

## **Lecture 6.**

### **Representation of aerosol processes in models.**

1. Major processes involving aerosols.
2. Example of aerosol treatments in WRF-Chem.

#### **Required reading:**

Fast, J.D., W. I. Gustafson, E. G. Chapman, R. C. Easter, J. P. Rishel, R. A. Zaveri, G. A. Grell, and M. C. Barth, The Aerosol Modeling Testbed: A Community Tool to Objectively Evaluate Aerosol Process Modules. BAMS, doi: 10.1175/2010BAMS2868.1 (in press).

McFiggans, G., et al., The effect of physical and chemical aerosol properties on warm cloud droplet activation. *Atmos. Chem. Phys.*, 6, 2593–2649, 2006.

#### **Additional reading:**

Grell, G.A., S.E. Peckham, R. Schmitz, and S.A. McKeen, G. Frost, W.C. Skamarock, and B. Eder, Fully coupled “online” chemistry within the WRF model. *Atmos. Environ.* 39, 6957-6976, 2005.

#### **Aerosol sources/emissions:**

Primary aerosols: emitted directly into the atmosphere as particles (e.g., dust, soot, sea-salt)

Secondary aerosols: formed in the atmosphere through chemical processes involving gaseous species (SO<sub>2</sub> -> sulfates; DMS-> sulfates)

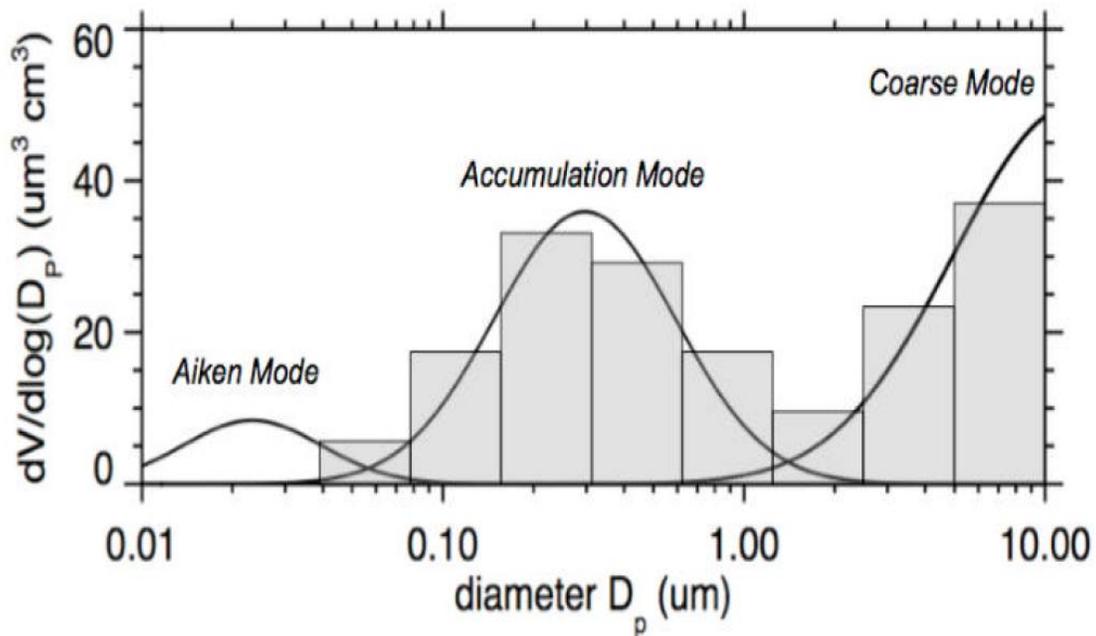
- ✓ Some aerosol and gas emissions are modeled online or available as gridded datasets
- ✓ Assessments of historical, present and future emissions have significant uncertainties , no single data set exists which would describe the geographical and temporal distribution of emissions for all species relevant to climate modeling

- ✓ Calculations of emission datasets involve a variety of steps: identifying the source of emission (e.g., fossil fuel combustion), an emission factor (e.g., how much of a given chemical species is emitted for specific mass of a given fuel burned in a specific technological process), and a procedure for mapping onto a geographical grid (e.g., the location of a source point such as a power plant)
- ✓ Ongoing efforts under IPCC AR5 assessments: development of continuous and consistent gridded emissions datasets from 1850 to 2100.

*Example:* The Global Emissions Inventory Activity (GEIA)

<http://www.geiacenter.org/>

**Representation of particle size distribution:**

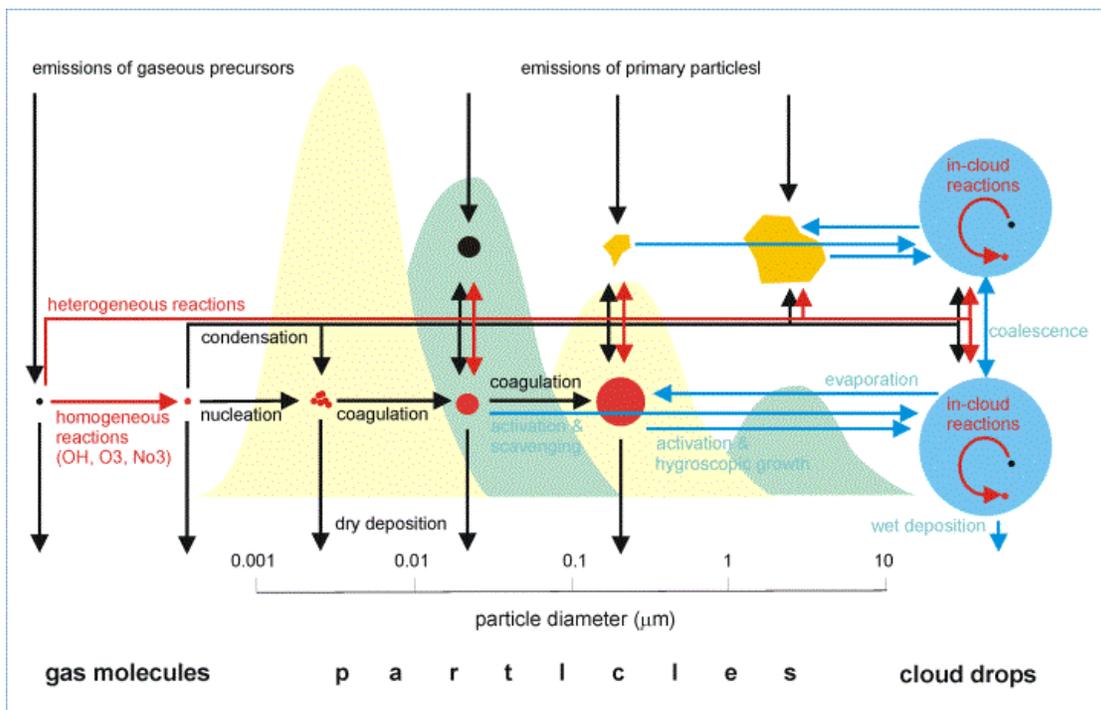


**Figure 6.1** Different representations of size distribution in models: modal (lines) vs sectional (or bin) (boxes).

**The particle size distribution** of aerosols represented by a sum of three log-normal functions:

$$N(r) = \sum_i \frac{N_i}{\sqrt{2\pi} \ln(\sigma_i)} \frac{1}{r} \exp\left(-\frac{\ln(r/r_{0,i})^2}{2\ln(\sigma_i)^2}\right) \quad [6.1]$$

where  $N(r)$  is the particle number concentration,  $N_i$  is the total particle number concentration of  $i$ -th size mode with its median radius  $r_{0,i}$  and geometric standard deviation  $\sigma_i$ .



Raes et al., *Atm. Env.*, 2000

(see fig. 5.4)

**Aerosol removal processes:**

- Dry deposition
- Gravitational settling
- Wet removal (wash-out)

The dry deposition flux,  $F_d$ , is calculated as the product of the concentration,  $m_d$ , and a deposition velocity,  $V_d$ , computed at a reference height,  $z_r$ :

$$F_d = m_d * V_d \quad [6.2]$$

$F_d$  = dry deposition flux ( $\mu\text{g}/\text{m}^2/\text{s}$ ),

$m_d$  = concentration ( $\mu\text{g}/\text{m}^3$ ), calculated at reference height,  $z_r$ ,

$V_d$  = deposition velocity (m/s),

$z_r$  = deposition reference height (m) =  $z_o+1$ , and

$z_o$  = surface roughness length for the application site (m), from the meteorological file.

NOTE:  $m_d$  and  $V_d$  depend of particle size

For a given size category, the particle deposition velocity,  $V_{dp}$ , is given as,

$$V_{dp} = \frac{1}{R_a + R_p + R_a R_p V_g} + V_g \quad [6.3]$$

$V_{dp}$  = deposition velocity for particles (m/s),

$R_a$  = aerodynamic resistance (s/m),

$R_p$  = quasilaminar sublayer resistance (s/m), and

$V_g$  = gravitational settling velocity for particles (m/s).

The aerodynamic resistance,  $R_a$ , is calculated as follows:

for stable and neutral conditions ( $L > 0$ ),

$$R_a = \frac{1}{(ku^*)} \left[ \ln \left( \frac{z_r}{z_o} \right) + \frac{5z_r}{L} \right] \quad [6.4]$$

for unstable conditions ( $L < 0$ ),

$$R_a = \frac{1}{(ku^*)} \ln \frac{(\sqrt{1-16\frac{z_r}{L}} - 1)(\sqrt{1-16\frac{z_o}{L}} + 1)}{(\sqrt{1-16\frac{z_r}{L}} + 1)(\sqrt{1-16\frac{z_o}{L}} - 1)} \quad [6.5]$$

$k$  = von Karman constant (0.4),

$u^*$  = friction velocity (m/s) from the meteorology, and

$L$  = Monin-Obukhov length scale (m) from the meteorology.

Wet deposition flux

$$F_{wp} = 10^{-3} \rho_p W_p r_{rain} \quad [6.6]$$

$F_{wp}$  = flux of particulate matter by wet deposition ( $\mu\text{g}/\text{m}^2/\text{hr}$ ),

$\rho_p$  = column average concentration of particulate in air ( $\mu\text{g}/\text{m}^3$ ),

$W_p$  = particle washout coefficient (dimensionless), and

$r_{rain}$  = water or water equivalent precipitation rate (mm/hr), from the meteorology.

The particle washout coefficient,  $W_p$ , is calculated as follows:

$$W_p = \frac{3z_p E}{2D_m} \quad [6.2]$$

$E$  = collision efficiency (dimensionless), and

$D_m$  = mean diameter of raindrop (m) =  $rain^{0.232}/905.5$  with  $r$  in mm/hr.

Coagulation is the sticking together of two particles. It is the result of particles coming into contact due to Brownian diffusion, turbulence or some force (electrostatic, phoretic effects *etc.*). Note that contact does not necessarily lead to coagulation, but must happen as a pre-requisite. This happens more quickly for Aitken mode (i.e., nucleation mode) particles with large aerosol than for coagulation of two Aitken mode particles.

Coagulation is also enhanced in shearing or turbulent flows, as these induce fast relative particle motion.

Condensation. As long as the partial pressure of a compound in the gas phase is higher than the vapor pressure of that compound in aerosol, growth will occur. The opposite situation is possible, where particles outgas certain compounds, but the growth tends to be the dominant process. Condensational growth is another mechanism by which aerosol can leave the nucleation mode.

Cloud processing. Cloud drops undergo aqueous chemical reactions. Because of their larger surface area, reaction rate per drop is usually higher than reaction rate per condensation nucleus. If a drop that has been involved in such reactions subsequently evaporates, the condensation nucleus is left behind and may be considerably larger than it

was before entering cloud. This process is called cloud processing, and can considerably increase the rate at which accumulation mode aerosol grow. Cloud processing generally affects accumulation mode rather than coarse mode aerosol, as the former tends to be more hygroscopic.

### **Aerosol treatments in WRF-Chem.**

<http://ruc.noaa.gov/wrf/WG11/>

#### **Aerosol schemes in WRF:**

##### **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)

#### **Aerosol module MADE-SORGAN**

[http://ruc.noaa.gov/wrf/WG11/made\\_sorgam.htm](http://ruc.noaa.gov/wrf/WG11/made_sorgam.htm)

#### **Biogenic emission modeling: MEGAN**

[http://ruc.noaa.gov/wrf/WG11/wrf\\_tutorial\\_2010/Wiedinmyer\\_megan\\_12jul10.pdf](http://ruc.noaa.gov/wrf/WG11/wrf_tutorial_2010/Wiedinmyer_megan_12jul10.pdf)