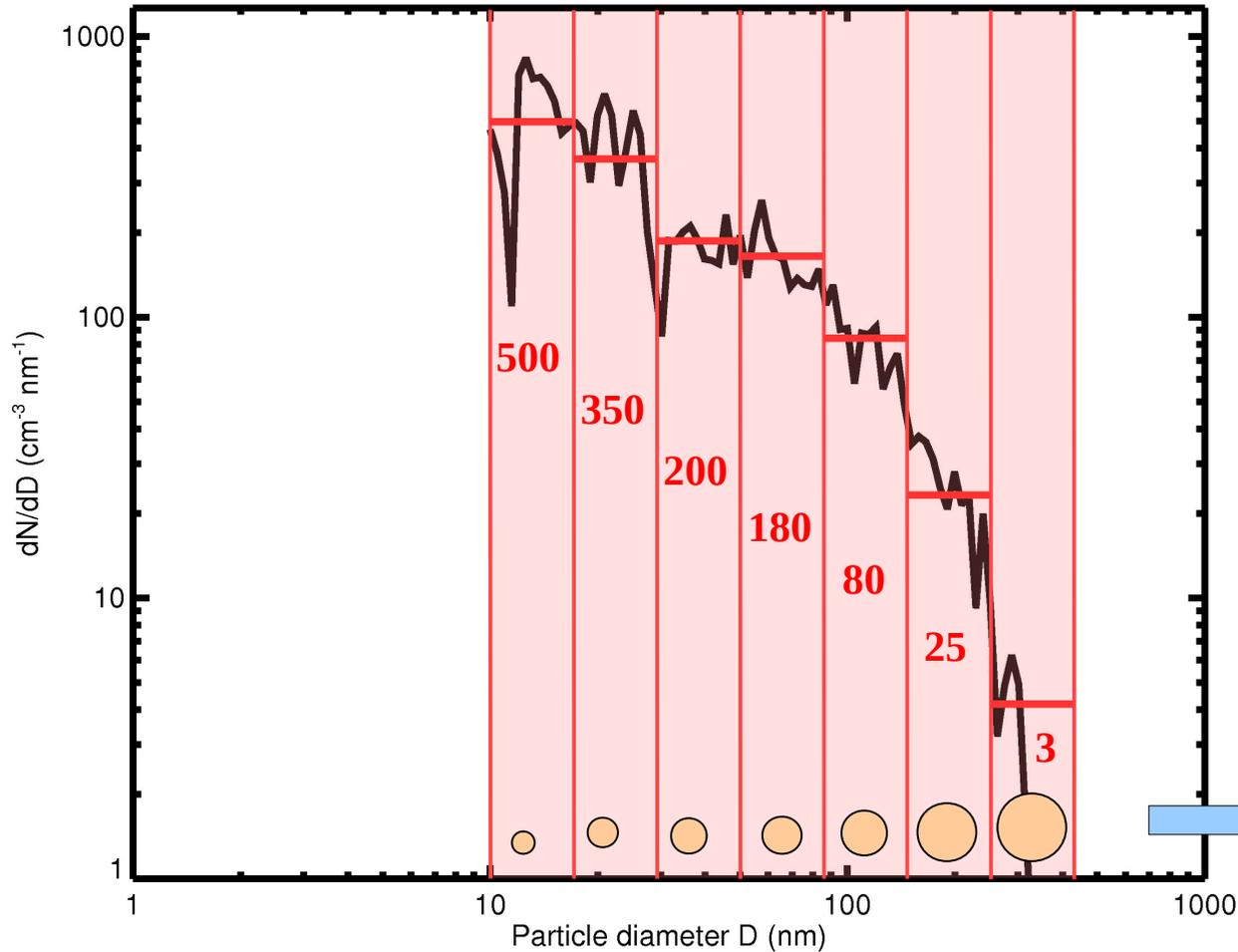
Modal aerosol schemes

Twin Otter data (black)

→ **MADE and MAM**

Sectional aerosol schemes

Twin Otter data (black)

→ **MOSAIC, volcanic ash, (GOCART)**

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 $\rightarrow$ SO$_2$ + ...**

- **DMS + OH $\rightarrow$ MSA + ...**

- **DMS + NO$_3$ $\rightarrow$ SO$_2$ + ...**

- **SO$_2$ + OH $\rightarrow$ 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 secondary organic aerosol (SOA)**

MADE aerosol module

Modal **A**erosol **D**ynamics Model for **E**urope
(Ackermann et al., Atm. Env., 1998)

- **3 log-normal aerosol modes: Aitken, accumulation, coarse**
- **Mode width σ is fixed**
- **Aerosol number and mass variable**
- **Interaction with radiation:**
  - ■ **Direct aerosol effect**
  - ■ **Effect on photolysis**
- **Interaction with clouds:**
  - ■ **Aerosol number determines cloud drop number and size**
  - ■ **Radiative response → 1st indirect aerosol effect**
    - ◆ **only for resolved clouds (Sc)**
  - ■ **Aqueous chemistry**
  - ■ **Wet removal (scavenging)**

MADE aerosol module

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

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** (**R**egional **A**cid **D**eposition **M**odel version **2**)
  - **RACM** (**R**egional **A**tmospheric **C**hemistry **M**echanism)
  - **RACM** NOAA/ESRL version
  - **CBMZ** (**C**arbon-**B**ond **M**echanism version **Z**)
- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MARS** (**M**odel for an **A**erosol **R**eacting **S**ystem)
  - **SORGAM** (**S**econdary **O**rganic **A**erosol **M**odel)
  - **VBS** (**V**olatility **B**asis **S**et)
- **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

H_2O H_2SO_4

$SO_3^=$

H_3O^+ HSO_4^-

NH_4HSO_4

H_2O $(NH_4)_2SO_4$

$SO_4^=$

NO_3^- NaCl NH_4^+

SOA

HNO_3 NH_3
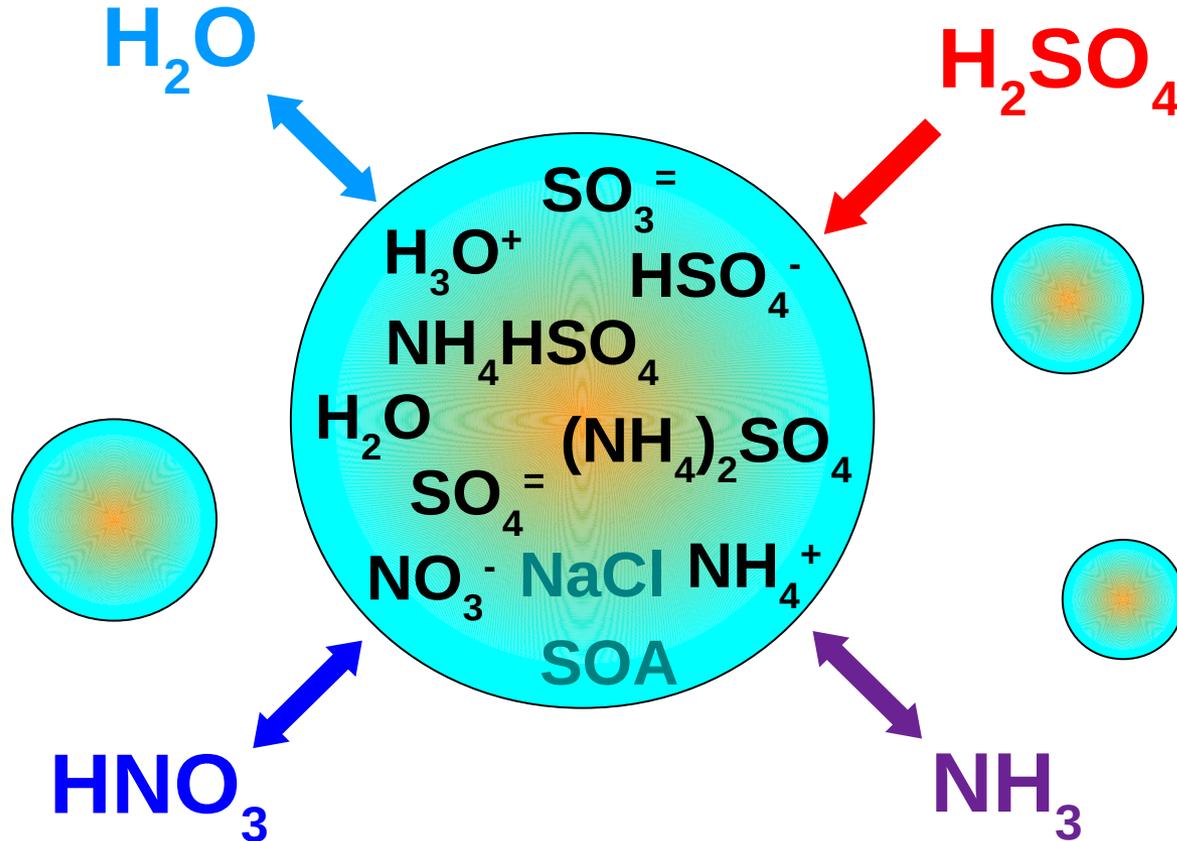
MARS (**M**odel for an **A**erosol **R**eacting **S**ystem),
Saxena et al., Atm. Env., 1986
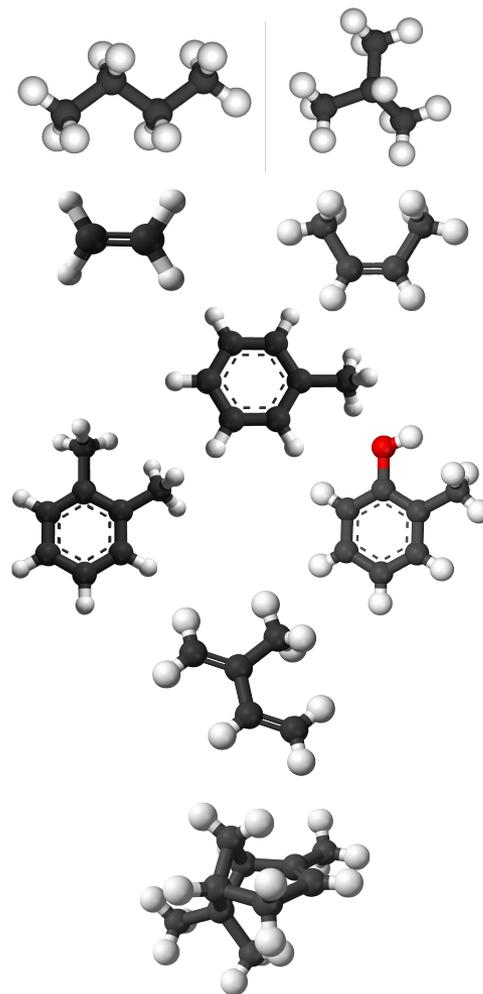
MADE/SORGAM

Gas phase scheme (RADM2, RACM)
Alkanes
Alkenes
Toluene
Xylene, cresole, ...
Isoprene
Sesquiterpene
Alpha-pinene, limonene

$\longrightarrow$ **OH, O_3, NO_3**

Semi-volatile organics
$X_1, X_2, X_3, X_4, X_5, ..., X_n$

SOA

H_3O^+ HSO_4^-
NH_4HSO_4
H_2O $(NH_4)_2SO_4$
$SO_4^=$
NO_3^- $SO_3^=$ NH_4^+
$NaCl$

SORGAM (**S**econdary **Org**anic **A**erosol **M**odel), Schell et al., JGR, 2001

MADE/VBS (Volatility Basis Set)

Gas phase scheme (RACM)

Alkanes

Alkenes

Toluene

Xylene, cresole, ...

Isoprene

Sesquiterpene

Alpha-pinene, limonene

OH, O_3, NO_3

Products

Volatile

Semi-volatile

Volatility

H_2O

NO_3^-

H_3O^+

$SO_4^=$

HSO_4^-

$SO_3^=$

NH_4^+

$NaCl$
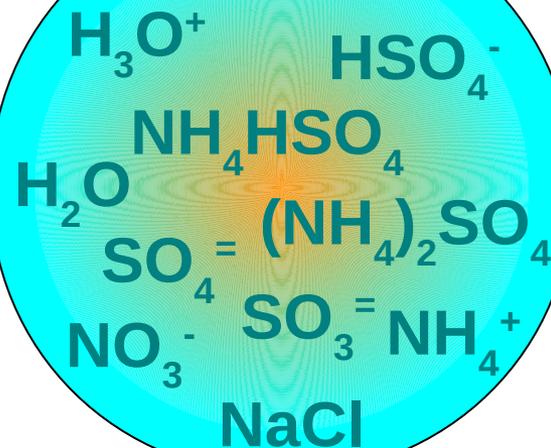
Ahmadov et al., JGR 2012
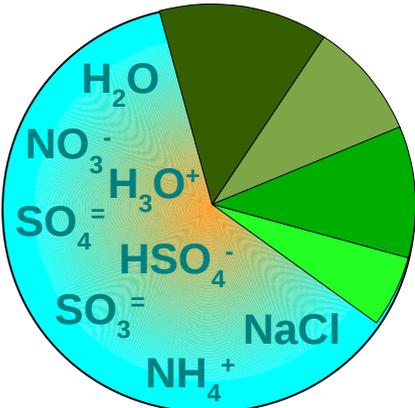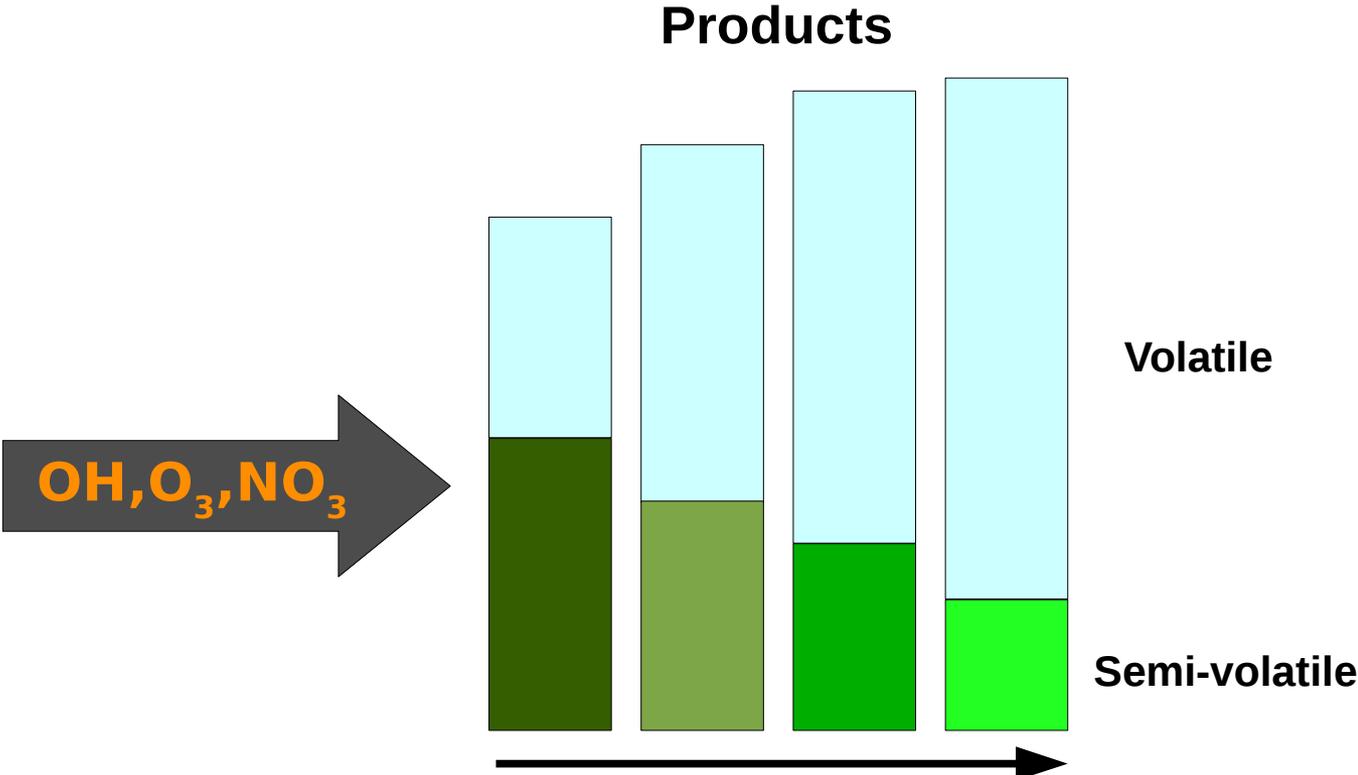
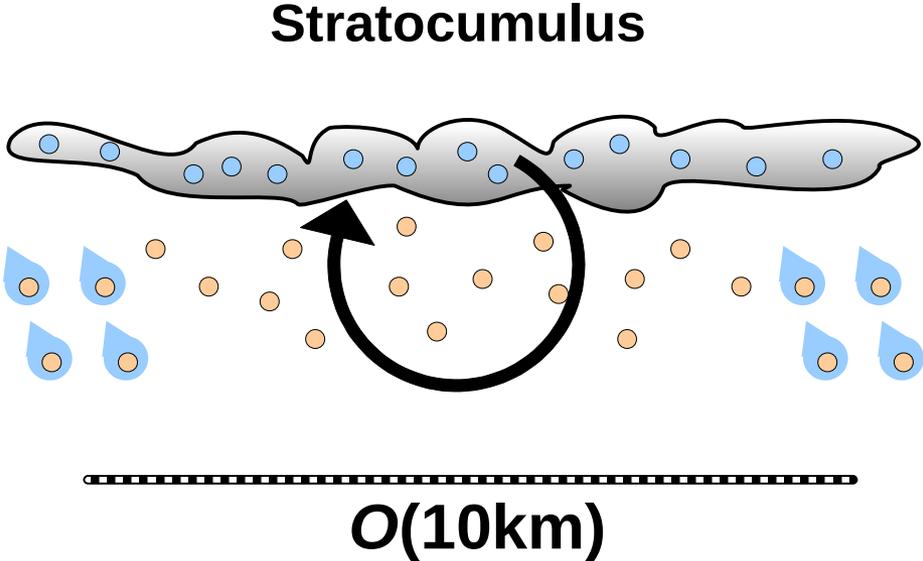# MADE/VBS (Volatility Basis Set)
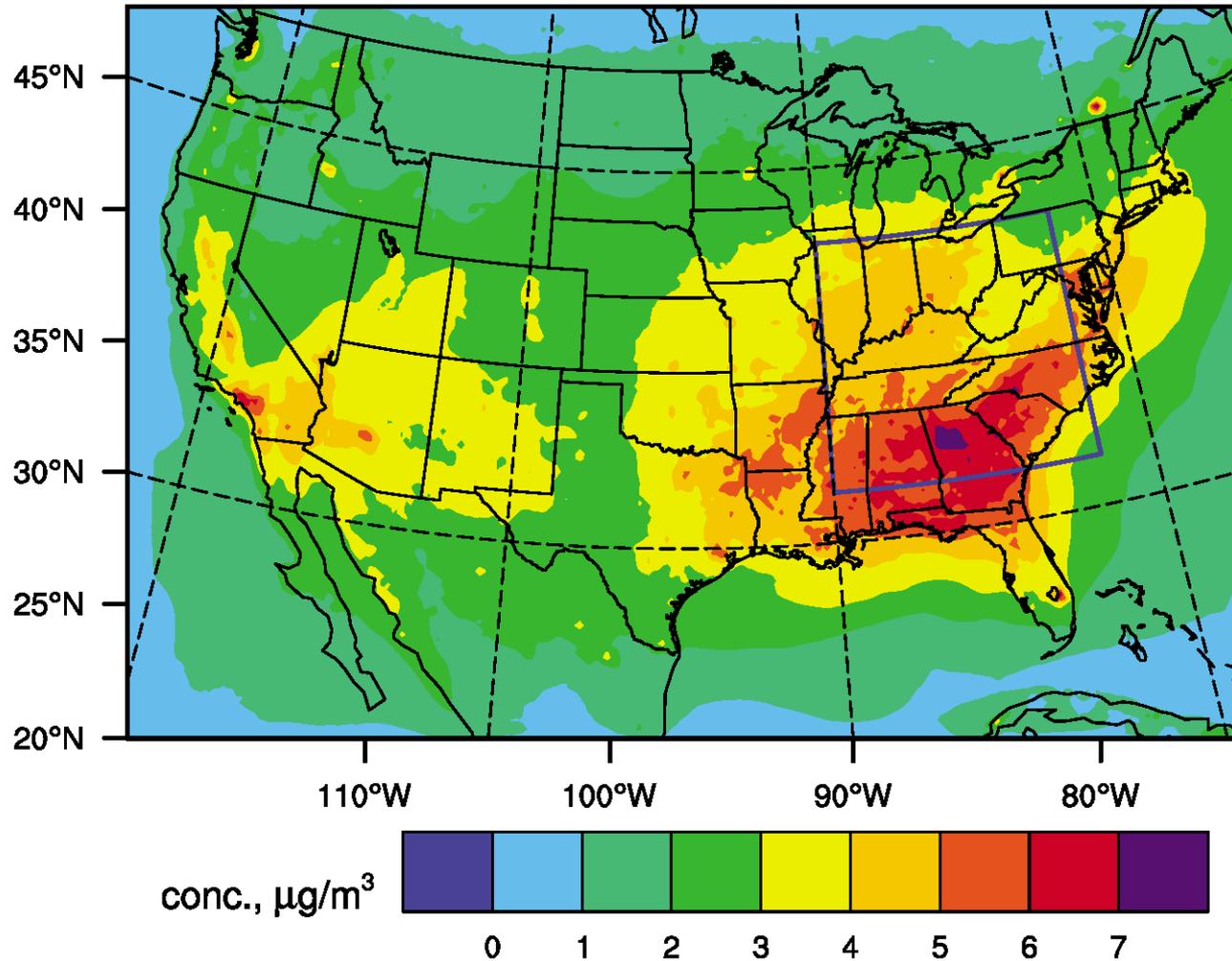
Organic aerosol mass in the surface layer (August - September 2006)

Ahmadov et al., JGR 2012

How clouds are simulated in WRF(Chem)

Details of aqueous chemistry depend on cloud type

Cumulonimbus

Cumulus

Stratocumulus

O(10km)

O(100m)

O(1km)
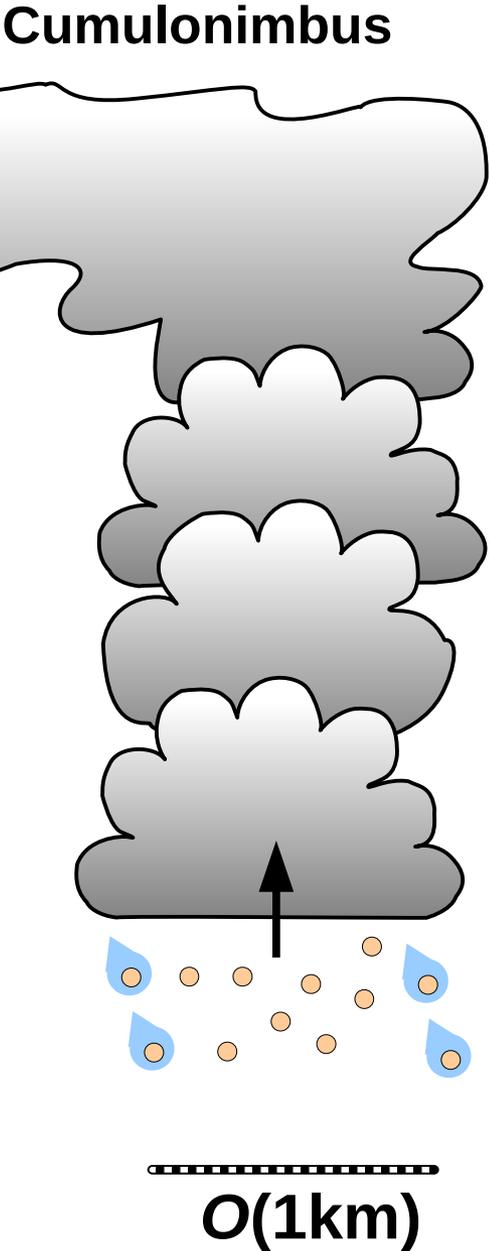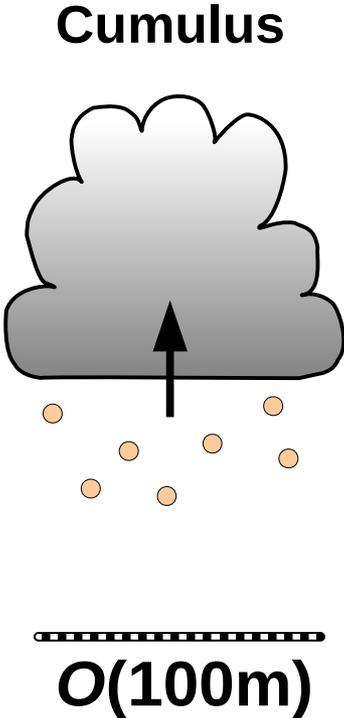
MADE and aqueous chemistry

- **CMU aqueous chemistry**
  - **(Fahey & Pandis, Atm. Env., 2001)**
  - **Slow, only for resolved clouds (Sc)**
- **CMAQ aqueous chemistry**
  - **(Walcek & Taylor, JAS, 1986)**
  - **Relatively fast**
  - **In both resolved (Sc) and parameterized (Cu) clouds**
  - **Can generate wet deposition of $SO_4^=$ and NO_3^-**
  - **In file "registry.chem", set "h" (history) flag of**
    - **wd_so4_sc, wd_so4_cu**
    - **wd_no3_sc, wd_no3_cu**
   - **Recompile**

MADE and aqueous chemistry

CHEM_OPT	Stratocumulus	Cumulus
1		AQCHEM **
11	CMU *	AQCHEM **
12	CMU *	AQCHEM **
105		AQCHEM **
106		AQCHEM **
107		AQCHEM **
108		AQCHEM **
41	AQCHEM *	AQCHEM **
42	AQCHEM *	AQCHEM **
42	AQCHEM *	AQCHEM **

```
 *  cloud_chem_onoff = 1 : Aqueous chemistry in Sc clouds on
** conv_tr_aqchem   = 1 : Aqueous chemistry in Cu clouds on
** wetscav_onoff    = 1 : Wet scavenging on in Sc clouds
** conv_tr_wetscav  = 1 : Wet scavenging in Cu clouds
```
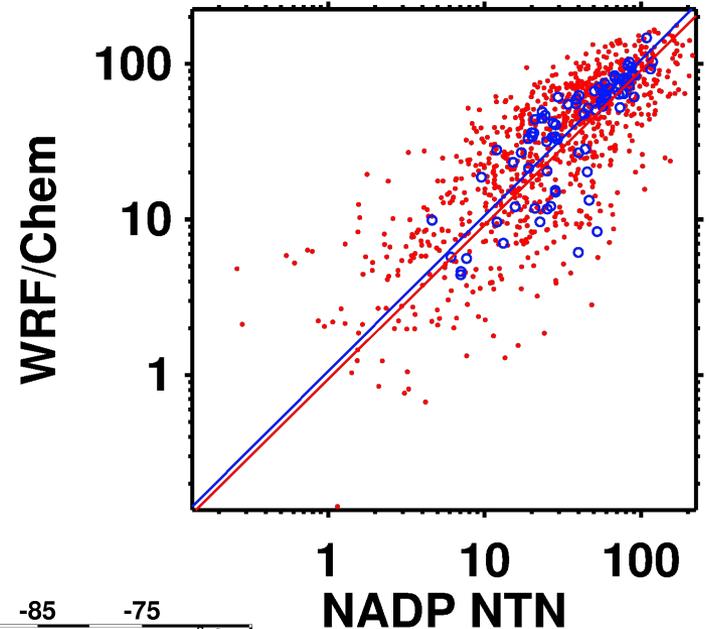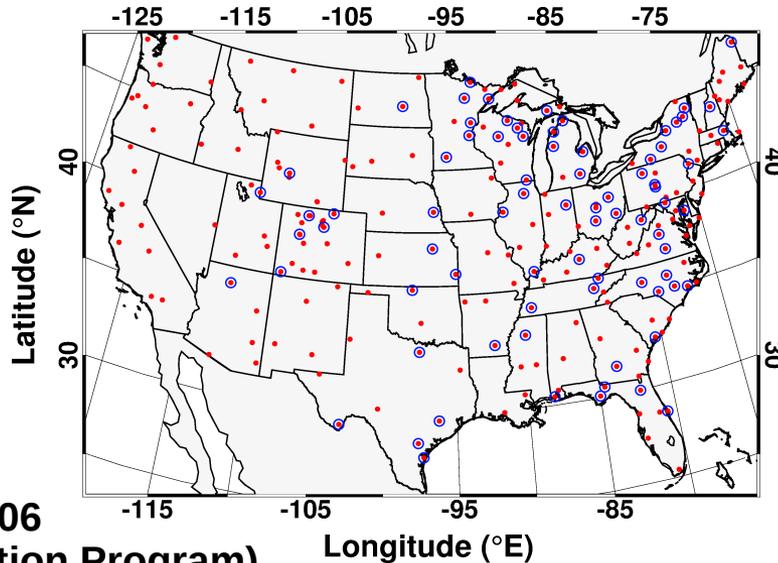
Wet deposition example

Rainfall (mm d^{-1})
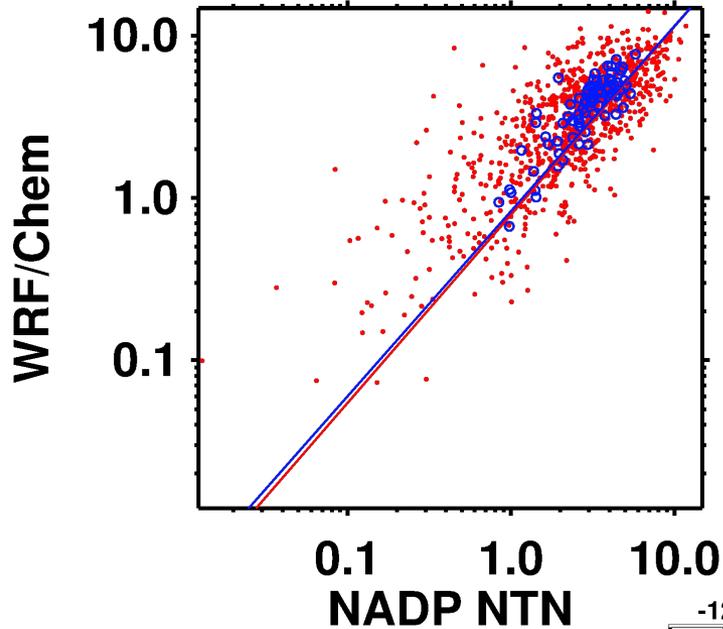
SO$_4^=$ wet deposition (mol km^{-2} d^{-1})

Rainfall	
r	model/obs.
0.80	1.24

SO$_4^=$ wet dep.	
r	model/obs.
0.89	1.04

**May-September 2006
(National Atmospheric Deposition Program)**

MOSAIC aerosol module

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

- **Modern aerosol scheme in WRF/Chem**
- **4 or 8 aerosol size sections (bins) 39 nm – 10 μm**
- **Interaction with radiation:**
  - **Direct aerosol effect**
  - **Effect on photolysis**
- **Interaction with clouds:**
  - **Aerosol number determines cloud drop number and size**
  - **Radiative response → 1st indirect aerosol effect**
  - **Aqueous chemistry**
  - **Wet removal (scavenging)**

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** (**C**arbon-**B**ond **M**echanism version **Z**)
    - ◆ "Standard" gas phase chemical scheme for MOSAIC
  - **SAPRC99** (extensive VOC chemistry)
    - ◆ Works with the VBS SOA scheme
  - **MOZART** (**M**odel for **Oz**one and **R**elated chem. **T**racers)
    - ◆ Works with the VBS SOA scheme
- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MTEM** (**M**ulticomponent **T**aylor **E**xpansion **M**ethod)
  - **MESA** (**M**ulticomponent **E**quilibrium **S**olver for **A**erosols)
  - **VBS** (**V**olatility **B**asis **S**et)
- **Aqueous chemistry:**
  - **CMU aqueous chemistry, only for resolved clouds (Sc)**

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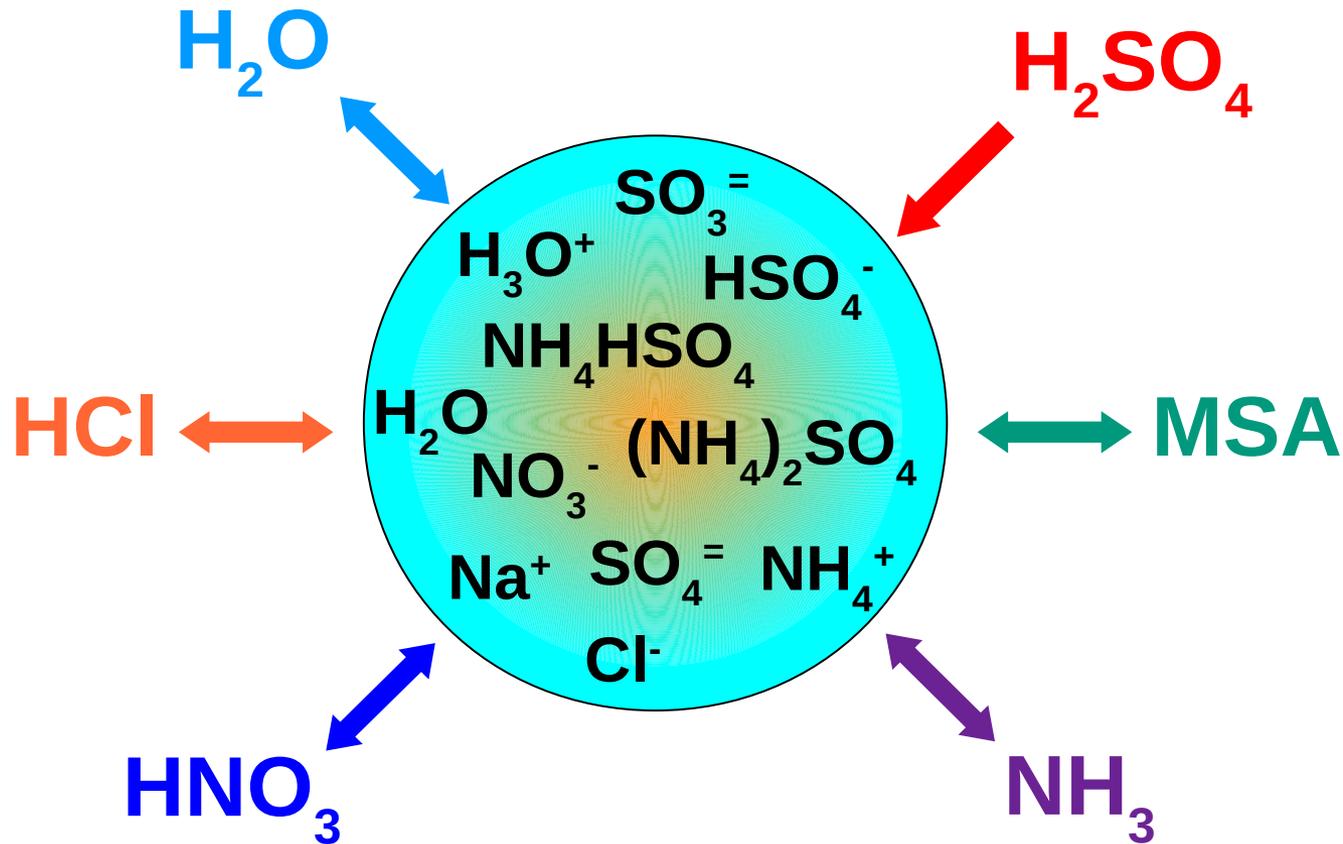
MTEM calculates activity coefficients
MESA solves ion-equilibria in the liquid phase
For SOA: VBS (Volatility Basis Set) scheme

MTEM (**M**ulticomponent **T**aylor **E**xpansion **M**ethod), Zaveri et al., JGR 2005a
MESA (**M**ulticomponent **E**quilibrium **S**olver for **A**erosols), Zaveri et al., JGR 2005b

MAM aerosol module

Modal Aerosol Model from CAM5

- **3 or 7 log-normal aerosol modes: MAM3 and MAM7**
- **Mode width σ is fixed**
- **Aerosol number and mass variable**
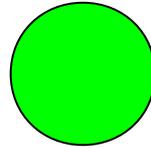- **Liu et al., Geosci. Model Dev., 5, 709-739, 2012**

MAM 3

Aitken mode **Accumulation mode** **Coarse mode**

Coagulation, condensation

●**Sulfate ($SO_4^=$)**
●**SOA**
●**Sea salt**

●**Sulfate ($SO_4^=$)**
●**SOA**
●**Primary organic matter**
●**Black carbon**
●**Mineral dust**
●**Sea salt**
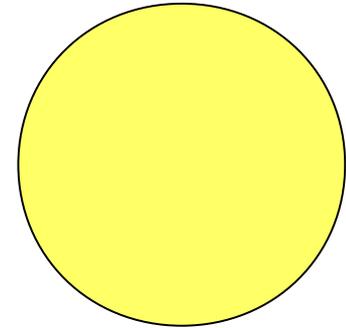
●**Sulfate ($SO_4^=$)**
●**Mineral dust**
●**Sea salt**

15 – 53 nm   **58 – 270 nm**   **0.8 – 3.65 µm**

Dry particle diameter

MAM 7

Fine sea salt, SO$_4^=$

Aitken mode

Accumulation mode

Coarse sea salt, SO$_4^=$

Coagulation,
condensation

- Sulfate (SO$_4^=$)
- SOA
- Sea salt

- Sulfate (SO$_4^=$)
- SOA
- Primary organic matter
- Sea salt
- Black carbon

Fine dust, SO$_4^=$

Primary carbon

Coarse dust, SO$_4^=$

- Primary organic matter
- Black carbon
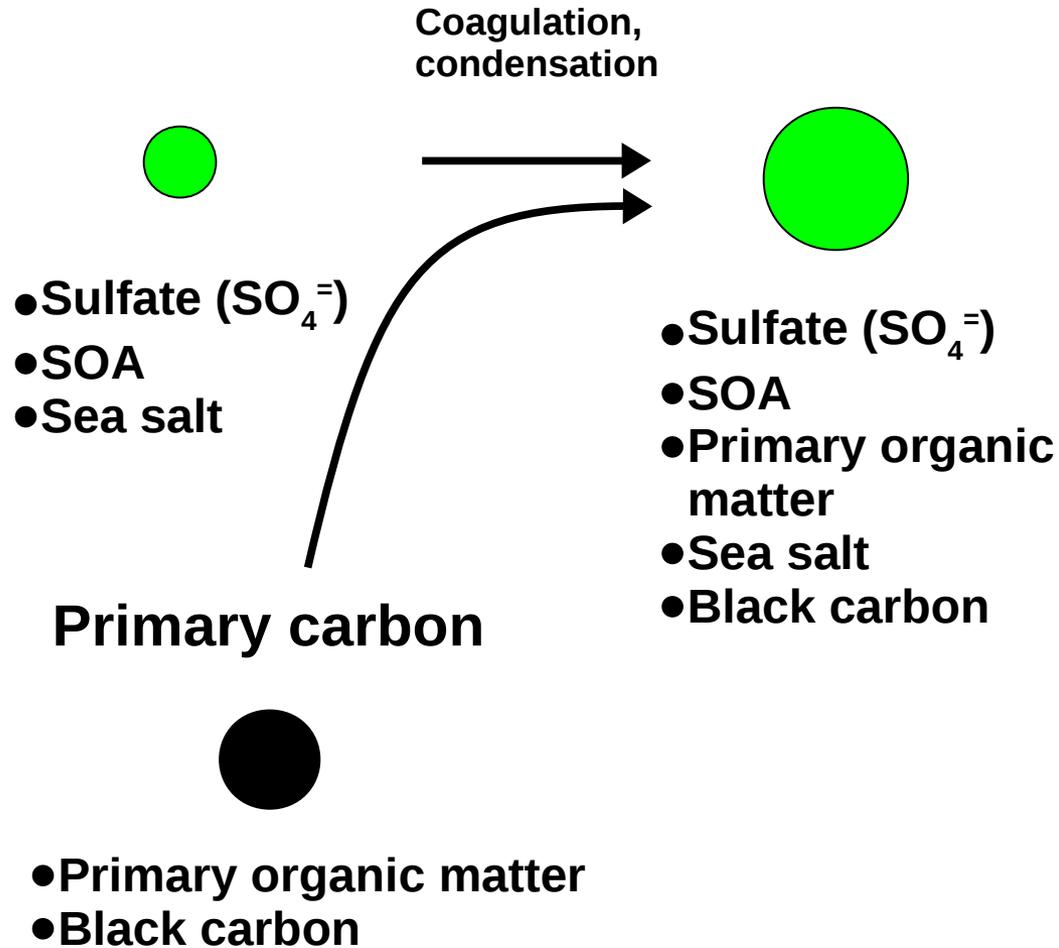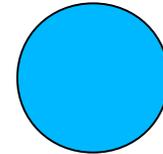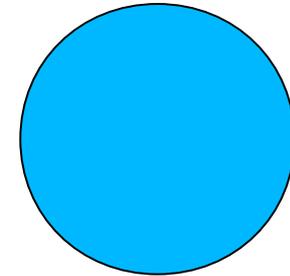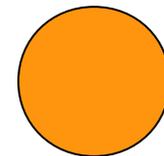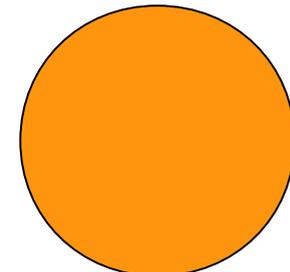
MAM aerosol module

- **Currently only one gas phase chemistry scheme**
  - **CBMZ (Carbon-Bond Mechanism version Z)**
- **Interaction with radiation:**
  - **Coupled to RRTMG radiation → Direct aerosol effect**

As in CAM5:

- **Gas phase/particle partitioning (aerosol chemistry):**
  - **Condensation of water vapor and of the 4 inorganic trace gase species: NH_3, H_2SO_4, HNO_3, HCl**
- **Interaction with clouds only resolved clouds (Sc):**
  - **Coupled to Morrison & Gettelman cloud microphysics**
  - **Radiative response → 1st indirect aerosol effect**
  - **Wet removal (scavenging)**
  - **Aqueous chemistry**
- **Dry deposition**

Volcanic ash

- **10 bins for volcanic ash aerosol**
- **Transport, settling, dry deposition**
- **Currently no other aerosol**
- **Single active volcano**
- **Database of 1535 volcanoes (latitude, longitude, height)**

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        = 43
  photdt          = 0.25
  chemdt          = 0
    ...
aerchem_onoff   = 1
    ...
conv_tr_aqchem = 1
```

MADE/SORGAM, RACM-ESRL, CMAQ aqueous chemistry

Switches all aerosol processes on/off

CMAQ aqueous chemistry on 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)**